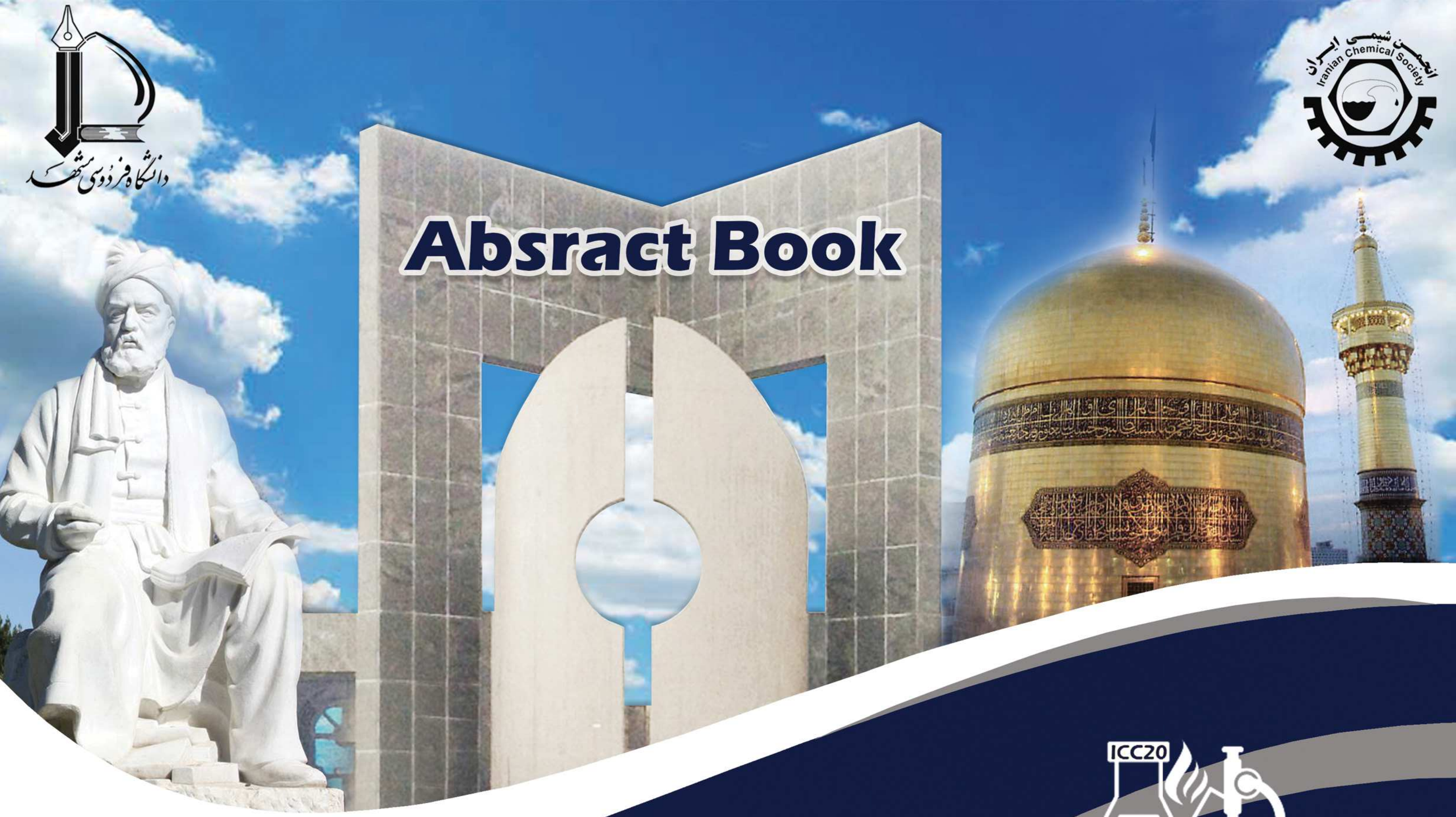
دانشگاه فردوسی مشهد

انجمن شیمی ایران
Iranian Chemical Society



Absract Book

ICC20
بیستمین کنگره شیمی ایران
۲۸-۲۶ تیرماه ۱۳۹۷
دانشگاه فردوسی مشهد

بیستمین کنگره شیمی ایران

20th Iranian Chemistry Congress

۲۸- ۲۶ تیرماه ۱۳۹۷ دانشگاه فردوسی مشهد
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17-19 July 2018 Ferdowsi University of Mashhad

http://icc20.um.ac.ir
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- سنتز ترکیب‌های آلی و دارویی
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تلفن: ۰۵۱-۳۸۸۰۵۵۴۶
دورنما: ۰۵۱-۳۸۷۹۶۴۱۶

In name of Allah, the compassionate, the merciful

20th Iranian Chemistry Congress

17-19 July 2018

Ferdowsi University of Mashhad, Iran

By:
Department of Chemistry, Faculty of Science
Ferdowsi University of Mashhad

In collaboration with:
Iranian Chemical Society

Editorial Note

We would like to note that the abstracts are printed with a minor revision by applying a general format and references style. Therefore, the content of each abstract is the responsibility of the authors, and the organizing committee of the conference assumes no responsibility for the statements and opinions advanced by contributors.

Proceedings of the 20th Iranian Chemistry Congress

𝒪 **By:** The Secretariat of 20th Iranian Chemistry Congress
𝒪 **Editor:** Prof. Hossein Eshghi
𝒪 **Cover Designer:** Mojtaba Tarin

Dear Colleagues,

It is my great pleasure to welcome you on behalf of the Congress Organizing Committee for participating in 20th Iranian Chemistry Congress (ICC20) sponsored by Ferdowsi University of Mashhad (FUM). ICC20 would be held in Mashhad on 17-19 July 2018.

This congress goes to the heart of all scientific matters relating to chemistry and it brings together the best scientists and researchers from all universities and industries from Iran allowing you to hear and meet those working on all branches of chemistry in one place. There will be delegates not only from top universities, but one feature is that delegates come from developing universities in Iran. We hope you will find the lectures and posters are a great resource for your future studies and knowledge.

I gratefully acknowledge FUM staffs, especially Prof. M. Kafi, the president of FUM, and Prof. A. R. Bahrami, the Vice-Chancellor of Research Council of FUM for their incomparable supports for holding of ICC20.

I also wish to appreciate the generous efforts of the organizing committee, especially my kind colleagues in Department of Chemistry as well as the BSc, MSc and PhD Students, the Iranian Chemical Society (ICS), and the sponsors, whose tireless efforts and financial help makes the ICC20 achievable.

I hope you will find here an enjoyable city to see the beauties and culture of Mashhad.

Prof. Hossein Eshghi
Chairman of ICC20
July 2018

Contents

به نام خداوند جان و خرد   کزین برتر اندیشه برنگذرد

از روزی که ایرانیانی چون جابرابن حیان و محمدبن زکریای رازی شیمی تجربی را پایه گذاری نمودند و فردوسی بزرگ پژوهش و نقد را پی نهاد تا روزی که لاوازیه و پریسلی شیمی جدید را بنا نهادند، چه یافته های با ارزش تر از کیمیا متولد شدند و چه اکسیرها که برپایه شیمی نوین افزایش امید به زندگی را در جامعه همچون آب حیات به کام انسان هدیه نمودند. بشر خواسته یا ناخواسته مدیون علم شیمی و معادلاتش گردید که در این رشد و نمو تصاعدی به سرعت اجازه ایجاد شاخه های جدید علمی منشعب از آن ساقه تنومند را داد تا این علم پایه زیربنای اکثر رشته های علمی از قبیل شیمی دارویی، داروسازی، شیمی کشاورزی، شیمی مواد و متالوژی، مهندسی شیمی، شیمی پلیمر، بیوشیمی، نانوشیمی و صنایع مرتبط با علم شیمی گردد.

علم کهن شیمی که از اولین تجربه های بشر در همآوردی سنگ و آتش آغاز شده اکنون در جایگاهی است که زمان و زمین را مجذوب یافته های خویش کرده و حرارت علمش توان همآوردی با اکثر مجهول های انسان هزاره سوم را دارد. در کشور ما نیز شیمی از علوم پیشرو در تأسیس دوره های دکتری بوده و امکان بروز خلاقیت ها و خودباوری نسل جوان را ابتدا این رشته ی علمی فراهم نموده و این خود باوریها باعث شده تا ایران در سال ۲۰۱۵ جایگاه دوازدهم جهان و اول منطقه را به خود اختصاص دهد. اکنون بیستمین کنگره شیمی ایران فرصتی را فراهم آورده تا اساتید، دانشجویان تحصیلات تکمیلی دانشگاه ها ، صنعتگران و شاغلین در صنایع شیمیایی در همآوردی دوسالانه گرد هم آیند تا با تبادل نظر در مورد یافته ها و مشکلات پیش رو امکان رشد و تعالی علم شیمی را در حوزه دانشگاه و صنعت فراهم آورند.

بدون شک بیستمین کنگره شیمی ایران (icc20) که به همت گروه شیمی دانشگاه فردوسی مشهد، برگزار خواهد شد، فرصتی بی بدیل برای تبادل داده های علمی به روز اساتید، دانشجویان و پژوهشگران این رشته، ایجاد نماید و معرفی شرکت های دانش بنیان و مراکز رشد، فرصتی را برای تبدیل دانش شیمی به کاربردهای صنعتی و دارویی، در این حوزه فراهم خواهد نمود.

مفتخریم کنار ملجأ شریف و نورانی امام مهربانی ها، حضرت امام رضا علیه السلام، با برگزاری بیستمین کنگره شیمی ایران (icc20) در روزهای بیست ششم تا بیست و هشتم تیرماه ۱۳۹۷ در دانشکده علوم دانشگاه فردوسی مشهد، میزبان کلیه اساتید، دانشجویان، پژوهشگران، متخصصین دانشگاهی، مراکز پژوهشی و صنایع شیمیایی سراسر کشور باشیم و یقین داریم که با حضور پرشور تمامی صاحب نظران، این همایش بزرگ علمی به بهترین شکل ممکن انجام خواهد گردید.

ما بدان مقصد عالی نتوانیم رسید   هم مگر پیش نهد لطف شما گامی چند

حسین عشقی

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درباره حامی ویژه بیستمین کنگره شیمی ایران

در دنیای پرشتاب و تحول‌گرای امروز، پیشرفت علم و فن‌آوری و دستیابی به تکنولوژی‌های نو یکی از پایه‌ای‌ترین و اصلی‌ترین نیازهای هر کشوری می‌باشد. کشور عزیزمان ایران نیز همواره در عرصه پیشرفت علوم و تکنولوژی نوین پیشتاز بوده و می‌باشد. در راستای این تحولات و نیاز روز افزون محققین و اساتید محترم دانشگاهها و مراکز تحقیقاتی و تلاشگران عرصه صنعت به تجهیزات روز دنیا و دستگاههای پیشرفته و لزوم تامین آنها در کمترین زمان ممکن شرکت شایگان سرمد تاسیس گردید. یکی از اهداف اولیه شکل گیری این شرکت تهیه دستگاهها و تجهیزاتی است که در سالهای اخیر بعضا تامین آنها با مشکلاتی مواجه بوده است. شرکت شایگان سرمد افتخار دارد با پشتوانه سالها تجربه مدیران و متخصصین آن در جهت مشاوره و تامین کلیه دستگاه ها و تجهیزات آزمایشگاهی و تحقیقاتی مورد نیاز عرصه صنعت و تحقیق کشور گام بردارد. شرکت شایگان سرمد با دارا بودن کادر علمی و فنی مجرب، توانایی انجام خدمات پس از فروش ، تامین قطعات و تعمیر دستگاه‌های ارائه شده را دارا می باشد .

در ذیل لیست کمپانی‌ها و زمینه‌های فعالیت این شرکت تقدیم حضور می گردد .

- دستگاههای پتانسیواستات، گالوانواستات، میکروسکوپ روبشی الکتروشیمیایی (SECM) ، مجموعه اسپکتروالکتروشیمی، الکترود و قطعات از کمپانی CH Instruments آمریکا و ALS ژاپن
- سیستم های کروماتوگرافی شامل HPLC، GC، GCMS و تامین قطعات آنها از کمپانی‌های Waters و Agilent Technologies آمریکا
- سیستم های اسپکتروسکوپی مولکولی و اتمی شامل UV/Vis، FTIR، AA ، ICP-OES ، ICP-MS و تامین قطعات آنها از کمپانی های PerkinElmer و Agilent Technologies آمریکا
- سیستم های اسپکترومتری، منبع نوری، مترولوژی و فیبر نوری از کمپانی Ocean Optics آمریکا
- سیستم های میکروسکوپ الکترونی روبشی SEM از کمپانی Zeiss آلمان
- سیستم های رزونانس مغناطیس هسته ای NMR از کمپانی Bruker آلمان
- انواع دستگاه های دانه بندی پودرها به روش لیزر، خردایش مواد و آماده سازی نمونه در رده آزمایشگاهی و صنعتی از کمپانی *Fritsch* آلمان
- دستگاه‌های Karl Fischer، Potentiometric Titration، EC Meter ، PH Meter از کمپانی Hach
- تجهیزات خلا و پایپینگ از کمپانی *EDWARDS* آمریکا
- سایر دستگاههای آزمایشگاهی شامل: آون، انکوباتور، ترازو، کوره و ... از کمپانی های GFL، Nabertherm، Carbolite، Thermo، Memmert، Sartorius، IKA ، ....
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کمپانی VWR ارائه کننده تجهیزات و مواد آزمایشگاهی از ده ها برند جهانی


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- ارائه خدمات آزمایشگاهی و تحقیقاتی به متخصصین در حوزه های سخت افزاری، نرم افزاری و نکات کاربردی از طریق دستگاه های موجود در آزمایشگاه شرکت
- برگزاری دوره های مدون آموزشی و کاربردی در داخل و خارج از کشور
- پذیرش مقالات تخصصی در ژورنال با درجه کیفی بالا

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Speeches Program

برنامه سخنرانی‌های بیستمین کنگره شیمی

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آقای دکتر صادق رستم‌نیا (دانشگاه مراغه)	Nano-pumice hybrid porous materials for catalytic organic & inorganic compounds assembling	۱۷:۳۰ الی ۱۸:۱۰	۴۰ دقیقه	۱۲۰۹
آقای دکتر حمید بیضائی (دانشگاه زابل)	Green Multicomponent Synthesis, Antimicrobial and Antioxidant Evaluation of Novel 5-Amino-isoxazole-4-carbonitriles	۱۸:۱۰ الی ۱۸:۳۰	۲۰ دقیقه	۶
دکتر محمود زارعی (postdoc)	Rational design, synthesis and application of task-specific materials in organic synthesis	۱۸:۳۰ الی ۱۸:۵۰	۲۰ دقیقه	۱۲۷۳
خانم فرزانه ملیجی	Synthesis and characterization of a new ferrocene-based calix[4]arene as electrochemical sensor	۱۸:۵۰ الی ۱۹:۱۰	۲۰ دقیقه	۵۰۲

روز سه شنبه ۱۳۹۷/۴/۲۶ – بعدازظهر – شیمی فیزیک – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
سخنرانی شیمی‌دان برجسته رشته شیمی فیزیک آقای دکتر عبدالخالق بردبار (دانشگاه اصفهان)	Binding of small molecules to proteins: An old problem with new insights	۱۵:۰۰ الی ۱۵:۴۰	۴۰ دقیقه	۱۲۷۷
آقای دکتر افشین شفیعی (دانشگاه صنعتی شریف)	Study of some recent research topics in the quantum field	۱۵:۴۰ الی ۱۶:۲۰	۴۰ دقیقه	۱۲۶۷
خانم دکتر سیده سمیه آسمانی	Theoretical Study on the Kinetics and Dynamics of the Reaction of HNO ($^{3}A''$) with HO_2 ($^{2}A''$)	۱۶:۲۰ الی ۱۶:۴۰	۲۰ دقیقه	۱۳

روز سه شنبه ۱۳۹۷/۴/۲۶ – بعدازظهر – شیمی تجزیه – سالن دکتر سعادت

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
سخنرانی شیمی‌دان برجسته رشته شیمی تجزیه آقای دکتر ابراهیم نوروزیان (دانشگاه شهید باهنر کرمان)		۱۵:۰۰ الی ۱۵:۴۰	۴۰ دقیقه	
آقای دکتر عبدالرئوف صمدی (دانشگاه مازندران)	ZnS@CdS core/shell quantum dots as photokilling agents for pathogenic bacteria	۱۵:۴۰ الی ۱۶:۰۰	۲۰ دقیقه	۸۸۶
خانم مهسا امیری	Organic/inorganic photoconductive hybrid films based on polypyrrol-cadmium sulfide quantum dot nano-composites	۱۶:۰۰ الی ۱۶:۲۰	۲۰ دقیقه	۳۸۷
آقای حامد توکلی	Liver cancer cells monitoring using a novel CNTs-based biosensor	۱۶:۲۰ الی ۱۶:۴۰	۲۰ دقیقه	۲۱۷
سخنرانی شیمی‌دان برجسته شیمی تجزیه آقای دکتر بهزاد رضائی (دانشگاه صنعتی اصفهان)	Recent approaches and advancements in energy production, conversion and storage systems using electrochemical methods	۱۷:۳۰ الی ۱۸:۱۰	۴۰ دقیقه	۱۲۵۸
خانم منیره کرمی	Automated EME-DLLME Method on a disk	۱۸:۱۰ الی ۱۸:۳۰	۲۰ دقیقه	۶۲۸
خانم فاطمه کردانی	Simultaneous determination of β-sitosterol and cholesterol in food samples by using solid phase microextraction fibers based on monolithic molecular imprinted polymer followed by HPLC–UV	۱۸:۳۰ الی ۱۸:۵۰	۲۰ دقیقه	۹۱
خانم گلنار احمدی بنکدار	Colorimetric determination of fexofenadine in biological samples after solid phase extraction by molecularly imprinted polymer	۱۸:۵۰ الی ۱۹:۱۰	۲۰ دقیقه	۴۳۲

روز سه شنبه ۱۳۹۷/۴/۲۶ – بعدازظهر – شیمی معدنی – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
سخنرانی شیمی‌دان برجسته رشته شیمی معدنی آقای دکتر حسن حدادزاده (دانشگاه صنعتی اصفهان)	Recent Research on Nanobioinorganic Chemistry	۱۷:۳۰ الی ۱۸:۱۰	۴۰ دقیقه	۱۲۷۹
خانم دکتر فاطمه بامحرم (دانشگاه آزاد اسلامی واحد مشهد)	Application of Heteropolyacids in Nanoscience for the Development of Green Catalytic Reactions	۱۸:۱۰ الی ۱۸:۵۰	۴۰ دقیقه	۱۲۸۱
آقای سهیل محمودی	Crystal engineering and interaction energy calculation of some new rhenium(I) tricarbonyl complexes bearing bidentate NN-donor ligand	۱۸:۵۰ الی ۱۹:۱۰	۲۰ دقیقه	۳۳۲

روز چهارشنبه ۱۳۹۷/۴/۲۷ – صبح – شیمی آلی – سالن دکتر رحیمی‌زاده

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر محمد رمضانی **(دانشگاه علوم پزشکی مشهد)**	Smart silica-based nanoparticles for targeted drug delivery	۸:۳۰ الی ۹:۱۰	۴۰ دقیقه	۱۲۸۸
آقای دکتر کمال‌الدین حق‌بین **(پژوهشگاه ملی مهندسی ژنتیک و زیست فناوری)**	New Insight in Medicinal Chemistry of Human tyrosinase; Based on a comparative study on Mushroom tyrosinase and Human tyrosinase	۹:۱۰ الی ۹:۵۰	۴۰ دقیقه	۷۴۶
خانم مریم نعیم آبادی	Diastereoselective synthesis of spirocyclopropane-linked pyrazolones from azomethine ylides via C(sp3)-H activation	۹:۵۰ الی ۱۰:۱۰	۲۰ دقیقه	۴۵۵
آقای دکتر بابک کریمی **(دانشگاه تحصیلات تکمیلی زنجان)**		۱۱:۰۰ الی ۱۱:۴۰	۴۰ دقیقه	
آقای دکتر محمود نصرالله‌زاده **(دانشگاه قم)**	Biosynthesis of Ag/MgO nanocomposite using Acalypha hispida extract and its application in the reduction of nitroarenes and organic dyes	۱۱:۴۰ الی ۱۲:۰۰	۲۰ دقیقه	۹۷۱
خانم محمره شیخی	Selenopheno[2,3-e][1,2,4]triazolo[4,3-c]pyrimidine: A novel tricyclic selenium containing heterocyclic system	۱۲:۰۰ الی ۱۲:۲۰	۲۰ دقیقه	۳۲۸
خانم مهری دانا	A new approach for silane curing metallocene-based polyethylene-octene copolymers by Monosil and Sioplas processes	۱۲:۲۰ الی ۱۲:۴۰	۲۰ دقیقه	۳۷

روز چهارشنبه ۱۳۹۷/۴/۲۷ – صبح – شیمی تجزیه – سالن دکتر سعادت

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
خانم دکتر محبوبه شیرانی (دانشگاه جیرفت)	Ultrasound assisted desulfurization of fuel oil with choline chloride based deep eutectic solvent and magnetic NaY zeolite	۸:۳۰ الی ۹:۱۰	۴۰ دقیقه	۲۷۰
خانم الناز مرزی خسروشاهی	Electrodeposition of carbon nitride nanosheets on the graphanized pencil lead as an effective SPME fiber for extraction of PAHs in edible samples	۹:۱۰ الی ۹:۳۰	۲۰ دقیقه	۵۱۳
آقای محمد مهدی ختائی	Fabrication of Covalent Organic Framework-based Composite as Advanced Adsorbent for Removal of Cationic and Anionic Dyes from Water	۹:۳۰ الی ۹:۵۰	۲۰ دقیقه	۳۰۶
خانم مریم نظری	Using ZnO-Al2O3 ceramic nanofibers and graphene oxide to simultaneously detect catechol and hydroquinone	۹:۵۰ الی ۱۰:۱۰	۲۰ دقیقه	۵۱۶

روز چهارشنبه ۱۳۹۷/۴/۲۷ – صبح – شیمی معدنی – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر علی مرسلی (دانشگاه تربیت مدرس)	Pillar-layered MOFs: Functionality, Interpenetration, Flexibility and Applications	۸:۳۰ الی ۹:۱۰	۴۰ دقیقه	۱۲۲۴
سخنرانی آقای دکتر رضا کشاورزی (دانشگاه اصفهان)	Mesoporous templated films in dye sensitized and perovskite solar cells	۹:۱۰ الی ۹:۵۰	۴۰ دقیقه	۱۲۸۶
خانم ناهید لطفیان	Purposeful molecular design of inorganic-organic hybrid architectures based Keggin-type polyoxometalates: luminescence properties and Monte Carlo simulation studies	۹:۵۰ الی ۱۰:۱۰	۲۰ دقیقه	۱۱۳۰
آقای دکتر سید حسن علم‌الهدایی (پارک علم و فناوری خراسان)	University entrepreneurship, a force for science-based economy	۱۱:۰۰ الی ۱۱:۴۰	۴۰ دقیقه	۱۲۸۳
خانم دکتر مونا علی‌بلندی (دانشگاه علوم پزشکی مشهد)	Thermo-pH-Dual-Responsive Smart Polymersomes for Controlled Release of Doxorubicin	۱۱:۴۰ الی ۱۲:۲۰	۴۰ دقیقه	
خانم زهرا یکه قاسمی	Synthesis of new dithiocarbazate Sn(IV) complex; investigation of the crystalline structure and cytotoxic activity	۱۲:۲۰ الی ۱۲:۴۰	۲۰ دقیقه	۵۷۰

روز چهارشنبه ۱۳۹۷/۴/۲۷ – صبح – شیمی فیزیک – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر سید مرتضی موسوی خوشدل (دانشگاه علم و صنعت تهران)	Quantum computational (QC) study of Supercapacitors and Li-ion batteries	۱۱:۰۰ الی ۱۱:۴۰	۴۰ دقیقه	۱۲۸۵
خانم نجمه مصطفوی	Lichexanthones as G-Quadruplex Stabilizing Ligands: the docking and DFT calculations	۱۱:۴۰ الی ۱۲:۰۰	۲۰ دقیقه	۱۲۵۱
خانم یلدا صباحی	Molecular dynamics as a tool to study effect of Na^+ cations on diffusion of SO_2 in Y zeolite	۱۲:۰۰ الی ۱۲:۲۰	۲۰ دقیقه	۱۲۰
آقای وحیدرضا داروگر	Tautomeric Equilibria Studies by UV-Vis Spectroscopy in β-diketones	۱۲:۲۰ الی ۱۲:۴۰	۲۰ دقیقه	۴۹۲

روز چهارشنبه ۱۳۹۷/۴/۲۷ – بعدازظهر – شیمی معدنی – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر محسن گلبن حقیقی (دانشگاه شهید بهشتی)	The Binuclear Organoplatinum(II) Complexes with Diphosphine Bridging Ligands; Synthesis and Optical Properties	۱۵:۰۰ الی ۱۵:۴۰	۴۰ دقیقه	۱۲۱۷
آقای علی سمیع	Packing Problem (Z′=2) in Mercuric Halide Complexes Containing the Most Stable Polymorph of Ester Ligands; Directionalized by Robust C−H···πe Synthon	۱۵:۴۰ الی ۱۶:۰۰	۲۰ دقیقه	۱۰۵۴
خانم معصومه محمودآبادی	Synthesis and theoretical studies of two new Co(III) and Cu(II) macroacyclic Schiff-base complexes containing piperazine moiety	۱۶:۰۰ الی ۱۶:۲۰	۲۰ دقیقه	۳۳۴
خانم سارا اخوین انصاری	Synthesis of a novel catalyst based on Ag nanoparticles on mesoporous silica for reduction nitro aromatic compounds in aqueous solution	۱۶:۲۰ الی ۱۶:۴۰	۲۰ دقیقه	۸۱۶

روز چهارشنبه ۱۳۹۷/۴/۲۷ – بعدازظهر – شیمی فیزیک – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر علی نخعی‌پور **(دانشگاه فردوسی مشهد)**	Role of chemistry knowledge in know-how development of industrial catalysis; petroleum refinery case study	۱۵:۰۰ الی ۱۵:۴۰	۴۰ دقیقه	۱۲۷۴
خانم منصوره پارسا	Cytotoxicity of Zinc Oxide Nanoparticles Synthesized in the Presence and Absence of Ultrasound on Saos-2 Cancer Cell Line	۱۵:۴۰ الی ۱۶:۰۰	۲۰ دقیقه	۲۷۶
خانم سپیده قلیزاده خاصوانی	Novel MIL-88A(Fe)@g-C3N4 core@shell nanocomposites: fabrication, characterization and application as a photocatalyst	۱۶:۰۰ الی ۱۶:۲۰	۲۰ دقیقه	۱۱۷۵
خانم زهره نیازی	TiO2@ graphene quantum dots nanocomposite as an efficient photocatalyst for degradation of RB5 under sunlight irradiation	۱۶:۲۰ الی ۱۶:۴۰	۲۰ دقیقه	۴۹۹
آقای دکتر علی نیک اختر **(دانشگاه بیرجند)**	Investigation of accelerated sulfur vulcanization by irreversible consecutive mechanism	۱۷:۳۰ الی ۱۷:۵۰	۲۰ دقیقه	۸۱۰
خانم دکتر مرضیه سادات معصوم‌پور	Theoretical studies on the kinetics and mechanism of the unimolecular reactions of hydrogen thioperoxide	۱۷:۵۰ الی ۱۸:۱۰	۲۰ دقیقه	۴۹
خانم دکتر فروغ ارکان (postdoc)	Energy conversion efficiency in the solar cells based on the methylammonium lead halide perovskites: Molecular Approach	۱۸:۱۰ الی ۱۸:۳۰	۲۰ دقیقه	۳۳
خانم فریبا مقدسی	Molecular Dynamics Simulation of Self-assembly Soybean Oil- based Nanoemulsion System	۱۸:۳۰ الی ۱۸:۵۰	۲۰ دقیقه	۵۹
آقای عباسعلی عربی	Kinetics and thermodynamics of Rhodamine B adsorption by $La_{0.7}Ca_{0.3}MnO_3$	۱۸:۵۰ الی ۱۹:۱۰	۲۰ دقیقه	۱۱۵۹

روز چهارشنبه ۱۳۹۷/۴/۲۷ – بعدازظهر – شیمی تجزیه – سالن دکتر سعادت

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر میرفضل‌الله موسوی (دانشگاه تربیت مدرس)	Electrochemical Energy Storage: A Survey of Our Research Group Activities Over the Past Two Decades	۱۵:۰۰ الی ۱۵:۴۰	۴۰ دقیقه	۱۲۸۴
خانم مریم گوهرجو	A new, facile and efficient agarose gel based electromembrane extraction for preconcentration, clean up and determination of propranolol in blood serum	۱۵:۴۰ الی ۱۶:۰۰	۲۰ دقیقه	۱۰۱۴
خانم اکرم حاجی‌نیا	Evolution of paper based analytical devices for fire assay- fluorimetric determination of gold in geological samples using camera smart phone	۱۶:۰۰ الی ۱۶:۲۰	۲۰ دقیقه	۱۰۳۰
خانم هنگامه بهرامی	Inhibition activity modeling of CINPA1 analogs as novel inverse agonists of constitutive androstane receptor	۱۶:۲۰ الی ۱۶:۴۰	۲۰ دقیقه	۵۲۴
آقای دکتر غلامحسین رونقی (دانشگاه فردوسی مشهد)	Chemical sensors, biosensors and bioprobes	۱۷:۳۰ الی ۱۸:۱۰	۴۰ دقیقه	۱۲۸۲
آقای دکتر علی‌رضا فخاری زواره (دانشگاه تربیت مدرس)	Simultaneous chiral separation of tramadol and methadone in tablets, human urine, and plasma by capillary electrophoresis using maltodextrin as the chiral selector	۱۸:۱۰ الی ۱۸:۳۰	۲۰ دقیقه	۱۱۰۸
آقای امیر اسماعیل‌زاده	Pesticides determination in crops by solvent assisted stir bar dispersive solid phase microextraction based on magnetic nano-composites	۱۸:۳۰ الی ۱۸:۵۰	۲۰ دقیقه	۹۸۷
آقای دکتر نوید نصیری‌زاده	Design and Manufacture of a Solid State Supercapacitor with PVA-KOH-KNO3 Gel Polymer Electrolyte and Carbon-Ceramic Nanocomposite Electrodes	۱۸:۵۰ الی ۱۹:۱۰	۲۰ دقیقه	۷۸۸

روز چهارشنبه ۱۳۹۷/۴/۲۷ – بعدازظهر – شیمی آلی – سالن دکتر رحیمی زاده

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر سعید بلالایی (دانشگاه خواجه نصیرالدین طوسی)	Designing of Novel Multicomponent Reactions using 3-Formyl Chromone for the Synthesis of Functionalized Heterocyclic Skeletons	۱۷:۳۰ الی ۱۸:۱۰	۴۰ دقیقه	۱۲۷۰
خانم دکتر الهه کوثری (دانشگاه صنعتی امیرکبیر)	Innovative applications of ionic liquids in Chemistry and chemical engineering	۱۸:۱۰ الی ۱۸:۵۰	۴۰ دقیقه	۱۲۰۸
خانم دکتر محبوبه رستمی	Synthesis of Tocopherol succinate-PolyoxomolybdateHybride Bio-Conjugate as potential anti cancer agent	۱۸:۵۰ الی ۱۹:۱۰	۲۰ دقیقه	۳۰۵

روز پنج‌شنبه ۱۳۹۷/۴/۲۸ – صبح – شیمی آلی – سالن دکتر رحیمی زاده

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر علی‌رضا مدرسی عالم **(دانشگاه سیستان و بلوچستان)**	Synthesis of superparamagnetic nanocomposite of poly(m-amino benzenesulfonic acid) and Fe_3O_4 and its high efficiency in solar cell	۸:۳۰ الی ۹:۱۰	۴۰ دقیقه	۴۱۳
آقای دکتر علی دره‌کردی **(دانشگاه ولی‌عصر رفسنجان)**	Trifluoromethylated Compounds: Synthesis and Evaluation of their Biological Activities	۹:۱۰ الی ۹:۵۰	۴۰ دقیقه	۱۲۵۳
خانم دکتر الهه مصدق **(دانشگاه تحصیلات تکمیلی صنعتی و فناوری پیشرفته – کرمان)**	Synthesis and characterization of a novel colloidal ceramic nanocomposite coated by Ag nanoparticles	۹:۵۰ الی ۱۰:۱۰	۲۰ دقیقه	۱۰۲۵
خانم دکتر آسیه وفایی شعرباف	Synthesis, characterization and molecular docking study of new 4-acetamidoalkyl pyrazoles as B-raf /COX-2 inhibitors	۱۰:۱۰ الی ۱۰:۳۰	۲۰ دقیقه	۱۲۴۵

روز پنج‌شنبه ۱۳۹۷/۴/۲۸ – صبح – شیمی فیزیک – سالن دکتر اسماعیل بیگی

نام و نام خانوادگی سخنران	عنوان سخنرانی	زمان	مدت زمان سخنرانی	کد مقاله
آقای دکتر امین‌رضا ذوالقدر **(دانشگاه شیراز)**	Interactions of nanoparticles with lipid membrane: simulations and experiments	۸:۳۰ الی ۹:۱۰	۴۰ دقیقه	۱۲۷۶
آقای دکتر علی‌رضا برنجی **(دانشگاه گناباد)**	Structure and vibrational analysis of copper (II) heptane-3,5-dione	۹:۱۰ الی ۹:۳۰	۲۰ دقیقه	۱۱۱۶
آقای دکتر هادی سالاری **(دانشگاه شیراز)**	Gold nanoparticles supported on magnetic Metal Organic Framework: kinetics and mechanism of alkenes oxidation by dioxygen	۹:۳۰ الی ۹:۵۰	۲۰ دقیقه	۹۳۱
آقای محمد ابراهیم ایزدی	Reactive molecular dynamics simulation for isotope exchange reactions in H/D systems: ReaxFFHD development	۹:۵۰ الی ۱۰:۱۰	۲۰ دقیقه	۱۵۷

Posters Program

راهنمای تفکیک گرایش‌های اصلی بر اساس رنگ				
شیمی آلی	شیمی تجزیه	شیمی فیزیک	شیمی معدنی	سایر

زمان ارائه پوستر بخش (A) شامل (شیمی آلی-شیمی فیزیک-شیمی تجزیه)

سه شنبه ۹۷/۴/۲۶ ساعت ۱۶:۵۰ الی ۱۷:۳۰

شماره	کد مقاله	ارائه دهنده	عنوان مقاله
۱	۵	حمید بیضائی	Multicomponent Solvent-free Synthesis of Novel 2-((Benzylthio)((alkyl or arylamino)thio)methylene)malononitriles as Antimicrobial Agents
۲	۶	حمید بیضائی	Green Multicomponent Synthesis, Antimicrobial and Antioxidant Evaluation of Novel 5-Amino-isoxazole-4-carbonitriles
۳	۷	مژگان حسین نژاد	Synthesis of an Organic Dye for Dye-sensitized Solar Cells
٤	۸	مژگان حسین نژاد	Preparation of Dye-sensitized Solar Cells Based on New Organic Dye
٥	۳۸	هاله نوری پور صادقی	One-Pot Synthesis of Functionalized 1,4-Dihydropyridines Catalyzed by Deep Eutectic Solvent
٦	۴۲	هدی ملاباقر	An Efficient Method for the Synthesis of Neuroprotective Drug Riluzole
۷	۴۵	کاظم محمدیان نژاد	The Synthesis of Formylated-Triarylmethanes and Their Use in the Preparation of Hydrazone and Azine Derivatives
۸	۵۰	سحر غلامی	An efficient method for the one-pot synthesis of 4-phenyl-hydrazineyl thiazole derivatives using nano-SiO_2
۹	۷۹	صدیقه شیخی محمره	One-pot procedure for the synthesis of diverse derivatives of novel heterocyclic system benzo[e]pyrazolo[5,1:2,3]pyrimido[5,4-b][1,4]diazepine

۱۰	۹۶	عالیه خواجه خضری	A regioselective synthesis of novel oxo-thioxo[3.3.3]propellanes
۱۱	۱۴۸	مریم محمدی	Nano $SnCl_4/SiO_2$ as a Green and Reusable Catalyst for the Synthesis of Azo Dyes Based on 2-Naphtol under Grinding Conditions
۱۲	۴۴۲	پروین پورامیری	A One-pot, efficient synthesis of Polyfunctionalized 5 -hydroxybenzo[a]phenazin-6-yl)-1,3-dimethylpyrimidines by nano-Fe_3O_4/PEG/succinic anhydride
۱۳	۱۵۶	پروین حاجی عباس تبار امیری	Synthesis of cyclopropane derivatives via an efficient stereoselective trimerization procedure
١٤	۲۹۱	پروین حاجی عباس تبار امیری	Copper-catalyzed coupling of aryl boronic acids with hydrazine hydrate
۱۵	۱۶۵	زرین قاسمی	Hantzch reaction for the synthesis of 4-(2-pyrrolyl)-dihydropyridines in the presence of Fe_3O_4@Chitosan–SO_3H nanoparticles as catalyst
١٦	۱۶۹	سمیرا رزم آرا	Synthesis and spectroanalytical studies of a new heterocyclic acid-base indicator
۱۷	۱۷۹	زرین قاسمی	Application of Fe_3O_4@Chitosan–SO_3H nanoparticles as efficient catalyst for synthesis of 4H-isoxazol-5-ones in aqueous medium
۱۸	۱۹۲	رضا دژانگا	One-pot Synthesis of Some Novel 1,8-dioxooctahydroxanthenes Catalyzed by PVPP-OXA
۱۹	۲۰۰	مائده دست مرد	Synthesis of 2-substituted Perimidine Derivatives using Nanosawdust/ $TiCl_4$ as a Green Catalyst under Solvent-free Condition
۲۰	۲۰۶	حسن رئیسی آهوان	Synthesis of Substituted Pyrroles by using Choline Carboxylate Deep Eutectic Solvent
۲۱	۲۱۲	سلیمه عبدی نسب	Synthesis (perchloropyridin-4-yl)(aryl)methanones
۲۲	۲۱۳	شیما نصری	Solvent-Controlled Highly Dehydration-Selective Synthesis of Indenone-Fused Thiazolo[3,2-a]pyridines Using Ketene Dithioacetals
۲۳	۲۱۵	شیما نصری	A Catalyst-free Approach to Synthesis of Polysubstituted Pyrano[3,2-c]chromene and Benzo[g]chromene Derivatives
٢٤	۲۳۰	رضا عراقی	Fe_3O_4@SiO_2-$SnCl_4$ promoted synthesis and screening of Pyrimido[4,5-b]quinolins as antifungal agents
۲۵	۲۳۹	رضا عراقی	A simple and green approach for the synthesis of substituted dihydro-2-oxypyrroles catalyzed by

			nano-Fe_3O_4@SiO_2/$SnCl_4$ super paramagnetic nanoparticles
٢٦	**۲۳۲**	تکتم افروغ	A New Multi-Component Synthetic Route to Hexahydropyrido[2,3-d]pyrimidine Derivatives
٢٧	**۲۳۱**	وحیده خرم آبادی	synthesis of 1-and 5- substituted 1H tetrazoles catalyzed by separable ligand complex of copper (Ⅱ) supported on Fe_3O_4@SiO_2 nanoparticles
٢٨	**۲۴۱**	مریم آرین نژاد	Novel efficient heterogeneous copper (II) nanoparticles for the synthesis of 1-and 5-substituted 1H tetrazoles
٢٩	**۲۵۵**	حسن واشقانی فراهانی	Synthesis of Novel Thiazolo[2,3-b]pyrimidine Derivatives Catalyzed by Nano- SiO_2 as a Reusable Heterogeneous Catalyst
٣٠	**۳۹۴**	حسن واشقانی فراهانی	Regioselective Synthesis of New Aryloyl-functional Thiazolo[3,2-a]pyridine Using Ketene Dithioacetals in Ethanol Media
٣١	**۲۶۸**	مریم محمودیانی گیلان	Magnetic based piconaldehyde-melamine copper complex for the one-pot synthesis of hexahydroquinolines via Hantzsch four component reactions
٣٢	**۲۷۳**	راضیه حسینی مهدی آباد	Synthesis of N, N'-bis (tetra fluoropyridyl)sulfonicdiamide
٣٣	**۱۶۳**	محمد ایزدی	Bromination of Phenol and Anillin derivatives in Presence of [MdPd].$(Br_3)_2$
٣٤	**۳۰۱**	سمیه حیدری	Efficiet one-pot synthesis of pyrazoles catalyzed by Nano silica sulfamic acid, Graphene oxide and Cobalt titanate(III) using green chemistry
٣٥	**۳۶۴**	سمیه حیدری	Efficiet one-pot synthesis of pyrazoles catalyzed by nono particles Graphine/iron oxid(hematite), Hollow zine ferrite nanosphere, Au nano particles using green chemistry
٣٦	**۳۱۲**	طاهره مرادی	reaction of 2-cyano-acetamides with tetrafluoro-4-(phenylsulfonyl)pyridine
٣٧	**۴۳۱**	زهرا واری	The reaction of three component isoquinoline and dimethyl acetylenedicarboxylate with pentachloropyridine
٣٨	**۳۱۶**	مهدی دادخواه	Synthesis of Hyperbranched Polyglycerols using Ascorbic acid as Activator
٣٩	**۳۲۰**	فاطمه عموزاد خلیلی	Iodine-catalyzed synthesis of 1,4-dihydropyridines and pyrido[1,2-a]quinoxalines
٤٠	**۳۲۳**	حدیثه یزدانی نیاکی	Novel Nano synthesis of 5,5-diphenyl hydantoins Synthesis and their Chracterization

٤١	۳۲۸	امید کهندل	Selenopheno[2,3-e][1,2,4]triazolo[4,3-c]pyrimidine: A novel tricyclic selenium containing heterocyclic system
٤٢	۴۸۱	امید کهندل	Synthesis of various S-alkylated derivatives of newly synthesized tricyclic selenium containing heterocyclic system
٤٣	۳۳۷	ایمان شاطر خبازی	A Catalyst-Free Synthetic Route to Thiazolo[3,4-a]benzimidazol Dreivatives through a Three-Component Reaction
٤٤	۳۴۰	فاطمه جلیلی	Design and synthesis of SBA-15 with phosphorous acid tags as a new nanostrucured catalyst: Application in the synthesis of novel pyrido [2,3-d]pyrimidines
٤٥	۳۵۱	زهرا رضایی	Synthesis a new series of potential biological activities compounds by reaction of imidoyl chlorides and GBP drug
٤٦	۳۵۲	فاطمه کریمی راد	One-pot three-component synthesis of Acridine derivatives in glycerin media
٤٧	۳۵۶	مریم منصوری	Synthesis of azo compounds by reaction between trifluoroacetimidoyl chlorides and hydrazinhydrat
٤٨	۳۵۷	غزل نظری	Nano BF_3/SiO_2: a Novel Acid Catalyst for the Synthesis of Pyrroles by the Paal–Knorr Condensation at Room Temperature
٤٩	۳۶۰	طیبه طالبی میمند	Synthesis of pyrido[1,2-b][1,2,4]triazine-7,9-dicarbonitrile derivatives
٥٠	۳۶۳	مینا حاجی پور	An efficient, four-component reaction for synthesis of dihydropyrimidin derivatives from malononitrile, arylglyoxal, arylamine and benzonitrile
٥١	۳۶۷	مهدی روزبهانی	Synthesis of sucrose stearate and its application as emulsifier
٥٢	۳۶۹	مهدیه طالبی زاده	Synthesis of new trifluoromethylated indole derivatives
٥٣	۳۷۵	فرزانه نژاد خراسانی	Synthesis of 2,2,2-trifluoro-N-phenyl-1-tosylethan-1-imine derivatives
٥٤	۳۷۸	فرزانه علیزاده بمی	An efficient synthesis of quinoxaline derivatives via arylglyoxal, o- phenylenediamine and meldrum\'s acid as catalyst
٥٥	۴۵۰	فرزانه علیزاده بمی	Synthesis of pyrazole derivatives via three-component reaction
٥٦	۳۸۰	فاطمه کریمی راد	An efficient synthesis of 1,8-dioxodecahydroacridine derivatives in the presence of glycerin

۵۷	۳۸۴	الهام کاظمی	Synthesis of new selective ligand from N-Aryltrifluoroacetimidoyl chlorides and aniline derivatives
۵۸	۴۰۱	فاطمه کاردوست	Synthesis pyrimidin- 5-yl-pyrroles derivatives
۵۹	۴۰۷	فهیمه السادات حسینی	Synthesis of spiro-fused heterocyclic scaffolds through multicomponent reactions involving nitro ketene aminal (HKA
٦٠	۴۰۸	فهیمه السادات حسینی	New approaches for the synthesis of imidazopyridine carboxamide and pyridopyrimidine carboxamide derivatives
٦١	۴۱۱	میلاد معصومی	An efficient and rapid synthesis of functionalized quinoline derivatives
٦٢	۴۱۲	میلاد معصومی	A mild and efficient one-pot synthesis of new indenone-fused heterocyclic compounds
٦٣	۴۲۷	سمیه قربانی	Nef/Perkow Cascade towards Imidazo Phosphate Derivatives
٦٤	۷۹۵	سمیه قربانی	Fabrication of Hollow Silica Structured Organic−Inorganic Hybrid Nanocatalyst for the Oxidation of Alcohols to Aldehydes and Ketones
٦٥	۴۳۰	فاضله لطف اله زاده	Survey reactivity of some bidentate nucleophile toward 2, 3, 5, 6-tetrafluoro-4-(phenylsulfonyl) pyridine
٦٦	۴۴۳	عفت اسماعیلی شهری	A facile one-pot green synthesis of piperidines by acidic ionic liquid (4-sulfobutyl)-tris (4-sulfophenyl) phosphonium hydrogen sulfate
٦٧	۴۹۷	عفت اسماعیلی شهری	L (+) Arabinose as a catalyst for efficient and simple synthesis of Dibenzo[a,c]phenazine in ethanol
٦٨	۴۴۵	مهری سلیمی ابراهیم سرایی	Iodine catalyzed mild 4CR protocol for synthesis of Tetrahydroimidazo[1,2-a]pyridines
٦٩	۴۴۷	زهرا امیدشفیعی	A one-pot, efficient synthesis of non-cyclized adducts by aldehydes, 1,3-dicarbonyl compounds, and 6-aminouracils
٧٠	۴۴۹	فرشته نژادشاهرخ ابادی	Unexpected products in the multicomponent reaction of sodium azide, barbituric acid, and arylglyoxal
٧١	۴۶۳	عاطفه روستا	Synthesis of Thieno[2,3-b]quinolin-2-yl methanone Derivatives via Sequential Multi-component Reaction
٧٢	۴۸۶	لیلا سادات میر جعفری	A New Approach to the Synthesis of Acylals Using Nano Sawdust/BF_3 as Green Catalyst at Room Temperature under Solvent-free Condition

٧٣	۴۹۳	محمدرضا شهبازی منشادی	Three-component reaction between Indole with Arylglyoxals and amidines
٧٤	۵۳۲	سارا شیخی	Synthesis of poly functionalized pyridine derivatives from sulfonolketenimines, tetramethylguanidine and acetylenic esters
٧٥	۴۹۴	سیده فرشته موسوی زاده	Reaction of arylglyoxals with acetylacetone in aqueous media: facile synthesis of 3-acetyl-1-argiopent-2-ene-1,4-dione
٧٦	۴۹۶	ماندانا علوب	The synthesis of new boronic acid fluorescent chemosensors based on carbazole for sugars
٧٧	۴۹۸	فاطمه تاختی	Synthesis of pegilated and tetrazolo-functionalized mesoporous SiO_2/APTES nano particles as a novel nanocarrier for gene delivery application
٧٨	۵۰۰	فاطمه تاختی	Synthesize and functionalize of the novel SiO_2/APTS derivatives for applications in enzyme stabilization
٧٩	۴۴	مریم عابدی	Thermodynamic modeling of NaCl+RbCl electrolytes in water-Ethanol solvent mixtures based on the electrochemical data and the Pitzer theory
٨٠	۴۶	مریم عابدی	Investigation of Ion-Pair Association for KCl Electrolyte in Methanol Based on Conductance Method
٨١	۱۰۲	شیوا اصل مرز	Electrochemical oxidation of some dihydroxybenzene derivatives in the presence of some Meldrum's acid derivatives: Mechanistic and thermodynamic study
٨٢	۱۲۶۴	فریبا جعفری ثقیه	Comparison of thermal and mechanical properties of epoxy networks cured with α,ω-diamino polyoxytetramethylene and isophorone diamine
٨٣	۱۲۶۵	فریبا جعفری ثقیه	Effect of surface- modified Sio2 nanoparticles compared to surface- modified magnetic iron oxide nanoparticles on improving theal and mechanical properties of DGEBA/IPD epoxy networksrm
٨٤	۲۵۹	سارا فیاض زاده	Micellization parameters of a novel cationic urethane gemini surfactant in the presence of insulin: Conductivity measurements
٨٥	۲۶۰	طاهره مرادیان	Volumetric and Acoustic Studies of L-valine in Polyethylene Glycol Aqueous Solutions
٨٦	۳۵۰	محسن محمدیان	Thermodynamic investighation of the ternary ([BMIm]Br + LiBr + H_2O) system using potentiometric measurements

۸۷	۱۱۲۲	مینا جامی	Synthesis, Structure and vibrational assignment of bis(3-amino-1- phenyl-2-buten-1-onato) nickel(II)
۸۸	۷۲۵	فهیمه عباسی نهوجی	Thermodynamic study of malachite green by nanomaterial $LaMnO_3$
۸۹	۷۳۴	فهیمه عباسی نهوجی	$LaMnO_3$ High-speed adsorbent to remove methyl orange from aqueous solutions
۹۰	۷۹۴	سمیرا کمالی مرغزار	Soret coefficients for binary mixtures of Helium and hydrogen isotopes: The nonadiabatic effects
۹۱	۸۲۷	محمد نادر لطف اللهی	Solubility of salicylic acid in ethanol, acetone and ethyl acetate solvents at temperature ranging from 298 to 313K
۹۲	۸۳۰	محمد نادر لطف اللهی	An Experimental Study of the Loading and Controlled Release of Salicylic Acid on Zeolite Nanocomposite
۹۳	۸۳۴	مدینه شفیعی	Thermodynamic modeling of the solubility of cholesteryl acetate and cholesteryl butyrate in supercritical carbon dioxide: Evaluation of cubic equation of states
٩٤	۱۰۸۴	روح الله قراگوزی	A Computational Study of all mono-chlorostyrenes
٩٥	۱۰۸۶	روح الله قراگوزی	Comparative analysis on all di-chlorostyrenes; a DFT-B_3LYP study
٩٦	۱۱۲۹	حدیثه معصومی	Investigation of effective factors in separation process with ATPS and PEG 8000
۹۷	۷۹۷	صفرعلی جعفری	Ultrasound assisted salting-out extraction of antioxidant phenolics from some pharmaceutical plants
۹۸	۱۴	سیده سمیه آسمانی	Dynamics Study on an Interpolated Potential Energy Surface of the Imidogen with Hydroxyl Radical Reaction
۹۹	۲۵	مرضیه رفیعی	Kinetic Monte Carlo Simulation of hydrogen production from formic acid decomposition on Ni(100) catalyst
۱۰۰	۴۸	مرضیه سادات معصوم پور	Multichannel RRKM-SSA and CVT Rate Constant Calculations for the Reaction of $H_2S(^1A_1)$ with $HO_2(\,^2A'')$
۱۰۱	۷۵	فاطمه کشاورز	Is single-reference calculation adequate to address kinetics of CH(X2Π) reaction with N_2(1Σg)
۱۰۲	۸۱	الهام مزارعی	Application of Master Equation to Multi Well System of CH_3OH+HO_2

١٠٣	۸۲	سمانه موسوی	Direct Dynamics Study on the Reaction of CH_3^+ with O(1P) Atom
١٠٤	۱۵۸	هادی سالاری	Antibacterial activity investigation of magnetic metal nanoparticles decorated ionic liquids
١٠٥	۶۹۴	عادله افروزان	Kinetic investigation on Sono-degradation of Methylene blue by La:ZnO/GO nanocomposite
١٠٦	۷۳۳	افسانه نظری	Theoretical kinetic studies on the unimolecular decomposition of CH_3O_2 radical
١٠٧	۷۶۸	علی نیک اختر	Applying the Laplace transform to solve the kinetic equations of rubber vulcanization
١٠٨	۸۱۰	علی نیک اختر	Investigation of accelerated sulfur vulcanization by irreversible consecutive mechanism
١٠٩	۷۷۹	فاطمه صالحیان	Fast removal of Methyl orange (MO) by hollow $LaMnO_3$
١١٠	۸۱۵	الهام طریقه دار	Investigation of the hydrogenation reaction of imidazopyrimidinecarbene and Si /Ge heavier analogues using by computational methods
١١١	۸۱۴	الهام طریقه دار	Investigation of the carbene structure and stability of Imidazopyrimidine isomers by using quantum mechanics and NBO analysis
١١٢	۹۰۰	اسماعیل دهستانی	The study of anaerobic reaction kinetics by comparing the removal of BOD and the production of biogas in the ECSB anaerobic reactor
١١٣	۷۷	سمانه برومند	Permeability-Solubility Compensation by Molecular Dynamics Simulation
١١٤	۳۳۰	هدیه طاهری نیا	Interactions between water and dye atoms in the adsorption process of Acid Red-88 on graphene nanosheet: A molecular dynamics simulation
١١٥	۷۵۰	هدیه طاهری نیا	The effect of functionalizing graphene nanosheets on Hydroxynaphtol Blue center of mass adsorption, A molecular dynamics simulation
١١٦	۳۵۵	فهیمه علیرضاپور	The Thermophysical Properties of Imidazolium Based Ionic Liquids from Tao- Mason Equation of state and Artificial Neural Network
١١٧	۳۷۷	سمانه اسماعیلی شیخ آباد	In silico study on the effects of Glucosamine group on Thermal stability of Yarrowia lipolytica Lip_2 lipase
١١٨	۵۱۷	زهرا تابنده	Canonical Monte Carlo Simulation Study of Noble Gas Adsorption onto the SiNT
١١٩	۵۴۳	نرجس شیبانی	The effect of slit size on stress tensor components

۱۲۰	۸۰۲	مریم قربانی سنگلی	The effect of glycosylation on the chloroperoxidase structure: A molecular dynamic simulation analysis
۱۲۱	۱۰۲۷	مژگان سبزه زاری	Determination of the Stable Structures and Phase Transitions of Adamantine Nanoclusters by Molecular Dynamics Simulation
۱۲۲	۴	زهرا شمس الدین آزاد	<u>Simultaneous detection of L-cysteine and tryptophan as two important amino acids using a MgO nanostructure-based electrochemical sensor</u>
۱۲۳	۱۵	زینب رجب دیزاوندی	determination of tetracycline by adsorptive differential pulse cathodic stripping voltammet
۱۲٤	۴۷۵	زینب رجب دیزاوندی	Polymerization and characterization of para-nitrophenol in sodium acetate medium on pb electrode
۱۲٥	۱۹	مرضیه نودهی	Designing and fabrication of electrochemical aptasensor based on a novel MWCNTs@Au nanocomposite for bisphenol A detection
۱۲٦	۲۰	مرضیه نودهی	Design of an electrochemical bisphenol A sensor based upon magnetic nanoparticles modified with Au
۱۲۷	۲۱	لاله عباسی	Electrochemical synthesis of $CuCo_2O_4$ nanosheets on Ni foam as a binder-free electrode for supercapacitors
۱۲۸	۳۹	زهرا اصغرپور گلفزانی	Electrochemical synthesis of S-doped cobalt–copper layered double hydroxide for energy storage systems
۱۲۹	۶۶	ابوالفضل ناصر صدرآبادی	Developing a modified bipolar electrode for selective measurement of nitrate ion based on palladium nanoparticles deposited on a cathode pole
۱۳۰	۹۷	محسن اکبری فیض آبادی	Preparation of Fe_3O_4@silica sulfuric acid/MWCNT-modified electrode for detection of acetaminophen in the presence of ascorbic acid
۱۳۱	۱۰۷	سیامک کیانی شاهوندی	pH assisted homogeneous liquid-liquid microextraction followed by electrochemical detection on MWCNTs modified electrode for the determination of 4-nitrobenzaldehyde in water samples
۱۳۲	۱۲۳	سمیه کریمی	Electrochemical determination of gallic acid using nano Co_3O_4/MWCNTs modified carbon paste electrode
۱۳۳	۱۶۰	مسعود قپانوری	Sensitive determination of imatinib in human biological samples by differential pulse

			voltammetry based on carbon paste electrode modified by MWCNTs
١٣٤	۲۲۱	فاطمه حسین زاده	Study of the electrochemical behavior of Gabapentin at surface of glassy carbon electrode modified by Prussian blue and carbon nanotube
١٣٥	۲۴۳	عارفه گرگیج	An electrochemical method for the detection of hydrogen peroxide using glassy carbon electrode modified with Cu/Fe layered double hydroxide@Fe_3O_4 nanoparticles
١٣٦	۲۶۱	علی اسماعیل نیا	Electrochemical determination of bisphenol A using a cobalt oxide sensor
١٣٧	۳۲۴	نجمه صباغی	Simultaneous Voltammetric Measurement of Dopamine, Acetaminophene
١٣٨	۳۳۸	منصوره میرکی	Fabrication of nanostructure electrochemical sensor for simultaneous determination of sulfite and nitrite in real samples
١٣٩	۳۹۸	ملیحه مجرب	Computational design of a molecularly imprinted electrochemical sensor for determination of amlodipine via multivariate optimization technique
١٤٠	۵۰۶	فریبا بیگ مرادی	New glassy carbon modified electrode with MXene/ZnO for electrochemical measurement of bilirubin
١٤١	۵۰۷	فریبا بیگ مرادی	A novel MXene/ZnO nanocomposite modified glassy carbon electrode for rapid voltammetric detection of bisphenol A
١٤٢	۵۱۴	فاطمه مدرسی زاهد	Fabrication and c haracterization of polyaniline nanotubes/silver composite for the electrochemical sensing of anticancer drug, 5 -Fluorouracil
١٤٣	۵۲۲	آمنه امانی	Electrochemical Oxidation of 3,4-Dihydroxycinnamic acid in the Presence of Barbituric Acids Derivatives
١٤٤	۵۲۳	آمنه امانی	Electrochemical evidences in Drug-Drug interaction of acetaminophen with the Duloxetine and Fluvoxamine
١٤٥	۵۲۵	کوروش محمودزاده	An electrochemical sensor for the determination of Cd(II) using a modified gold electrode with organic-inorganic hybrid polyoxotungstate
١٤٦	۵۲۶	کوروش محمودزاده	Electrochemical determination of lead(II) on modified gold electrode by square wave voltammetry

١٤٧	۵۳۵	خدیجه قنبری	Electrochemical sensor based on graphene oxide/chitosan/ZnO/Au nanocomposite for the determination of losartan
١٤٨	۵۳۶	خدیجه قنبری	Electrochemical sensor for simultaneous determination of dopamine and epinephrine based on reduced graphene oxide/TiO_2 nanocomposite
١٤٩	۵۳۹	راضیه کاردوست پاریزی	Voltammetry determination of Tramadol by using of glassy carbon electrode modified with Alizarine Red S
١٥٠	۶۵۵	راضیه کاردوست پاریزی	Application of poly-Alizarin red s/ Multi-Walled Carbon Nanotubes-Modified electrode for detection of tramadol and dopamine
١٥١	۵۴۹	ستاره اکبری	Termodynamics of Ag^+ Cation complexation With N,N′-bis (salicylidene)-1,3-propane diamine in Some Binary Mixed Non-aqueous Solvents
١٥٢	۵۵۰	ستاره اکبری	Separation study of seven heavy metal cations through a bulk liquid membrane containing N,N’,N” -Tri-(4-ethyl benzene) phosphoric triamide
١٥٣	۵۶۱	مینا روحانی	Adsorptive stripping voltammetry determination of methyldopa at a pencil graphite electrode modified with Fe_3O_4 nanoparticle/reduced graphene oxide-chitosan in biological and pharmaceutical samples
١٥٤	۵۹۷	حیدر النجار	Preparation of gC_3N_4–Pt photoelectrocatalyst for electrooxidation of ethanol
١٥٥	۶۶۳	محمد الخفاجی	Electrooxidation of methanol using lanthanum cobalt oxide/platinum photoelectrocatalyst
١٥٦	۶۷۳	زهرا شفیعی	Determination of D-penicillamine at the sonogel-carbon electrode modified with cerium oxide nanoparticles
١٥٧	۶۷۸	نیلوفر رحمانی	Electrochemical oxidation of acetaminophen in the presence of clonazepam
١٥٨	۶۸۲	فرزانه کیا	Electrochemical synthesis of hollow gold nanoparticles on the surface of pencil graphite electrode as high efficient cathode material in the fuel cells
١٥٩	۶۸۶	زهرا رحیمی	Determination of Diuron using platinum nanoparticle and molecularly imprinted technology
١٦٠	۶۹۶	فریبا ملا رسولی	ZnTe/Quinhydrone nanocomposite-modified glassy carbon electrode as a promising ethanol

			electro-oxidation catalyst in acid media for fuel cell applications
١٦١	۷۱۳	حمیده ایمان‌زاده	Electrocatalytic Activities of the Pt/CNP Nanocomposite on Carbon Ceramic Electrode for Ethanol Oxidation
١٦٢	۷۱۹	شراره سیار	Visible light photoelectrochemical sensor for determination of progesterone based on polydopamine/quantum dots nanocomposites
١٦٣	۷۵۷	اياد الساعدی	Electrooxidation of ethanol on a lanthanum cobalt oxide/platinum modified FTO electrode
١٦٤	۷۶۷	علی حمزه‌لوی	Investigation of expander formulation in the negative active material on key performance characteristics of lead-acid batteries
١٦٥	۷۶۹	عبدالحمید هاتفی مهرجردی	Voltammetric determination of sulfasalazine by using glassy carbon electrode modified with 2,4-dinitrophenyl hydrazine
١٦٦	۷۷۰	عبدالحمید هاتفی مهرجردی	Multi-walled carbon nanotube/ polypyrrol nanocomposite modified glassy carbon electrode as a new sensor for determination of Buprenorphine
١٦٧	۷۷۴	لیدا فتوحی	Sensing platform for adefovir based on molecularly imprinted polymer- coated carbon nanocomposite
١٦٨	۷۷۶	لیدا فتوحی	Sensitive nonenzymatic electrochemiluminescence hydrogen peroxide sensor using polypyrrole/ ployluminole / titanium dioxide nanoparticles
١٦٩	۸۰۸	سیده مهرانگیز اطیابی	Decolorization of Industrial Wastewater Using Some Coagulants by Electrochemical Method
١٧٠	۸۱۷	فاطمه ابراهیمی	Electrochemical detection of phenol using semiconductor based modified electrode
١٧١	۸۸۵	حسین محمدزاده	A high-capacitance flexible solid-state super capacitor based on polyvinyl chloride, carbon nanotubes and polyaniline
١٧٢	۹۱۹	علی محمدی	Cobalt-Nickel Loaded on Hydroxyapatite Wrapped Multiwalled Carbon Nanotubes as a New Catalyst for Oxygen Evolution Reaction
١٧٣	۹۲۰	فردین ناصرپور	Designing and fabrication of novel electrochemical sensor for simultaneous determination of hydroxylamine and phenol
١٧٤	۹۹۶	فردین ناصرپور	Voltammetric determination of hydrazine at the surface of a modified carbon paste electrode with TiO_2 nanoparticles

۱۷۵	۹۴۴	سمیه میرگل	Modified Graphite Paste Electrode with Strontium Phen-Dione Complex for Simultaneous Determination of a Ternary Mixture of 4-aminophenol, Uric Acid and Tryptophan
۱۷۶	۹۴۵	سمیه میرگل	Modified Graphite Paste Electrode with Strontium Phen-Dione Complex for Simultaneous Determination of a Ternary Mixture of Dopamine, Acetaminophen and Xanthine
۱۷۷	۹۶۸	سیده زینب حسینی	Potentiometric Determination of HPO_{42}- with Chitosan- Cu by Carbon Paste Electrode
۱۷۸	۹۶۹	سیده زینب حسینی	Potentiometric Determination of HPO_{42}- with Chitosan-Zn by Carbon Paste Electrode
۱۷۹	۱۰۲۰	مریم محمدآبادی	High-Performance Visible-Light-Driven Ag–gC_3N_4/Pt Photoelectrocatalysts for Methanol Oxidation
۱۸۰	۳۹۱	محدثه بیابانی	Preparation of polypyrrole/TiO_2 nanocomposite via surface molecular imprinting technique and its photocatalytic activity under UV irradiation

راهنمای تفکیک گرایش‌های اصلی بر اساس رنگ				
شیمی آلی	شیمی تجزیه	شیمی فیزیک	شیمی معدنی	سایر

زمان ارائه پوستر بخش (B) شامل (شیمی آلی-شیمی تجزیه-شیمی معدنی)

چهار شنبه ۹۷/۴/۲۷ ساعت ۱۰:۲۰ الی ۱۱:۰۰

شماره	کد مقاله	ارائه دهنده	عنوان مقاله
۱	۶۰۴	شادی قلعه نوی	Synthesis and Antibacterial activity evaluation of two 2-Aminothiophene derivatives
۲	۶۱۸	زین العابدین سپهر	Preparation of Polystyrene Containing Photochromic Functional Group
۳	۶۲۱	زین العابدین سپهر	Preparation of Photochromic polyvinyl chloride
۴	۶۲۴	ساناز قره حسنلو	Aqua three-component synthesis of new isoxazole-5(4H)-ones catalyzed by sodium malonate

۵	۶۳۰	ایرج سروی	Highly dispersed palladium nanoparticle loaded catalyst for suzuki reaction in water
٦	۶۳۳	فاطمه مرادی	Metal-Free Assembly of Four C-N and Two C-C Bonds: Diestereoselctive Synthesis of Pyrido[1,2-a]pyrimidines via a FiveComponent Reaction
۷	۶۳۵	سیده لیلا الهقلی پور	Synthesis of MgO nanoparticles supported on ionic liquid-based periodic mesoporous organosilica as a nanocatalyst for the synthesis of novel spirooxindole
۸	۶۵۸	طیبه داودیان	Reactions of chlorinated pyridines at 4-position: synthesis, structure and reactivity of a variety of tetrachloropyridyl niterene
۹	۶۶۱	طیبه داودیان	Survey reactivity of enaminones derivatives with pentafluoro(chloro)pyridine
۱۰	۶۹۳	غلامحسن ایمانزاده	Synthesis of new derivatives of pyrazole using three component reactions
۱۱	۷۱۷	حنانه رحیمی	Synthesis of a novel pyridine-2,6-dicarboxamide as a fluorescent chemosensors for recognition of ions
۱۲	۷۲۷	سیما درویشی	Pd Immobilized on a Nano Worm-like Silica Network Catalyzed Coupling reactions
۱۳	۷۳۲	پریسا چگینی	Metal modified beta-cyclodextrin (MMC) exhibits high reactivity in synthesis of fused pyrimidines
١٤	۷۳۹	امیر احسانی	Introducing an efficient method for preparation of 2,8-bis(methylthio)-5- propyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-4,6-diol (L)
۱۵	۷۶۴	مینو خدامرادی	The preparation and characterization of BNPs-SO3H: a highly efficient and reusable nanocatalyst for the preparation of 5-substituted 1H-tetrazoles
١٦	۷۷۸	سهیلا بلندی	Desulfurization by Metal Oxide/Graphene Composites
۱۷	۷۹۰	فاطمه شاه محمدی مهرجردی	Cetyltrimethylamonium hydrogensulfate catalyzed synthesis of quinoxalines in aqueous media at room temperature
۱۸	۷۹۲	فاطمه شاه محمدی مهرجردی	Copper acetate/sulfadiazine complex as a highly active catalyst for 1,2,3-triazoles synthesis in aqueous polyethylene glycol media at room temperature
۱۹	۷۹۸	آسیه امیراحمدی	Synthesis of Pyrimidine-4-thiones and Thiazoles from TMG Adducts and Isothiocyanates

۲۰	۸۲۵	فهامه محمودی	Five-component synthesis of dihydropyridines based on diketene
۲۱	۸۴۴	مهین ولایتی هوشنگ	The Synthesis of Epoxy Polyuretheane -Silica Nanocomposites
۲۲	۸۴۵	زهره طاهری	A synthesis of (arylthio-ethylidene)indolin-2-ones via S-arylation of oxoindolin-ethanethiolates with aryl halides
۲۳	۸۴۶	ناهید موسی وند	κ-Carrageenan: An efficient, green and reusable catalyst for the one-pot synthesis of 3, 4-dihydropyrimidin-2(1H)-ones and their corresponding 2(1H)thione
٢٤	۱۱۲۵	ناهید موسی وند	κ-Carrageenan as an efficient, green, bifunctional and reusable catalyst for one-pot synthesis of Hantzsch 1,4-dihydropyridine
٢٥	۸۵۰	میثم پسندیده ندامانی	Light-induced switching of azo-imidazoles on gold nanoparticles
٢٦	۸۵۵	رزا ادریس عامری	Quinolin-4(1H)-one promoted synthesis of functionalized trifluoro methylated ketenimines and 1-azabuta dienes via isocyanide based multicomponent reactions
۲۷	۸۶۰	فاطمه حسنی باقری	Synthesis of novel amino and pyrrolyl acridine 1, 8-dione derivatives
۲۸	۸۶۷	سعید ایرانپور	Sodium Formaldehyde Solfoxylate, Synthesis, Optimization and Performance Evaluation
۲۹	۶۸۸	سعید ایرانپور	Comparison of different analytical methods for measuring salt in crude oil
۳۰	۸۷۴	ملیحه کمالپور	Condensation reaction between 3-acetylcumarine and arylaldehydes in the presence of L-proline
۳۱	۹۰۱	محمدرضا جعفری	Formic acid catalyzed One-pot synthesis of αaminophosphonates: an efficient, inexpensive and environmentally friendly organocatalyst
۳۲	۹۰۲	حسین صارمی	Hydroxy ethyl methyl morpholinium azide [HEMMorph][N_3] as a novel and highly efficient ionic liquid for three components Click Huisgen cycloaddition
۳۳	۹۴۱	اسرین پاکروان	Chemo-photothermal therapy of cancer cells using gold nanocages covered by smart polymers for controlled release
٣٤	۹۴۷	پروین اسدی	Preparation, characterization and antimicrobial properties of some s-triazine/quinazolinone hybrids

٣٥	۹۵۱	معصومه جدیدی نژاد	Guanidine Acetic Acid Functionalized Magnetic Nanoparticles: Recoverable Green Catalyst for Transamidation
٣٦	۹۵۲	الهام سنجری	A one‑pot protocol for the construction of chromenoimidazopyridines and chromenopyridopyrimidines containing intramolecular hydrogen bonds
٣٧	۹۷۶	سپیده خائف	C−S Bond Formation Via C-H Bond Activation Catalyzed by Co(ll)-Immobilized Silica- Based Magnetic Retrievable Nanocatalyst
٣٨	۹۸۱	فاطمه رضایی منش	Synthesis of new derivatives of 2-alkynylamino-6-substituted-pyrimidine-5-carbaldehyde catalyzed by Pd-Cu
٣٩	۹۸۲	فاطمه رضایی منش	Efficient synthesis of novel 1,2,3-triazole-linked pyrimidine via copper-catalyzed click reactions
٤٠	۹۹۰	سحر عباسی	Synthesis of novel derivatives of 1,2,3-triazole-linked pyrazole catalyzed by copper(I)
٤١	۹۹۳	سحر عباسی	Catalyst-free method for the synthesis of pyranopyrazoles in magnetized water
٤٢	۹۹۲	فاطمه زهرا خورسی دامغانی	Synthesis and Characterization of Fe_3O_4@C-SO_3H as a highly efficient Nano-Catalyst for the preparation of 2/aminobenzothiazolomethylnaphthols and 1-amidoalkyl-2-naphthols
٤٣	۸۰۶	فاطمه زهرا خورسی دامغانی	Fe_3O_4@C-SO_3H: Synthesis, Characterization and Its application on benzo[4, 5]imidazo[1, 2-*a*]-pyrimidines synthesis
٤٤	۹۹۴	زهره حسنلو	Catalytic method for the synthesis of 2-amino-4-aryl-3-cyano-4H-pyran derivatives
٤٥	۹۹۷	زهرا علی محمدی	Synthesis of new azo compounds based on thiazolidinone derivatives
٤٦	۹۹۹	ظهیر شکوه سلجوقی	Antibacterial activity of AgO- chitosan composite against aquaculture pathogenic bacteria (case study: Edwardsiella tarda)
٤٧	۱۰۰۰	ظهیر شکوه سلجوقی	Surfactant modified clinoptilolite as novel antifungal agents against Saprolegnia sp
٤٨	۱۰۱۱	لیلا محمدزاده قشلاقی	Electrospun Soluble Eggshell Membrane Protein/Galatin/Polycaprolactone for Tissue Engineering Applications
٤٩	۱۰۱۸	رضا رضائیه راد	A Sequential One-pot Three-component Synthesis of 2-Oxindole Scafold Containing Dihydropyrazine by Using Triethylammonium thiolates

٥٠	۱۱۰۵	فاطمه رمضانی گماری	Protic acidic ionic liquids: green, efficient and reusable catalyst for synthesis of dihydropyridines
٥١	۱۰۳۹	عاطفه زینعلی	4H-benzochromene derivatives catalyzed by KCC-1@SO_3H nano heterogeneous solid acid
٥٢	۱۰۴۳	عاطفه زینعلی	A new application of KCC-1@SO_3H as a heterogeneous catalyst in crossed-aldol condensation reaction under solvent-free conditions
٥٣	۱۰۴۷	سیما عباس پور	A novel access to new pyrrolo[1,2-a]quinoxalines through palladium- catalyzed multi-component reactions
٥٤	۱۰۵۱	سیما عباس پور	One-pot Synthesis of Pyrrolo[1,2 a]quinoxaline Derivatives via Palladium-catalyzed reactions
٥٥	۱۰۴۸	سعید لشکری	Novel multi-component synthesis of 4-ethynyl substituted pyrrolo[1,2-a]quinoxalines through palladium-catalyzed coupling-coupling reactions
٥٦	۱۰۵۰	سعید لشکری	A one-pot synthetic approach for construction of thiazolo[3,2- *a*]benzimidazole-linked quinoxaline scaffold via palladium-catalyzed reactions
٥٧	۱۰۷۳	غزاله ابارشی	A Green and Efficient Synthesis of 2-Thioxoquinazolinone Derivatives in Water Using Potassium Thiocyanate
٥٨	۱۰۹۸	آرزو اکبری	Magnetic Propylsulfonic Acid-Anchored Isocyanurate-Based Periodic Mesoporous Organosilica (Fe_3O_4@PMO-PrSO_3H): A Novel and Highly Efficient Nanoporous Catalyst in the Synthesis of Spirooxindoles
٥٩	۱۱۲۷	آرزو اکبری	Sulfonic Acid-Anchored Isocyanurate-Based Periodic Mesoporous Organosilica (PMO-SO_3H): A Highly Efficient and Recoverable Nanoporous Catalyst in Biginelli reaction
٦٠	۱۱۰۷	زینب حمیدی	Synthesis a polymer-supported Fe_3O_4 nanoparticles and its application as a novel route for the synthesis of imidazole derivatives
٦١	۱۱۰۹	مریم کمال زارع	Simple and efficient strategy for the synthesis of pyridone derivatives
٦٢	۱۱۱۵	مریم کمال زارع	Synthesis of highly functionalized 6-amino-4-(aryl)-5-nitro-2-oxo-1,2-dihydropyridine-3-carbonitrile derivatives
٦٣	۱۱۴۹	عالمه مصلحی	Application of Magnetic Fe_3O_4 Nanoparticles in the Synthesis of β-Lactams Contain Amino Group

٦٤	۱۱۴۷	رقیه سلطانی	Metal-Free Aerobic Oxidative Esterification of Aldehydes in the Presence of Potassium Fluoride
٦٥	۱۱۵۲	اشرف مرادی	Synthesis of Xanthene and Dihydroquinazolin-4(1H)-ones by fructose catalyst
٦٦	۱۱۵۳	فاطمه پیرانی	An Efficient Green Synthesis of Pyrimidine and Pyridopyrimidine Derivatives In The Presence of Eutectic Solvents
٦٧	۱۱۷۸	فاطمه میرهاشمی	Synthesis of Pyrimidin derivatives using Fe_3O_4@Ag-β-CD nanoparticles as a green and magnetically recyclable nanocatalyst
٦٨	۳۴۷	فاطمه میرهاشمی	Fe_3O_4@Cu-β-CD nanoparticles-catalyzed synthesis of pyrazole derivatives
٦٩	۵۰۴	سهیلا حیدری پرستار	Study on the peri- and stereoselectivity of cycloaddition reaction of disulfonyl diene with cyclopentadiene by computational methods
٧٠	۵۰۵	سپیده معصومی فر	DFT study on the mechanism of the cross Diels-Alder of monosulfonyl-1,3-dienes
٧١	۲۱۸	معصومه رضائی	Hydrogen Production from Biomass derived-Formic acid Catalyzed by Pt-TiO_2: A Periodic DFT Analysis
٧٢	۲۷۷	سمانه علی نیا	Conformational analysis of bistetrazole energetic compound in neutral and anionic forms
٧٣	۴۵۲	محمدرضا زمانلو	Investigation of Optical and Solution Properties of Azo-dyes Derived from Ethylacetoacetate and Aromatic Amines
٧٤	۵۸۶	سمیه صفایی	Factors affecting on the acidic site of prunasin in gas phase, water and DMSO
٧٥	۵۴۲	نازنین محبی	Substituent effects on thermodynamic parameters of new plumbylenes at DFT
٧٦	۹۰۴	الهام توکلی	Synthesis of titanomagnetite nanoparticles functionalized with sulfamic acid groups and applications for the synthesis of quinazolin derivatives
٧٧	۱۸	مهناز محمودی فرد چگنی	Nano γ- Alumina supported boron trifluoride as a novel solid acid catalyst for the synthesis of pyrroles at room temperature under solvent-free condition
٧٨	۱۰۲۱	مریم محمد آبادی	A novel visible light photoelectrochemical aptasensor for detection of bisphenol A
٧٩	۱۰۳۴	فرشته سالکی	Basic charge storage mechanism of cobalt sulfide electrode material for supercapacitor
٨٠	۱۰۳۵	ایمان رضوی پناه	Pt–Os–TiO_2 photoelectrocatalyst for methanol oxidation

٨١	۴۲۸	فهیمه زارعیان جهرمی	Removal of Brilliant green dye from aqueous solution using Au-Fe_3O_4 ,B cyclodextrin nanocomposite as a novel sorbent
٨٢	۶۷	مهناز قرقلو	Method Validation for the Quantitative Analysis of Aflatoxins (B1, B2, G1, and G2) in Rice by HPLC with Fluorescence Detection
٨٣	۱۱۸	عاطفه امام جمعه	Process analysis of chabahar maritime university reverse osmosis desalination plant
٨٤	۱۲۶	مژگان صالحی	Introducing a new pH assisted homogeneous liquid-liquid microextraction method based on switchable-hydrophilicity solvents followed by GC-MS for the determination of PAHs in water samples
٨٥	۱۲۸	ملیحه میر	Study of supported liquid membrane transport of 2,4-Dichlorophenoxyacetic acid (2,4 D) using Nano material as new support
٨٦	۱۳۱	ملیحه میر	Study of facilitated bulk liquid membrane transport of lithium ion from seawater and use of carbon nanotube as additive in membrane
٨٧	۵۶۹	فاطمه زمانی	Determination of nortriptyline in aqueous sample by dispersive liquid phase microextraction followed by ion mobility spectrometry
٨٨	۲۶۴	محبوبه شیرانی	Ultrasonic-assisted liquid-liquid microextraction linked deep eutectic solvent for determination of lead using flame atomic absorption spectrometry in water
٨٩	۳۷۲	نیلوفر جلیلیان	Synthesis of magnetic MIL-53(Fe) as an efficient sorbent for coextraction and determination of acidic, basic and amphiprotic pollutants
٩٠	۴۰۶	محبوبه قزاق میری	Urea-based porous organic polymer/graphene oxide hybrid sorbent for highly efficient extraction of bovine serum albumin
٩١	۴۵۶	پوریا نجواک	PVDF-HFP based polymer inclusion membranes composed of Aliquat® 336 and Cyphos® IL 101 for removal of Cr(VI) from sulfate solutions
٩٢	۴۵۸	غزال جوادیان	Lactose intercalated layered double hydroxide as a green sorbent for efficient and selective removal of heavy metals from aqueous solution
٩٣	۴۷۹	لیلی زارع	Modeling and optimization of Diclofenac extraction using Plackett–Burman method
٩٤	۵۰۸	آرزو نجفی	Homogenizer assisted dispersive liquid phase microextraction followed by corona discharge-ion mobility spectrometry for determination of Pramipexole

٩٥	۵۴۷	قمر سلامت	Ionic liquid-based supramolecular solvent microextraction for extraction of synthetic food dyes in foodstuff samples
٩٦	۶۴۸	الهه سالاری	Development of a new liquid phase microextraction method using a switchable solvent for the determination of polychlorinated bi-phenyls (PCBs)
٩٧	۶۶۸	کبرا سادات هاشمی نسب زواره	Use of switchable hydrophilicity solvents based liquid phase microextraction (SPs-LPME) followed by HPLC-UV for the determination of 17 amino acids in different samples
٩٨	۶۶۹	کبرا سادات هاشمی نسب زواره	Determination of glyphosate residues in wheat samples with switchable hydrophilicity solvents (based liquid phase microextraction (SPs-LPME
٩٩	۶۸۴	مهناز نوظهور یزدی	Multiwall carbon nanotube- zirconium oxide nanocomposite hollow fiber solid phase microextraction for determination of polyaromatic hydrocarbons in water, coffee and tea samples
١٠٠	۷۵۴	کبری زوار موسوی	Imidazolium-based bifunctional periodic mesoporous organosilicas as novel sorbent for microextraction by packed sorbent
١٠١	۷۸۳	سیده علیه حمیدی خرق	Synthesis of novel sorbent for the extraction and preconcentration of polycyclic aromatic hydrocarbons from aqueous samples
١٠٢	۷۸۷	زهرا نصرالهی خشکبار	Investigation of Zeolitic Imidazolate Frameworks Ability as Sorbent in Solid Phase Microextraction Method
١٠٣	۸۳۵	مژده اسماعیلی	Extraction of Caffeine from coffee by Homogenous Liquid-Liquid Extraction (HLLE) method and determination with Spectrophotometric UV-Vis
١٠٤	۸۴۹	مولود خسران نجف آبادی	Extraction of dopamine by DC potential-reinforced bulk-liquid membrane transport (PR-BLMT) combined with UV- Vis spectrophotometric method
١٠٥	۹۱۵	سحر بدرقه	Simultaneous determination and pharmacokinetic study of antidiabetic drugs by HPLC-UV using novel MSPE method
١٠٦	۹۶۵	زهره حمزه ای	Preconcentration and determination of phenylalanine in some pharmaceutical and food samples by cloud point extraction coupling with UV-Visible

١٠٧	۹۶۷	امیر اسماعیل زاده	Trace determination of nitrotoluenes in water by hollow fiber protected stir bar liquid phase microextraction based on magnetic ionic liquids
١٠٨	۹۸۰	عرفان براتی	Analysis of antidepressant drugs by using HS-SPME based on nano-structured conductive polymer fiber couple to ion mobility spectrometry
١٠٩	۹۹۸	نسرین مرادی	Combining magnetic solid-phase extraction and dispersive liquid-liquid microextraction methods for preconcentration environmental poll
١١٠	۱۰۳۷	عباس آبدار	Magnetic three-dimensional graphene solid-phase extraction coupled with gas chromatography-flame ionization detector for the determination of chlorophenols in water samples
١١١	۱۰۳۸	نگار امیرحقیان	A liquid chromatography method for determination of p-cresol in human plasma by in situ surfactant-based solid phase extraction
١١٢	۱۰۶۶	نگار امیرحقیان	A validated HPLC–FL method for estimation of metoprolol in exhaled breath condensate
١١٣	۱۰۴۵	مجتبی جعفری	Application of ligandless liquid phase microextraction based on deep- eutectic¬ solvent for determination of trace amounts of lead in edible oils by flame atomic absorption spectrometry
١١٤	۱۱۲۴	علی جهانبخش	Extraction of Dopamine by Homogeneous Liquid –Liquid Extraction method (HLLE) and determination with UV-Vis Spectroscopy
١١٥	۲۶۵	ساناز رضازاده	Modeling the retention behavior of some drugs in high performance affinity chromatography
١١٦	۵۴۱	امین همتی یادکوری	Using the CPE-scanometry method for the simultaneous preconcentration and determination of the Rhodamine B and Nile blue
١١٧	۶۵۰	نسترن حاجی حسینی	Paper-based colorimetric sensor array for detection of trinitrotoluene using chemometric methods
١١٨	۷۴۵	میلاد نمرودی	Alignment Independent 3D-QSAR Study of BACE1 Inhibitors as Anti-Alzheimer Drugs
١١٩	۹۰۵	عباس دادرس	Determination of pKa of Cinnamic acid using Net analyte signal as a chemometric method on the spectrophotometric data
١٢٠	۹۰۶	عباس دادرس	Spectrophotometric determination of acidity constant of Cinnamic acid using rank annihilation factor analysis (RAFA)

١٢١	۸۶۱	خلیل زرنوشه فراهانی	Simultaneous determination of N-acetylcysteine and acetaminophen at the modified electrode assisted by chemometeric approaches
١٢٢	۱۳۴	فائزه مجتبی زاده	Synthesis and structural determination of novel the Cu(II) nano coordination system
١٢٣	۱۳۶	فائزه مجتبی زاده	Sonochemical and the structural characterization of novel the Cd(II) nano metal-organic polymer
١٢٤	۲۸۸	بهنام قریب	Two Pillared Metal–organic Frameworks Comprising a Long Pillar Ligand used as fluorescent sensor for nitrobenzene and heterogeneous catalyst for Knoevenagel condensation reaction
١٢٥	۴۳۳	فرنوش زارع کاریزی	Cation exchange in an anionic nanoporous MOF for study of CO_2 adsorption
١٢٦	۴۳۴	حسین قاسم پور	Interplay Between Hydrophobicity and Basicity toward the Catalytic Activity of Isoreticular Organocatalyst MOFs
١٢٧	۸۰۳	نسرین شکوه فر	N-oxide Functionalization of UiO-66 via Solvent-Assisted Ligand Incorporation: Synthesis and Cr(VI) Adsorption Studies
١٢٨	۱۰۷۵	الهام رودباری	Competitive Adsorption of Metal Pollutants on Modified Silica gel
١٢٩	۱۰۵۶	الهام رودباری	Green Synthesis of Silver Nanoparticles from Berberis Integerrima Extract and Their Antihyperglycemic Properties
١٣٠	۲۴	رویا نظری	Mononuclear copper(II) complexes containing chelating ligand of 2-methyl-N-(pyridine-2-yl-methyl)propane-2-amine as chromotropic probes
١٣١	۶۸	عبدالله الظاهر	In situ oxidation of 2,9-dimethyl-1,10-phenanthroline for synthesis of nickel(II) complexes containing highly preorganized acidic ligand
١٣٢	۶۹	مصطفی عطایی	Mixed ligand coordination complex of Mn(II) containing oxidized pyridine-2,6-dicarboxylic acid and 1,10-phenanthroline: Synthesis and characterization
١٣٣	۷۱	الهام مومن زاده	Construction of two zinc and copper(II) coordination complexes containing pyridine-2,6-dicarboxylic acid N-oxide based on mixed-ligand synthetic strategy
١٣٤	۱۰۳	نسیمه جام گوهری	Interaction of CT-DNA/BSA With Ethylendiamine 2-pyridinecarboxcylatopaladium(II) ninarte and anti- tumor activity

١٣٥	۲۳۵	زهرا بیات	Synthesis and characterization of new binuclear complexes mercury(II) of pyridinium ylide
١٣٦	۲۳۸	زهرا بیات	Synthesis and characterization of silver(I) and mercury(II) complexes with pyridinium ylide and study on their antibacterial properties
١٣٧	۲۷۹	رامین کیانی	Anticancer activity of three novel Pt complexes with Amine and glycine ligand
١٣٨	۲۸۱	رامین کیانی	Synthesis, characterization and cytotoxicity of three novel amino acid Platinum (II) complexes against colon cancer cell line
١٣٩	۳۰۴	معصومه محمودآبادی	Synthesis and theoretical studies of Cadmium (II) macrocyclic Schiff-base complexes containing piperazine moiety
١٤٠	۳۰۸	محمدطاهر رضایی	Synthesis and characterization of macrocyclic complexes containing piperazine moieties with Mn(II), Cd(II) and Zn(II)
١٤١	۳۲۵	مریم نوری	Synthesis, characterization and photoluminescence studies of a new Schiff base ligand and its nickel(II) complex
١٤٢	۳۳۱	فاطمه فروزنده	Synthesis and Characterization of a new polyamine containing piperazine moiety and related potentially N_6O_2 donors ligands together with corresponding Zn(II) complexes
١٤٣	۵۰۱	سید علی یثربی	Synthesis and crystal structure of a novel mixed ligand copper complex
١٤٤	۵۴۰	زهرا محسنی افشار	Synthesis, characterization and chemiluminescence study of quercetin and its metal complexes
١٤٥	۵۴۵	فاطمه اسمی پور	Synthesis, characterization and electronic absorption spectra of new mononuclear cyclopalladated benzo[h]quinolinate complexes containing phosphorus ylides
١٤٦	۵۴۶	فاطمه اسمی پور	Cyclopalladated complexes derived from benzo[h]quinolinate and diphosphine ligands as highly efficient homogeneous pre-catalysts for the Suzuki reaction of aryl halides
١٤٧	۵۶۲	زهرا یکه قاسمی	Synthesis, structural characterization and cytotoxic activity of Mn(IV) complex of dithiocarbazate
١٤٨	۶۰۰	سعید دینی	New Molecular Azo-Azomethine Receptor for Colorimetric Detection of Inorganic Anions

١٤٩	۶۲۰	فاطمه گودرزی	Synthesis and characterization of new binuclear and polymeric complexes mercury(II) stabilized of pyridinium ylide
١٥٠	۶۲۳	فاطمه گودرزی	Synthesis and characterization of palladium(II) complexe derived from α-keto stabilized pyridine ylide and study on its catalytic properties
١٥١	۶۵۲	زهره سادات قوامی	Synthesis and characterization of polymeric Schiff base ligand and its vanadium complex
١٥٢	۷۱۱	رضا کاظم شعاردوزدوزانی	Geometrical aspects in coordination of an amino alcoholic ligand toward copper bromide
١٥٣	۷۱۴	رضا کاظم شعاردوزدوزانی	Synthesis and Spectral Study of a zinc(lI) Complex with NN'O-Donor Ligand
١٥٤	۷۳۰	جواد اسماعیل زاده	Structural and statistical investigation of the coordination behavior of the picolinate-based ligands using the CSD database
١٥٥	۱۱۳۱	جواد اسماعیل زاده	Structural and statistical investigation of the coordination behavior of the picolinate-based ligands using the CSD database
١٥٦	۷۵۵	سمانه صادق زاده بقمچ	Synthesis and characterization of cobalt complexes containing 1,10-phenanthroline-2,9-dicarboxylic acid
١٥٧	۴۴۰	سمانه صادق زاده بقمچ	Clinical investigations of cobalt, copper complexes containing 1,10-phenanthroline-2,9-dicarboxylic acid in some cancer therapy treatments
١٥٨	۷۷۷	فرزانه مروتی	Synthesis and characterization of metal complexes with tridentate Schiff base ligand (NNS) derived from Pyrrole-2-carbaldehyde
١٥٩	۸۰۹	سلیمه عبدی نسب	Synthesise and characterization of cadmium sulfide nanoparticles via a solvothermal method in the presence of a new sulfur source
١٦٠	۸۴۰	لیلا عبدالهی	Synthesis, characterization and biological activity of a new novel cis MoO_2 Schiff base complex
١٦١	۸۹۴	فاطمه سلیمانی راوندی	Synthesis and characterization of VO^{2+} and Mn^{2+} complexes containing a Schiff base ligand derived from Tryptamine and 2-hydroxy-1-naphtaldehyde

راهنمای تفکیک گرایش‌های اصلی بر اساس رنگ				
شیمی آلی	شیمی تجزیه	شیمی فیزیک	شیمی معدنی	سایر

زمان ارائه پوستر بخش (C) شامل (شیمی آلی-شیمی تجزیه-شیمی معدنی-شیمی فیزیک)

چهار شنبه ۹۷/۴/۲۷ ساعت ۱۶:۵۰ الی ۱۷:۳۰

شماره	کد مقاله	ارائه دهنده	عنوان مقاله
۱	۵۲	معصومه مظلومی	Facile synthesis of N,N′-diarylformamidines by acidic ionic liquid immobilized on nanoporous TiO_2
۲	۷۳	رقیه خنیور	Efficient synthesis of bis-coumarins using Isatin-N-sulfonic acid under solvent-free conditions
۳	۷۴	رقیه خنیور	Pyridinium-N-sulfonic acid hydrogen sulfate as a highly effective and dual-functional catalyst for the synthesis of 1-carbamatoalkyl-2-naphthols
٤	۱۰۸	مهدی بهبودی لایین	Synthesis of the Cu (II) Schiff base complexes supported on alumina nanoparticle; for preparation of 5-Substituted-1H-tetrazoles derivatives
۵	۱۲۵	علی سواری	One-Pot Synthesis Of 1,4-Benzodiazepine Derivatives Using Hetropoly acid Ionic Liquids Supported On Magnetic Nanoparticles Of $CoFe_2O_4$
٦	۱۳۰	زهرا نظامی	Synthesis of new tetrahydro pyridines catalyzed by Fe_3O_4@S-doped TiO_2 via one-pot multi component Mannich reaction
۷	۱۴۰	حسین آقاجانپور وشکی	Oxidation of alcohols and trimethylsilyl ethers to the corresponding carbonyl compounds by molybdic acid supported on $NaHSO_4.H_2O$ under solvent-free conditions
۸	۱۴۱	عاطفه بختیاری	L-Prolin anchored on mesoporous SBA-15: A new recyclable catalyst to the synthesis of pyrimidines
۹	۱۴۹	فاطمه عسکری جیرهنده	Facile and simple synthesis of pyrimido[4,5-b]quinolines catalyzed by [PVP- SO_3H]HSO_4
۱۰	۱۵۲	احمدرضا موسوی زارع	Isonicotinic acid as an efficient catalyst for the synthesis of hexahydroquinolines
۱۱	۱۶۸	زهرا جلیلیان	Tandem cyclocondensation-Knoevenagel–Michael reaction of phenylhydrazine, acetoacetate derivatives and arylaldehydes, using isonicotinic acid under neutral media

١٢	۱۶۴	امین خشنود	Highly efficient three-component synthesis of 5-substituted-1H-tetrazoles, in present of Cu(II) heterogeneous complex catalysts
١٣	۱۷۰	مهدیه حقیقت	Using a new magnetically separable nanocatalyst in the synthesis of [1,2,4]triazolo quinazolinone derivatives
١٤	۱۷۱	ریحانه پورحسن	Using a new superparamagnetic nanocatalyst for the N-Boc protection of amines
١٥	۱۷۲	محمد رضایی	The synthesis of 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s using boric acid aqueous solution system
١٦	۱۹۶	شادی نظری	Facile synthesis of aryl-azo dyes using a nano sized dicationic acidic catalyst
١٧	۲۰۱	شیلا درویش زاد	Introduction of a new piperazine-based ionic liquid as an efficient catalyst for the biginelli reaction
١٨	۲۰۸	زهرا شریفی	Application of a new dicationic ionic liquid catalyst in the efficient synthesis of 4H-pyran and pyrano[2,3-d]pyrimidinone derivatives
١٩	۲۱۴	زهره قدمیاری	Graphene Oxide Immobilized Zr-Organic-Framework: a New and Efficient Catalyst for Biginelli Reaction
٢٠	۲۲۰	سمانه محمودی گم یک	Immobilized Cu(II) Schiff-base complex supported on Fe_3O_4 magnetic nanoparticles: A highly efficient and reusable new catalyst for the synthesis of pyranopyridine derivatives
٢١	۲۳۴	نیلوفر صفری	An efficient three-component synthesis of triazolo[2,1-b]quinazolinone derivatives catalyzed by reusable DABCO-based dicathionic ionic liquid
٢٢	۲۷۵	عاطفه السادات موسوی سیاوشی	Facile and Efficient Multicomponent Synthesis of Some Trisubstituted 1,3,5-Triazine Derivatives Catalyzed by Various Nanocatalysts
٢٣	۳۱۰	فاطمه قربانی	Pomegranate juice as a green catalyst for the synthesis of 2-aminochromenes-3-carbinitriles
٢٤	۸۷۱	فاطمه قربانی	Nanocrystalline silica-H_2SO_4 as an efficient Heterogeneous catalyst for the synthesis of 2-aminobenzothiazolo-arylmethyl-2-naphthols under solvent-free conditions
٢٥	۳۱۱	علی رجایی	Application of Cellulose/Clay/ZnO/CeO_2 nanocomposite as a catalyst for oxidation of aniline derivatives

٢٦	۵۶	علی رجایی	TiO_2 nanoparticles supported on the Fe_3O_4/GO nanocomposite: a novel magnetic nanocatalyst for the synthesis of 2- Aminothiazoles
٢٧	۳۴۱	سید حسین بنی طبا	Nanosilica sulfamic acid catalyzed synthesis of 2-phenylbenzoxazole Derivatives as heterogeneous catalyst
٢٨	۶۶۰	سید حسین بنی طبا	A mild Synthesis of Pyrophthalone Derivatives Catalyzed by ZnO Nanoparticles under Solvent-free Conditions
٢٩	۳۴۴	اسماعیل عیدی	Synthesis of quinazolines over recyclable Fe_3O_4@SiO_2-APTES-Fe^{3+} nanoparticles: A green, efficient, and solvent-free protocol
٣٠	۳۴۶	بهاره عباس خاکیانی	Introduction of Benzimidazole-based ionic liquid as an efficient and reusable catalyst for the preparation of 1,8-dioxo xanthene derivatives
٣١	۴۸۲	سپیده عباسی	Copper oxide supported on magnetic nanoparticles (CuO@γ-Fe_2O_3) for addition of amines to carbodiimides toward synthesis of guanidines
٣٢	۳۵۴	زهرا نصراصفهانی	Ionic liquid-functionalized mesoporous silica nanoparticles ([pmim]$FeCl_4$/MSNs): Efficient nanocatalyst for solvent-free synthesis of N,N′-diaryl-substituted formamidines
٣٣	۴۰۳	معصومه محمدی	Solvothermal Synthesis of Surface-Passivated and Functionalized Carbon Quantum Dots with High Catalytic Activity for Selective Oxidation of Alcohols under Mild Conditions
٣٤	۴۰۵	فاطمه پاکپور رودسری	Synthesis of polyhydroquinoline derivatives in the presence of [PVP-SO_3H] HSO_4 under solvent-free conditions
٣٥	۴۲۶	داود الهامی فر	Magnetic mesoporous silica supported propyl amine: An efficient catalyst for Knoevenagel reaction
٣٦	۵۰۳	روح اله پرنیان	A novel and practical method for the selective synthesis of sulfonyl chlorides and thiosulfonates from thiols using Triazo-Cl-H2O2 as well as direct conversion of sulfonyl chlorides to sulfonamides
٣٧	۵۲۹	ملیحه السادات صفایی	Tannic acid: An efficient catalyst for one-pot synthesis of xanthene derivatives under solvent-free conditions

۳۸	۵۶۶	میثم یاری	Synthesis of pyridine derivatives using a novel nanostructured molten salt catalyst via anomeric based oxidation
۳۹	۵۶۷	میثم یاری	A novel nonosized molten salt catalyst for the preparation of dihydropyrano[2,3-c]pyrazole derivatives
٤٠	۵۷۳	سعیده پاک وجود	Synthesis and characterization of Pd(II) tetradentate Schiff base complex as an efficient catalyst for the oxidative coupling of thiols to disulfides using tert-BuOOH
٤١	۵۸۰	سمیه بهروز	One-pot synthesis of N-alkyl 9H-carbazole derivatives from alcohols using 1-tosylimidazole (TsIm)
٤٢	۵۸۱	سمیه بهروز	Docking study of some novel azole-oxime ether hybrids as potential antifungal agents
٤٣	۶۰۸	نسرین صفاجو	Fe_3O_4@nano-cellulose/TiCl as an efficient and magnetically nano-catalyst for the synthesis of indenopyrido[2,3-d]pyrimidine derivatives
٤٤	۶۰۶	نسرین صفاجو	Synthesis of 2,3-dihydroquinazolin-4(1H)-ones catalyzed by Fe_3O_4@nano-cellulose/$CuCl_2$ as a bio-based magnetic catalyst
٤٥	۶۳۸	آیدا منصوری	Green synthesis and characterization of Betti bases derivatives by NS-PCS and FHS as the catalyst via Mannich reaction
٤٦	۶۴۶	نرجس امام دادی	The effect of magnetized solvent on rate of oxidation reaction of phenols and aromatic amines compounds by horseradish peroxidase
٤٧	۶۵۹	فاطمه بقائی	Synthesis of 2-(1-(4-((2-hydroxyarylidene)amino)phenyl)ethylidene) anils
٤٨	۶۶۴	محدثه یوسف زاده	Cholinesulfuric acid drivatives as an efficient catalyst for reaction of aryl aldehydes, cyclic 1,3-diketones and malononitrile
٤٩	۶۶۵	محدثه یوسف زاده	ɣFe_2O_3@activated carbon: an efficient nano-catalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones under solvent free conditions
۵۰	۷۰۳	کاوه همت	Magnetically Recyclable $CoFe_2O_4$@SiO_2/Co (III) Salen complex as a Heterogeneous Nanocatalyst for the synthesis of di-indolyloxindole
۵۱	۷۰۸	کاوه همت	Three-component reaction of malononitrile, aldehydes and β-naphthol in the presence of Co-salen complex.

٥٢	۷۳۵	عیسی موسی زاده مقدم پور	Preparation of an agar-trapped ionic liquid using as catalyst in the synthesis of xanthene derivatives
٥٣	۷۳۶	صادق رحمتی	Catalytic Trimethylsilylation of alcohols and phenols by tribromoisocyanuric acid (TBCA) under mild and solvent free conditions
٥٤	۷۶۱	صادق رحمتی	Fabrication of Pd@gelatin/agarose nanoparticles: a new heterogeneous catalyst for heck reaction
٥٥	۷۴۱	فاطمه زراعت پیشه	Ultrasound promoted synthesis of spirocyclohexanones catalyzed by proline
٥٦	۸۲۱	فاطمه زراعت پیشه	Application of ultrasound waves for extraction of total phenols and flavonoids from Echinacea Purpurea (L.)
٥٧	۸۶۸	حمزه کیانی	One-pot, three-component synthesis of isoxazol-5(4H)ones using $NH_4H_2PO_4$ in aqueous medium
٥٨	۸۱۹	مرضیه منصوری	A highly efficient method for the synthesis of polyhydroquinoline by carbon-based solid acid catalyst
٥٩	۸۲۰	مهدی کلهر	A Facile Synthesis of quinoxalines and dicyano pyrazines using $Ca(IO_3)_2$ as efficient and recycling catalyst
٦٠	۸۳۸	بهشته حمیدی	A multicomponent synthesis of 2-amino-3-cyanopyridine derivatives by carbon-based solid acid catalyst
٦١	۹۴۰	فاطمه کیانی	Inorganic–organic hybrid nano magnetic as a novel, efficient and reuseable nanocomposite for the synthesis of biphenyl compounds
٦٢	۸۸۲	سعید بابایی	Phenanthroline-SO_3H as a novel nano-molten salt catalyst: Application in multi component synthesis
٦٣	۸۸۴	سعید بابایی	Phenanthroline based ionic liquids as a catalyst in the synthesis of 2‑ amino-8-oxo-4,8-dihydropyrano[3,2-*b*]pyran-3-carbonitrile in water
٦٤	۸۸۸	حسن سپهر منصوری	Application of novel uinoxaline–based nono molten salts in the synthesis of 3-amino-5-pyrazolone and pyrano [3, 2- *c*] pyrazoles
٦٥	۸۸۹	مرتضی ترابی	Application of novel phosphonium based ionic liquid at the synthesis amidoalkyl naphthols under mild and solvent free conditions
٦٦	۸۹۰	سیما کلهر	A novel magnetic nanoparticle with morpholine tags as a multi-rule catalyst for synthesis of hexahydroquinolines

٦٧	۸۹۷	عذرا زارعی	Catalytic application of a novel oxyammonium based nano ionic liquid at the preparation of pyrano[4,3-b]pyrans and tetrahydrobenzo[b]pyrans
٦٨	۸۹۹	فاطمه کریمی	A novel ionically tagged magnetic nanoparticles as a reusable catalyst for synthesis of pyridines via anomeric based oxidation mechanism
٦٩	۹۱۸	سعیده کمالی فر	Green synthesis of 1,8-dioxo-octahydroxanthene derivatives catalyzed by sulfacetamide
٧٠	۹۲۳	المیرا حمیدی حاجی آبادی	Synthesis,characterization and application of LaFeO$_3$ nano particle in the synthesis of heterocyclic compounds
٧١	۹۵۹	ثریا رحمتی نژاد	Nano magnetite supported iron–phthalocyanine as a promising catalyst for the synthesis of β-amido ketones
٧٢	۹۶۶	حکیمه سادات میرزایی حصاری	Palladium nanoparticles supported on natural polymer (silk fibroin): the efficient and recyclable catalyst for Heck reaction
٧٣	۹۹۱	عاطفه لیموزاده	Functionalized nickel ferrite nanoparticles with phthalocianine-nickel complex as nano catalyst for the synthesis of 1,2,4,5-tetra aryl imidazoles
٧٤	۱۰۰۴	مریم فرحناک ضرابی	Synthesis of hydroxyl naphthalene-1,4-dione derivatives using Cu (II) immobilized on hyperbranched polyglycerol functionalized graphene oxide catalyst
٧٥	۱۰۲۲	سمیرا سهراب نژاد	A New Method for the Preparation of thiosulfonates from H_2O_2–Me_3ClSi
٧٦	۱۰۴۱	مریم خلیلی	N1,N1,N2,N2-Tetramethyl-N1,N2-bis(sulfo)ethane-1,2-diaminium chloride as a highly effective catalyst for the synthesis of 3,4-dihydropyrimidin-2-(1H)-ones (-thiones)
٧٧	۱۰۴۴	مریم خلیلی	Sulfonic acid-functionalized phthalimide (SFP) as a highly Efficient catalyst for the synthesis of 4H-pyrano[2,3-c]pyrazole
٧٨	۱۰۵۸	کبری ولدی	Agar :a natural and environmentally friendly substrate composed with copper oxide nanoparticles for efficient synthesis of 1,2,3 triazoles
٧٩	۱۰۶۳	فاطمه رضایی	Simultaneous Evaluation of Factors Affecting the Size of Gold Nanoparticles by Response Surface methodology
٨٠	۱۰۶۱	فاطمه رضایی	Valuation of Syringe Pump’s Performance for Reproducible Synthesis of Gold Nanoparticles using Sodium Borohydride as-Reducer

٨١	۱۰۶۵	عباس آبدار	preconcentration of Reactive 194 Dye by magnetic carbon nanotube followed by its determination with smart Mobile Phone
٨٢	۱۱۷	سعید اسدپور	Preconcentration and trace determination of thallium(I) in water by Inductively coupled plasma mass spectrometry using TiO2 nanopartic
٨٣	۱۵۰	مژده مردانی	Magnetic Fe_3O_4/SiO_2 Nanoparticles for Ciprofloxacin Detection in Biological Samp
٨٤	۳۹۰	رضا محمدی	Multivariate optimization approach for Cu(II) ions selective extraction from a mixture of six (metal cations via benzyl bis(thiosemicarbazone
٨٥	۸۵۱	رضا محمدی تودشکی	Spectrophotometric determination of furazolidone in real samples after its microextraction using hollow fiber reinforced with MIP@MWCNT
٨٦	۴۲۳	فرزانه مراحل	Synthesis of graphitic carbon nitride nanosheet and its application for determination of 2-Mercapto benzo thiazole by resonance reighley scattering technique
٨٧	۴۲۵	فرزانه مراحل	Colorimetric determination of Formaldehyde based on localized surface plasmon resonance of gold nanoparticles
٨٨	۵۵۲	امین همتی یادکوری	Determination of the acid dissociation constant of Nile blue and metanil yellow by the solution scanometric method and comparison with spectrophotometric results
٨٩	۵۵۹	فهیمه توکلی	Electrochemical investigation of acetaminophen/amlodipine interactions
٩٠	۶۷۴	الهه جباری	Fluorescent determination of alprazolam via molecularly imprinted polymer embedded CdTe quantum dots sensor
٩١	۶۸۱	الهه جباری	Epitope imprinted polymer embedded CdTe quantum dots as a highly selective fluorescent receptor for recognition of cytochrome c in biological samples
٩٢	۷۸۵	شکوفه ملک زاده روستا	Host-guest complex of curcumin with beta-cyclodextrin and its antioxidant activity
٩٣	۷۸۹	شکوفه ملک زاده روستا	The application and formation of inclusion complex of γ-cyclodextrin with turmeric
٩٤	۸۱۸	ایسر نعمت سعید الهموندی	A novel microfluidic paper-based device with colorimetric assay for determination of catechol

			using poly(N-vinylpyrrolidone)-capped silver nanoparticles
٩٥	۸۶۵	محمد بهرامی	Spectrophotometric determination of brilliant green in aqueous samples after supramolecular solvent extraction
٩٦	۸۷۰	ساناز حامد شتربانی	Spectrophotometric Study of the Interaction Between Pyridoxine with Some Transition Metal Ions in Non-aqeuos Media
٩٧	۹۱۴	ریحانه نامداری	Designing paper biosensors to the colorimetric measurement of bisphenol A by using gold nanoparticles modified with aptamer
٩٨	۹۳۰	محبوبه وافی	Fabrication of an optical pH sol-gel sensor based on Thionine dye
٩٩	۹۳۶	زهرا آموزگار	Zn^{2+}-mediated fluorescent ZnS quantum dots as indirect sensor for selective and sensitive detection of glutathione
١٠٠	۱۰۲۸	حمیده یزدانی	A simple visual and highly selective colorimetric analysis of Dopamine based on decorated gold nanoparticles using smart camera phone
١٠١	۱۰۲۹	فاطمه ارجمندی	Dressed-up gold nanoparticles as the colorimetric nano-sensor for simple assay of acetaminophen in biological samples
١٠٢	۱۰۴۰	اکرم حاجی نیا	Application of smart camera phone for End point detection of precipitation titration technique
١٠٣	۸۷	سیده فاطمه نامی عنا	Bio-Metal Organic Framework Nanofibers Incorporated to Polyaniline as a High-Performance Room Temperature Carbon Monoxide Gas Sensor
١٠٤	۱۶۷	مریم شمسایی	Highly efficient and fast co-removal of heavy metal ions and oxyanions with zeolite@layered double hydroxides core-shell heterostructure
١٠٥	۳۷۴	رقیه ثقفی	Synthesis and Effect of (Dy, Ni) Co-doped on the Multiferrioc and Photocatalytic properties of BiFeo$_3$ on the degradation of Organic dyes
١٠٦	۴۳۶	مهسا نازراز	Solid sorbent based on natural polymer nanosheets for removal of antibiotics from wastewater
١٠٧	۵۱۵	الناز مرزی خسروشاهی	Walnut Bloom Powder as a novel green sorbent for cationic dyes removal: Equilibrium, Kinetic, and Thermodynamic Studies
١٠٨	۵۵۴	عصمت کوهساریان	Water Vapor Removal from Gas Streams Using Nano-Structured Zeolites

۱۰۹	۵۵۸	عصمت کوهساریان	Water Harvesting from Air Using Nano-composites
۱۱۰	۶۰۲	طیبه انصاری	Titanium Dioxide Nanoparticles: Synthesis and study of its modifying properties on acrylic paints
۱۱۱	۶۰۹	فرزاد نژادی	3D QSAR Study of Simultaneous AT1 and ETA Antagonists as Anti- hypertensive Drugs
۱۱۲	۷۳۸	راضیه موسوی	Preparation of Ag Nano Clusters as a Glucose Fluorescent Sensor
۱۱۳	۷۴۸	عاطفه درویش شاهمرادی	In-situ synthesis and characterization of reduced graphene Oxide and sulfonated graphene-polypyrrole nano-composites for use in gas sensor
۱۱٤	۸۱۳	عاطفه ابراهیمی	Process Variables in Phytosynthesis of Ag@AgCl Nanoparticles by Syzygium cumini Fruit Extract
۱۱۵	۸۵۳	ملیحه صمدی کاظمی	Effect of solvent, time and method on the amounts phenol, flavonoid and the anitioxidant activity of Ixiolirion tataricum (Pall.) Herb extract
۱۱٦	۸۵۹	ملیحه صمدی کاظمی	Optimization of extraction process of Arenaria hispanica L. using response surface methodology
۱۱۷	۸۶۶	مرضیه بانشی	Preparation of doxorubicin, gold and magnetic NPs loaded on Albumin NPs as well as in vitro treatment of MCF-7 breast cancer cells
۱۱۸	۸۸۷	حمیدرضا رجبی	A fast and green photodegradation approach based on functionalized quantum dots for removal of anthracene from aqueous media
۱۱۹	۹۱۷	حمیدرضا رجبی	Synthesis, characterization and antimicrobial activity of zinc oxide nanoparticles prepared by a green approach based on extract of Seidlitzia rosmarinus after microwave and maceration extraction method
۱۲۰	۹۱۳	علی خدایاری	Thermocatalytic activity of $CuCo_2O_4$ nanoparticles prepared by sol-gel method
۱۲۱	۹۱۶	مریم محمد آبادی	Design of headspace paper sensor for determination of Arsenic (III) in drinking waters using smart mobile phone based on chemical hydride generation
۱۲۲	۹۸۵	سعیده رسائی نژاد	The green synthesis of gold nanoparticles using extract of Dracocephalum kotschyi Boiss
۱۲۳	۱۰۰۸	مارال عجمیان	Synthesis of high yield gold nanosheets with electrocatalytic activity toward NADH and

			investigation of their self-assembly at toluene/water interface
١٢٤	۱۰۶۴	میلاد کاشمری	Comparison of different pretreatment on the recovery of gold and silver from sarcheshmeh copper anode slime
١٢٥	۱۱۰۴	عبدالرئوف صمدی	Sequential one-pot synthesis of high-quality magnetite@CdS type-II core/shell nanocrystals with improved photocatalytic activity
١٢٦	۷۲۴	سیده مهسا ترابی	Experimental Study of the Synthesized Mordenite Zeolite for Simultaneous Reduction of Lead, Zinc and Cadmium ions
١٢٧	۷۲۹	سیده مهسا ترابی	Synthetic and Thermodynamic Study of Ammonium Absorption on Clinoptinolite Zeolite
١٢٨	۹۵۸	فاطمه کریمی احمدآباد	A new phosphoric triamide structure: $(CF_3C(O)NH)P(O)(NHC_6H_4\text{-}4\text{-}CH_3)_2$
١٢٩	۱۰۷۰	سیدجواد معافی	Synthesis and Characterization of Fe(II), Co(II), Cu(II) and Zn(II) Complexes Containing a New Unsymmetrical Tetradentate Schiff-base
١٣٠	۱۰۸۲	سیدجواد معافی	Synthesis and Characterization of an Unsymmetrical Tetradentate Schiff Base and Its Co(II), Ni(II), Cu(II) and Zn(II) Complexes
١٣١	۱۰۷۷	غزل صالحی	Graphitic carbon nitride@nickel-aluminium layered double hydroxide nanocomposites
١٣٢	۱۱۸۳	مهرداد پورایوبی	Two single-enantiomer (R and S) Amidophosphoesters
١٣٣	۱۱۸۴	سولماز برزگر نوروزی	Preparation of sodium and potassium doped $LaCoO_3$ perovskite as adsorbent for wastewater treatment
١٣٤	۱۱۸۷	فرانک منطقی	Synthesis of Ni-Al LDH by co-precipitation method and its application in removal of dyes
١٣٥	۱۱۸۸	فرانک منطقی	Synthesis and identification of a Zr-MOF with carboxylate linker
١٣٦	۱۰۵۷	طناز شریفی	Removal of malathion and diazinon from wastewater by modified iron kaolin and UV / H_2O_2
١٣٧	۱۰۶۰	معصومه دیبازر	Removal of malathion and diazinon from wastewaters by iron-modified bentonite and uv H_2O_2
١٣٨	۱۰۵	سمیرا چمیانی	Pt–Au Complexes Built on a Diphosphine Scaffold: Cytotoxic Properties
١٣٩	۱۰۶	سمیرا چمیانی	Synthesis, Biological Evaluations and DNA Interaction Studies on Trans Platinum(II) Thiolate Complexes

١٤٠	۲۹۶	نسرین جمشیدیان	New Hydrazide Palladium Complexes, Synthesis, Characterization and biological studies
١٤١	۴۵۷	بهنام رضازاده	Co(II) Schiff base complexes encapsulated in the zeolite-Y as efficient and reusable nanocatalysts for epoxidation of styrene in mild conditions
١٤٢	۱۱۱۰	بهنام رضازاده	Mo(VI) Schiff base complex immobilized on graphene oxide nano-sheets as an efficient, selective and reusable catalyst for epoxidation of olefins
١٤٣	۷۰۵	میلاد مقدسی	Mononuclear and dinuclear complexes of stannyldimethylplatinum(IV) via oxidative addition reactions
١٤٤	۶۳۷	محمد پناهی مهر	Synthesis and spectroscopic characterization of Hg(II) complexes of new unsymetrycal Phosphorus ylide
١٤٥	۲۹	مریم منافی خیابانی	Synthesis, X-ray structural properties of hexacoordinate nickel(II) complex incorporating 4-methylpyrazole and azide ligands
١٤٦	۵۳	لیلا شیرمحمدزاده	Formation and Photocatalytic Activity of $BaTiO_3$ Nanoceramics via Solgel Process
١٤٧	۵۴	لیلا شیرمحمدزاده	Synthesis, Properties, and Photocatalytic Activity of Perovskite-Phase $Ba_{0.75}Sr_{0.25}TiO_3$ Nanoceramics
١٤٨	۳۱۹	شیوا باتمان قلیچ	Synthesis, characterization, structure determination and theoretical studies of some new dimethylglyoxime cobalt(III) complexes
١٤٩	۳۲۹	فرانک حشمت نیا	Synthesis, characterization and structural studies of some new homoleptic and heteroleptic diminic and diphosphine copper(I) complexes
١٥٠	۷۶۰	حجیه بسطامی	TiO_2 conjugated with molecules of Rose red dye as a photocatalyst towards salicylic acid
١٥١	۱۶	اعظم سبحانی	Effects of surfactant, ratio of Cd:surfactant, amount of reductant and time reaction in the sonochemical synthesis of CdSe nanostructures
١٥٢	۱۷	اعظم سبحانی	PbS nanostructures: thermal decomposition synthesis of [bis(thiosemicarbazide)lead(II)] precursor
١٥٣	۷۲	داود موسوی	Selective and mild oxidation of sulfides to sulfoxides with H_2O_2 catalyzed by copper(II) asymmetrical tetradentate Schiff base complex
١٥٤	۸۵	مرضیه دریانورد	Highly Efficient Ru(II)-based Electrocatalyst for Reduction of Carbon Dioxide to Carbon Monoxide

١٥٥	۸۶	مرضیه دریانورد	Zinc(II) Complexes: Synthesis, Characterization, Crystal Structure, and Antifungal Activity
١٥٦	۱۱۱	مائده کوهی	Design, Synthesis and Characterization of Gold(I) Complexes Containing Allyldiphenylphosphine as Improved Cytotoxic Agents
١٥٧	۱۰۹	مائده کوهی	Activation of C-I Bond by Cycloplatinated(II) Complexes Comprising Tricyclohexylphosphine ligand: Kinetics and Mechanism Investigations New Hydrazide Palladium Complexes, Synthesis, Characterization and biological studies
١٥٨	۱۶۱	فاطمه بشگزی	Heterogeneous activation of Oxone® by magnetic nanoparticles anchoring Schiff base complexes for water treatment
١٥٩	۱۶۲	فاطمه بشگزی	Non-immobilized water-insoluble Metallosalens as efficient heterogeneous catalyst for degradation of dyes in water
١٦٠	۱۷۵	حمید گودرزی افشار	Tandem Knoevenagel-Michael-cyclocondensation reaction of malononitrile, various aldehydes and barbituric acid derivatives using isonicotinic acid
١٦١	۱۸۲	زهرا فرهمند ملک آبادی	Preparation of Palladium nanoparticles from [Pd(aemptrz)Cl_2] by sonochemical method
١٦٢	۱۹۵	فرشته موزردزاده	Synthesis and Characterization of Nanozirconia via Interaction of Zirconium (IV) with Oxamid under Solvothermal Conditions
١٦٣	۲۰۲	الهام غیاثی	Structural Features of B-site Substituted Nano-Lanthanum Manganite
١٦٤	۲۶۶	فاطمه رفیع زاده ماسوله	Synthesis of two Cd(II) based metal–organic frameworks : sonochemical synthesis aspect and applications
١٦٥	۳۷۱	شیما شاهی	Synthesis and characterization of wurtzite ZnS nanoparticles via solvothermal method
١٦٦	۳۹۲	کوروش ادیب	Application of Chromium Tungsten/Reduced Graphene Oxide as an advanced electrode material for supercapacitors
١٦٧	۶۸۷	کوروش ادیب	Facile Chemical Synthesis of silver Tungstates and silver Tungsten/Reduced Graphene Oxide as High Performance Supercapacitor
١٦٨	۴۴۶	الهام عسگری	Effect of zinc oxide nanoparticles on azo dye
١٦٩	۴۸۹	رضا روشنی	A facile and green sonochemical route for the synthesis of $CuWO_4$ nanostructure

۱۷۰	۴۹۰	رضا روشنی	A facile and green route for the preparation of $ZnWO_4$ nanoparticles
۱۷۱	۵۳۰	آزاده مرادزاده	Synthesis of $SrZrO_3$ nanocomposites and their Photocatalytic property under visible light
۱۷۲	۵۳۱	آزاده مرادزاده	Investigation on Synthesis , Characterization and Photo catalytic properties of nano Composite Perovskites $SrTiO_3$ /Zn_2TiO_4 for degradation of Congo Red
۱۷۳	۶۱۵	علی حاجی زاده	New efficient visible light photocatalyst for degradation of phenol: Nano-particle of HAP/Bi_2O_3-Ag composite
۱۷٤	۶۵۱	سید حامد ادیانی	Green synthesis of Ag/RGO nanocomposite using Punica Granatum peel extract and its catalytic activity for the reduction of 4-nitrophenol
۱۷٥	۶۵۳	سید حامد ادیانی	Green synthesis of Ag/Fe_3O_4 nanocomposite using Citrus sinensis peel extract and its catalytic activity for the reduction of organic dyes
۱۷٦	۶۷۶	معصومه دولابی	Sol-gel synthesis of $LaFeO_3$/ZnO composite as promising photocatalyst
۱۷۷	۶۸۹	ساحل ظهیری	Synthesis of Dopant/hydroxyapatite/graphene oxide nano composites for dye degradation
۱۷۸	۷۶۶	بهروز الهی	Plant-based synthesis of ceria nanoparticles and its catalytic activity
۱۷۹	۷۹۶	فاطمه مرادی گرجی	Synthesis and characterization of Cu(II) Schiff base complex immobilized on magnetic Fe_3O_4/ .graphene oxide sheets as heterogeneous catalyst
۱۸۰	۸۴۳	نیلوفر پورناصر	Aerobic oxidation of alkenes in the presence of metalloporphyrines without any additives
۱۸۱	۸۹۲	لیلا کافی احمدی	Effect of synthesis temperature on the crystal structure of nano-sized CdS spheres synthesized by Ultrasonic assisted Hydrothermal method
۱۸۲	۹۵۷	ویدا عبدی	Efficient visible light photocatalytic activity based on magnetic
۱۸۳	۹۷۴	معصومه بلالی	Immobilization of dioxomolybdenum(VI) complex on the Schiff base coated magnetic nanoparticles: A highly active, selective and reusable catalyst in oxidation of sulfides to sulfoxides
۱۸٤	۹۸۶	معصومه بلالی	Synthesis of magnetically separable copper nanocatalyst and their application as an efficient catalyst for $C(sp^2)$–C(sp) and $C(sp^2)$–$C(sp^2)$ cross-coupling reactions

١٨۵	۱۰۵۵	آرین زمانی فرد	Aerobic oxidation of organic compounds in the presence of the free base porphyrins and porphyrins supported onto nanostructure solid as photosensitizer
١٨٦	۱۰۸۸	مرضیه ضیا سیستانی	Synthesis and Characterization of a New man-(sized Magnetic Core/shell of (Fe_3O_4@CuO)
١٨٧	۱۱۰	نجمه داستانی	Density functional calculations on the adsorption of Ampyra drug on graphene nanosheet
١٨٨	۱۱۴	نجمه داستانی	Molecular structure and electronic properties of adsorbed Ampyra drug on the functionalized graphene nanosheet: A DFT study
١٨٩	۱۱۹	عبدالرضا فرامرزی پلنگر	Theoretical investigation and comparison of Dielectric coefficient tautomerization process in gas and solution phase of 5-(x-amino)-1,3,4-oxadiazol -2(3H)-one(x=Br)
١٩٠	۱۳۳	سیده مهرانگیز اطیابی	The pristine and C, Si or Ge substituted (5, 5) BeO nanotube: A Computational DFT study of NMR parameters
١٩١	۱۸۷	زهره حسن زاده	Theoretical study on adsorption behaviour of Thioguanine anticancer drug on the surface of fullerene C60 nanocage
١٩٢	۱۸۹	زهره حسن زاده	Theoretical Study on Adsorption Of Methan Molecule on nanostructured functionalized Graphene with hydroxyl and epoxide
١٩٣	۲۰۹	فرزانه فرزاد	H_2S Capturing Based on hexagonal boron nitride: A DFT study
١٩٤	۲۱۰	فرزانه فرزاد	Investigation of adsorption properties of CS_2 on hexagonal boron nitride
١٩٥	۲۴۸	فاطمه سادات بنی جمالی	On the study of CO/H_2 separation in HKUST-1 MOFs using ab initio calculations
١٩٦	۲۷۱	اعظم مرتضوی فر	Investigation of HOMO-LUMO and quantum molecular descriptors in reactivity of Carmustine drug and boron nitride nanotube by DFT
١٩٧	۲۸۵	اعظم مرتضوی فر	A computational study on the electronic properties of single walled boron nitride nanotube as carrier for Carmustine molecule by DFT
١٩٨	۲۷۲	ندا خورشیدوند	Electronic effects on normal and abnormal acyclic, cyclic-saturated and cyclic-unsaturated diaminocarbenes at DFT
١٩٩	۲۶۹	ندا خورشیدوند	Synthesis and characterization of DCC supported on magnetic nanoparticles: a highly active and recyclable catalyst for the synthesis of polyhydroquinolines

٢٠٠	۲۸۲	مهناز شهابی چشمه موسی	Adsorption of Cr and Pd transition metal atoms on the pristine Zinc oxide nanotube: a DFT approach
٢٠١	۲۸۴	مهناز شهابی چشمه موسی	Sensitivity mechanism of single-walled carbon nanotube as a drug delivery system toward the anticancer drug molecules
٢٠٢	۳۵۹	فائزه مهدوی پژوه	2D&3D-QSAR studies on -di keto Acids Derivatives of Pyridinones as anti-HIV drugs
٢٠٣	۴۴۴	الهام ابراهیمی مکرم	Theoretical study of solvent effect on NLO property in $(\eta^6\text{-}C_6H_6)Cr(CO)_3$ complex
٢٠٤	۴۸۵	سعید نجاتی	A computational study of all di-fluoroazulenes
٢٠٥	۴۸۸	سپیده سدنی	Theoretical study of the molecule carbon monoxide adsorption on the Ni_4Sc and Ni_4Mo nanoclusters
٢٠٦	۴۸۷	سپیده سدنی	Using metal based electrochemical biosensors with nano-porous surfaces to identify phenol and phenolic compounds
٢٠٧	۵۰۹	مهدی رضایی صامتی	Interaction of NO gas with P-doped BNNTs: A DFT study
٢٠٨	۵۱۰	مهدی رضایی صامتی	The effect of Al atom doped and SO_2 adsorption on the electrical and structural parameters boron nitride nanotube: A quantum approach
٢٠٩	۵۴۸	مژگان ایوبی	Computational study of polycyclic unsaturated silylenes and their allenic analogs
٢١٠	۵۵۳	رضا فتح اللهی قشلاق	NBO analysis on all mono-fluorovinylbenzenes: A theoretical study
٢١١	۵۵۵	رضا فتح اللهی قشلاق	A DFT and NBO study of di-fluorovinylbenzenes
٢١٢	۵۵۶	توحید جابری	DFT study on mono-chloroazulenes
٢١٣	۵۵۷	توحید جابری	Comparative study on all di-chloroazulenes; a study of density functional theory
٢١٤	۵۹۸	مرضیه هاشمی	Strain and Ring Size Effects on the 1,3-dipolar Cycloaddition reactions of the Medicine Efavirenz Derivatives; A Theoretical Studies
٢١٥	۱۰۴۶	مرضیه هاشمی	Theoretical Studies of the H-Bonding Effect on the regiochemical outcome of the 1,3-DC reactions to the Medicine Ethisterone
٢١٦	۶۴۴	علی اکبر احمدی	Planar Stacking Interactions in the Binding of Type II Statins to HMG-CoA Reductase
٢١٧	۶۷۹	الناز رنج بخش	Theoretical prediction of nonmetal-doping effects on the photocatalytic performance of graphite-like carbon nitrides

٢١٨	۷۰۱	سید عبداله سید کتولی	Tautomerism, molecular structure, intramolecular hydrogen bond, and tautomery equilibrium of α-methyl and ethyl substituted 4-amino-3-penten-2-one; A theoretical study
٢١٩	۷۰۴	سید عبداله سید کتولی	Intramolecular hydrogen bond strength of 3-methyl-4-amino-3-penten-2-one, an experimental approach
٢٢٠	۷۰۶	محمود بذرافشان	Conformational stability, molecular structure, and intramolecular hydrogen bond of 2,2-dimethyl-5-amino-4-hexen-3-one
٢٢١	۷۸۲	طاهره خشتی	Evaluation of Geometries, Stabilities and optical Properties of Bn and Be©Bn (n=6-12) Clusters: Computational Assessment
٢٢٢	۱۱۱۷	طاهره خشتی	Electron Transport Properties of Defected Carbon Atomic Chains between Nano Capsule Electrodes
٢٢٣	۸۰۴	حسین هراتی	A Theoretical Study on the Kinetics and Thermodynamic Parameters of Chelotropic Dichlorophenylphosphine Reactions: Dienes with
٢٢٤	۸۲۲	سحر دزفولی	Ab initio study of fumagillin derivatives as potent anticancer compounds
٢٢٥	۸۵۴	فاطمه صفدری	Graphene Oxide Nanosheet as a Drug Delivery Vehicle For 5-Fluorouracil Anticancer Drug
٢٢٦	۸۶۲	سمیرا خندان	Study of Structural and Electronic Properties of Doped group ɪɪɪ (B, Al, Ga and In) on (6, 3) Chiral CNTs
٢٢٧	۸۹۳	آرزو قراچورلو	Chloropicrin sensor based on the doped-graphene: DFT studies
٢٢٨	۱۰۱۶	مهیا کیافر	Theoretical studies of pyramidality of nitrogen in (2-Cyclohexyl-vinyl)-methyl-amine, (2-Cyclopentyl-vinyl)-methyl-amine, (2-Cyclobutyl-vinyl)-methyl-amine and (2-Cyclopropyl-vinyl)-methyl-amine
٢٢٩	۱۰۷۱	مهیا کیافر	Theoretical studies of pyramidality of nitrogen in (2-Cyclohexyl-vinyl)-methyl-amine, (2-Cyclopentyl-vinyl)-methyl-amine, (2-Cyclobutyl-vinyl)-methyl-amine and (2-Cyclopropyl-vinyl)-methyl-amine

راهنمای تفکیک گرایش‌های اصلی بر اساس رنگ				
شیمی آلی	شیمی تجزیه	شیمی فیزیک	شیمی معدنی	سایر

زمان ارائه پوستر بخش (D) شامل (شیمی آلی-شیمی فیزیک-سایر)

پنج شنبه ۹۷/۴/۲۸ ساعت ۱۰:۲۰ الی ۱۱:۰۰

شماره	کد مقاله	ارائه دهنده	عنوان مقاله
١	۲۲	سحر شب زنده دار	Synthesis of superparamagnetic nanocomposite of poly(m-amino benzenesulfonic acid) and Fe_3O_4 and its high efficiency in solar cell
٢	۲۳	سحر شب زنده دار	Synthesis of p-Aminoazobenzene nanosheet via green chemistry and Study on its photovoltaic properties by preparation its solar cell
٣	۲۸	رضا محمدی پور	Synthesis of 3,4-dihydropyrimidin-2(1H)-ones via Biginelli reaction using nano($BF_3/Al_2O_3/SiO_2$) as a green catalyst under solvent-free condition
٤	۳۱	مهدی حسین زاده	Removal of Pb(II) From Aqueous Solutions Using New Carboxylic Acid- containing Absorbent Polymer
٥	۳۲	مهدی حسین زاده	Chemo-phototherapy of cancer cells using gold nanocage -cored pH-sensitive thiol-ended triblock copolymer
٦	۱۰۴	فاطمه جمالی	Esterification of levulinic acid to n-butyl levulinate using mesoporous zirconium phosphate
٧	۱۲۴	سمیرا عشیری	Synthesis of novel mixed- ligand palladium (II) based on graphene and oxime: its application as a recyclable catalyst
٨	۱۳۲	سمیرا عشیری	Preparation a novel catalytic hydrogel based on biopolymers and graphene oxide containing palladium nanoparticles

٩	۱۵۱	زهرا خلیلیان گورتانی	Catalytic oxidative desulfurization of model oil by TiO_2 nanotubes prepared by electrochemical anodizing
١٠	۱۸۱	محدثه شهابی نژاد	Two-dimensional functionalized graphene oxide anchored TPA: $H_3PW_{12}O_{40}$ and their application for reduction of organic dyes
١١	۲۳۷	محدثه شهابی نژاد	$RuCl_2$(p-cymene)$]_2$ complex immobilized on reduced graphene oxide as active catalyst for the synthesis of carboxylic acids from alcohol dehydrogenation
١٢	۲۲۶	نعیمه صالحی	Synthesis of highly substituted dihydro-2-oxopyrroles using Fe_3O_4@nano-cellulose-OPO_3H as a novel bio-based magnetic nanocatalyst
١٣	۲۲۸	نعیمه صالحی	Green Synthesis of Pyrano[2,3-c]pyrazoles and Spiro[indoline-3,4′-pyrano[2,3-c]pyrazoles] Using Nano-silica Supported 1,4-Diazabicyclo[2.2.2]octane as a Novel Catalyst
١٤	۲۲۷	سیده آزیتا فاضلی عطار	Application of Fe_3O_4@SiO_2/$TiCl_3$ for the synthesis of quinoxaline derivatives
١٥	۲۲۴	سیده آزیتا فاضلی عطار	Nano-BF_3/cellulose as a biodegradable catalyst for synthesis of highly functionalized tetrahydropyridines
١٦	۲۵۰	مهناز ایمانی	Synthesis of perimidines in the presence of Fe_3O_4@nano-cellulose/BF_3 as a super paramagnetic nanocatalyst
١٧	۲۵۴	رویا سلطانی	Preparation and application of kaolin-based magnetic nanocatalyst for the synthesis of 4H-pyrimido[2-1-b] benzothiazole derivatives
١٨	۲۵۷	الهه بابایی	One pot synthesis of five substituted tetrahydropyridines using nano-Al_2O_3/BF_3/Fe_3O_4 as a highly efficient nano-catalyst
١٩	۲۸۷	مهنوش رشیدی شریف آباد	Synthesis of novel Pd nanoparticle on Fe_3O_4@ZrO_2/5-amino-1,3,4-thiadiazole-2-thiol and its application for reduction Organic Dyes
٢٠	۱۱۲۰	مهنوش رشیدی شریف آباد	Synthesis of magnetic Pd nano composite and its application as recoverable catalyst for the C-C cross coupling Suzuki reaction
٢١	۲۹۴	مقدسه محمدیان	Synthesis of hydrogel beads based on tragacanth gum and graphene oxide through radical polymerization: study of Ca^{+2} and Mg^{+2} removal from drinking water
٢٢	۲۹۵	مهیار کریمی	Curing of DGEBA with MF resins in decorative impregnated Paper and investigation of laminates quality and kinetic parameters

٢٣	۳۰۰	آیدا ابراهیمی	Synthesis and characterization of conductive star copolymer of PANI/PAA with calix [4] resorcinarene core
٢٤	۳۰۷	فاطمه سیداقازاده	Synthesis and characterization of poly¬¬¬ (aniline-co-carbazole) conductive copolymer and its carbon based nanocomposite
٢٥	۳۱۴	دینا ملاح	Preparation and design of new protic ionic liquids supported on nano-magnetite and their applications in three-component synthesis of 1-amidoalkyl 2- naphthols
٢٦	۳۸۸	ندا سیدی	Synthesized of palladium nanoparticles supported on functionalized 2D-geraphene oxide and their application in reduction of organic dyes
٢٧	۳۸۹	ناهید سهیلی ارشدی	The Hg$^{2+/}$Al$_2$O$_3$ Nanoparticles for Adsorption of Thymine Nucleobase
٢٨	۴۲۱	مهسا خوشنویس	Diastereoselective three-component Mannich reaction catalyzed by prolinated MWCNTs
٢٩	۴۴۸	نینا حسینی محتشم	Application of Horsetail and Horsetail Ash as a Novel Natural Lewis Acid Catalyst for the One-Pot Synthesis of 2-Amino-4H-Chromene Derivatives
٣٠	۴۷۸	فرحناز حمدی هولاسو	Comparison of DSC curves Copolymerization of vinyl acetate- butyl acrylate with different initiators
٣١	۵۶۵	شیوا ولایتی هروانی	A phenobarbital molecularly imprinted polymer electrochemical sensor based upon a polyaniline/graphene oxide nanocomposite
٣٢	۶۱۶	حسین مهدی پور	Catalytic Epoxidation of Polybutadiene Rubber Using H_2O_2/CH_3COOH and Na_2WO_4
٣٣	۶۱۷	حسین مهدی پور	Synthesis of Aldehyde-Terminated Epoxidized Liquid Polybutadiene Rubber
٣٤	۶۱۹	مریم عباس زاده	A novel ligand-metal complex immobilized on magnetic graphene oxide as a magnetic nanocatalyst for the coupling reactions
٣٥	۶۳۱	محمد مهدی خاکزاد سیوکی	Cu nanoparticles immobilized on modified magnetic zeolite as a new efficient catalyst for the synthesis of 1,2,3-triazoles via click chemistry reaction
٣٦	۶۳۲	هما ترغان	Graphene Oxide-Supported Palladium Complex: Synthesis, Characterization and Application in Cross-Coupling Reactions

٣٧	۶۸۰	صدف فرجی سلیمانی	Fabrication of polyurethane rigid foam composites incorporated with phase change materials
٣٨	۷۰۲	فاطمه ترکیان	Extraction and Identification of the Alkaloids in Papaveraceae Endemic Plant Resources in Iran
٣٩	۷۵۳	شیوا عطایی کچویی	The comparative study of support effect in silver-graphene oxide nano magnetic catalyst
٤٠	۷۷۳	الهه یزدانی	Copper supported on citric acid modified magnetite nanoparticles as a novel superparamagnetic nanocatalyst for nitro reduction
٤١	۸۰۵	مسعود صادقی تکلو	Synthesis of 2-amino-4H-chromenes catalyzed by N,N-diethyl-N-sulfoethanaminium hydrogen sulfate
٤٢	۸۱۱	مسعود صادقی تکلو	N,N-diethyl-N-sulfoethanaminium hydrogen sulfate as an effective catalyst for the preparation of 14-aryl-14H-dibenzo[a,j]xanthenes
٤٣	۸۹۵	سمیه راثی	Immobilized Lipase on Graphene Oxide as Nanobiocatalyst for the Synthesis of Heterocyclic Compounds
٤٤	۹۲۹	کامران پورقاسم لامعی	Synthesis of nanoparticles within the modified pores of SBA-15: An efficient catalyst for reduction reaction
٤٥	۹۳۵	مرتضی ایمان پور	CuNPs–GO nano sheets for novel synthesis of N-(phenyl(4-phenyl-1H-1,2,3-triazol-yl)methyl)benzamine
٤٦	۶۸۳	مرتضی ایمان پور	AgNPs–GO nano sheets for Aerobic Aqueous Oxidations of Alcohols
٤٧	۹۴۸	بهارک پولادیان	Investigations of Flame-Retarded Poly(Imide–Urethane)s Containing Phosphorus Units
٤٨	۹۷۱	محمود نصرالله زاده	Biosynthesis of Ag/MgO nanocomposite using Acalypha hispida extract and its application in the reduction of nitroarenes and organic dyes
٤٩	۹۷۲	نگین مرتضایی	Effects of Palmitic Acid@SiO_2 on the Synthesis of Microcellular Polyurethane foam
٥٠	۹۸۴	مهناز قدیمی ماهانی پور	Green synthesis of graft copolymer of psyllium musilage with acrylamide/acrylic acid and investigation of properties of its hydrogel
٥١	۹۹۵	آیدا بهادری	synthesis of graft copolymer of itaconic acid/acrylamide on starch and investigation of water absorption behavior of its hydrogel
٥٢	۱۰۰۲	محدثه بوجاری نیا	Polyurethane nanocomposite for water filtration

٥٣	۱۰۱۰	وحیده رییس دسته حکم آباد	Elaeagnus angustifolia extract-Hydroxyapatite incorporated PCL based nanofibers for bone tissue engineering
٥٤	۱۰۱۲	مهدیه اسکندریان	Synthesis and characterization of Walnut shell/diopside nanocomposite for removal of Congo red dye: Experimental design and optimization
٥٥	۱۰۱۹	حکیمه ابراهیمی اصل	s-Triazinium-based ionic liquid immobilized on silica-coated Fe_3O_4 magnetic nanoparticles: an efficient and magnetically separable heterogeneous catalyst for synthesis of dihydropyrano[3,2-b]pyran-3-c
٥٦	۱۰۵۲	راحله دهقانی	Functionalized graphene oxide decorated with Au nanoparticles as a designed catalyst for reduction of organic dyes
٥٧	۱۱۱۹	نصیبه آناهیدزاده	Metal-organic framework composite membrane for fuel cell applications at high temperature and low humidity
٥٨	۵۱۲	امیر فرخنده	Copper-catalyzed click synthesis of 1,2,3-triazole-linked benzimidazole
٥٩	۹۷۸	امیر فرخنده	An efficient green method for synthesis of 1,8 dioxooctahydroxanthenes in magnetized water as a new solvent
٦٠	۵۳۴	زهرا منیری	Graphene oxide: An efficient recyclable solid acid for the synthesis of 2-substituted benzimidazoles from aldehydes and diamines at ambient temperature
٦١	۹۵۵	شهرزاد محسنی میبدی	Synthesis of a new spiro derivative Catalyzed by p-Toluenesulfonic acid and using three component reaction
٦٢	۹۱۱	محمود زارعی	Synthesis of a novel biological-based glycoluril with phosphorous acid tags: Application for synthesis henna-based compounds
٦٣	۹۱۲	محمود زارعی	Novel crabby biological-based glycoluril with sulfonic acid tags: Application for synthesis of new mono and bis-spiropyrans
٦٤	۵۶۸	پریوش جهانشاهی	An efficient one-pot three-component synthesis of novel derivatives of pyrido[2,3-d]pyrimidines by using nanocatalyst [γ-Fe_2O_3@HAp-SO3H]
٦٥	۵۷۱	محمد نوید سلطانی راد	Benzyl methyl morpholinium hydroxide [BMMorph][OH] as an ionic liquid media for efficient synthesis of carboacyclic nucleoside via Michael addition of purine and pyrimidine nucleobases with α,β-unsa

٦٦	۵۷۲	محمد نوید سلطانی راد	Benzyl methyl morpholinium ascorbate [BMMorph][Ascorb] as an efficient catalyst and media for ‘Click’ synthesis of 1,2,3-triazolyl based carboacyclic nucleoside
٦٧	۵۹۴	آفاق بنی فریدنی	Synthesis of dihydropyrimidine-4-one derivatives from amines, phenyl cyanides and acetylenedicarboxylates
٦٨	۵۸۷	جواد گتابی	Design and synthesis of a gelatin base ion imprinted polymer for selective extraction of Lead ion
٦٩	۵۹۶	اعظم میدانی	One pot, two-step synthesis of pyrimidine derivatives via arylamins, benzonitriles, benzaldehydes and Meldrum’s acid
٧٠	۳۵	افشین صادقی ایوریق	Solvent-free esterification of alcohols with carboxylic anhydrides using hexachloroacetone as an efficient catalyst
٧١	۳۶	ریحانه کریمی چایجانی	Immobilized ionic liquid on γ-Fe_2O_3 as an efficient and reusable nano-catalyst for the synthesis of pyrano[2,3-d] pyrimidinone derivatives
٧٢	۱۰۵۹	کبری ولدی	Mica as an efficient catalyst for the synthesis of benzoimidazole derivatives
٧٣	۱۰۸۹	عارفه سلامت منش	Mild and eco-friendly chemoselective acylation of amines in aqueous medium using superparamagnetic nanoparticles as a highly efficient and recyclable catalyst
٧٤	۱۰۹۷	سمیه محمدی	Stereoselective synthesis of spirooxindoles through multi component reaction catalyzed by Methanetriamine under mild condition
٧٥	۱۱۱۴	ریحانه سلماسی	Syntheses, characterizations, crystal structures and Hirshfeld surface of two new oxidation agents of 1, 2-Ethandiylbis (triphenyl phosphonium) cation including perchlorate and chlorate anions
٧٦	۱۲۰۴	مهراسا ترحمی	Synthesis of Tetrahydrobenzo[b]pyran Derivatives using SO_3H–functionalized Nano-MGO-D-NH_2 in Aqueous Media
٧٧	۱۱۹۰	هدی ملاباقر	A mild and efficient method for Synthesis of novel fused thiopyrano[2,3-b] indole derivatives
٧٨	۱۲۴۷	سیاوش حسنوندی	Tosylation of Cellulose Nanowhisker in Aqueous Solution
٧٩	۵۹۹	مریم پوریامهر	Synthesis and characterization of new palladium(II) complexes derived from pyridinium ylide and investigation of its catalytic activity

۸۰	۶۰۱	مریم پوریامهر	Synthesis and characterization of new mercury(II) complexes derived from α-keto stabilized new pyridinium ylide
۸۱	۳۰	فاطمه براتی دربند	Electron-hole transfer in the dye-based solar cells: A computational study on indoloquinoxaline and triphenylamine derivatives
۸۲	۱۴۷	فاطمه براتی دربند	Spectroscopic properties of a metal-free indoloquinoxaline-based dye
۸۳	۶۱	مرضیه محمدی	The theoretical study on the coumarin-based Mn(II) complex
۸٤	۴۵۹	علیرضا ناصری مود	Production of electronic content for the teaching of electron quantum composition of elements
۸٥	۴۶۰	علیرضا ناصری مود	Pyramid Modeling Teaching the Quantum Arrangement of Boron Electron Reconstruction in the Chemistry Curriculum of the Tenth Secondary School
۸٦	۴۶۱	طاهره روحانی بسطامی	Solar light driven magnetic-photocatalyst nanohybrid and photocatalytic degradation of pharmaceutical pollutants
۸۷	۴۶۲	طاهره روحانی بسطامی	A review on electrospun polymeric nanofibers and antibacterial wound dressing
۸۸	۴۶۸	راهله افضلی	DFT studies on the structure and intramolecular hydrogen bond strength in 1, 2-dibenzoylcyclopentadiene
۸۹	۴۶۷	راهله افضلی	Is there any correlation between some theoretical and experimental parameters at similar and dissimilar beta-diketone complexes?
۹۰	۵۱۱	فاطمه اسدی	Solar/visible photocatalytic degradation kinetics and mechanism of RB5 dye by g-C_3N_4 nanosheets
۹۱	۶۵۴	ساجده شعبان پناه	Thermal Analysis and Ion Exchange Capacity of Poly (Vinyl Alcohol)-Based Membranes Modified with 2-Nitroso-1-Naphthol-4-Sulfonic Acid for Direct Methanol Fuel Cell Applications
۹۲	۶۵۶	ساجده شعبان پناه	Effect of Crosslink Density on the Characteristics of the Poly (Vinyl Alcohol) Membranes having Boromo Ethane Sulfonic Acid
۹۳	۷۲۳	عفت مشفقی	Effect of CH_3NH_3I Concentration on Efficieny of Mesoporous Methylammonium Lead Iodide Perovskite Solar Cell
۹٤	۹۶۰	اسماء یوسف وند	Suggest of using activated carbon in structure of absorbent and catalyst BCT

٩٥	۹۶۲	شیدا خاکزاد	The effect of neutron radiation on the activity of urease enzyme
٩٦	۱۰۸۳	زهرا سخندان	A systematic study on the effects of Ni^{2+} and OH- ions on performance of direct ethanol fuel cell
٩٧	۱۰۶۲	هانیه ندیمی	Effect of alkyl chain length on aggregation behavior in amino acid ionic liquid surfactant by molecular dynamic simulation
٩٨	۱۱۳۶	هانیه ندیمی	The effect of temperature on cation aggregation in dodecyl betaine N-acyl glycinate ionic liquid surfactant by molecular dynamic
٩٩	۱۱۱۲	فاطمه جنتی فرد	The effects of sodium dodecyl sulphate on the behaviour of glucose oxidase enzyme
١٠٠	۱۱۱۳	ریحانه دهقانی	Can Prion and Aptamar Connect Stabemeter
١٠١	۱۱۵۱	زهرا شرفی	Study of thermodynamic properties and intermolecular forces in the formation of aqueous aggregation of Arachidonic acid
١٠٢	۱۱۵۴	زهرا شرفی	Investigation of the Formation of Arachidonic Acid Micelle in Aqueous Medium
١٠٣	۱۳۸	پرنیان جعفری چاشمی	The study of synergism between N-lauryl sarcosine sodium and lithium dodecyl sulfate using conductometric technique
١٠٤	۱۳۹	پرنیان جعفری چاشمی	A comparison between three methods for determination of the critical micelle concenteration in ionic surfactants
١٠٥	۲۶	محبوبه زارگزی	Forest like $BiFeO_3$ thin film obtained from Sol-EPD: photocatalytic and photoelectrochemical activities
١٠٦	۱۷۶	مریم اکبری	Optimization of synthesis parameters of iron oxide nanoparticles prepared by reverse microemulsion method
١٠٧	۵۷۵	مریم خسروی	Synthesis of superhydrophobic ZnO micro-rods on carbon cloth
١٠٨	۱۰۷۹	ساجده محمودی صالح اباد	Corrosion inhibition behavior of collidine on aluminium in hydrochloric acid solution
١٠٩	۳۴	فروغ ارکان	Carrier lifetime improvement in D-π-A systems; Molecular engineering of the dye-sensitized solar cell
١١٠	۴۷	سمیه رحمتی	N-Heterocyclic germylenes in focus: Steric effects on nucleophilicity of novel tetrazole-5-germylenes at DFT
١١١	۱۰۴۹	ترلان مهذب لیقوانی	VX gas sensor based on the doped-nano cage: DFT studies

١١٢	۱۰۵۳	مونا خیرالهی	Mechanical Properties of Graphene, Silicen, Germanen and mixtures of them
١١٣	۱۰۳۱	صفورا حریری	3D-QSAR Study of Human DHFR Inhibitors Based on GRIND Descriptors and Designing of New Inhibitors
١١٤	۱۱۵۶	علی کاکش پور	Study of inter- and intra- molecular interactions on conformational stability of N-(1,3-thiazol-2-yl) benzamide
١١٥	۲۴۴	زهرا سیار	The I–V Characteristics of dimethyl 3,5-heptane Nano-Molecular Wire Induced by Hydrogen Transfer
١١٦	۴۹۱	وحیدرضا داروگر	Application of Hammett equation to intramolecular hydrogen bond strength in para-substituted phenyl ring in some β-diketones and schiff bases
١١٧	۲۲۹	وحید کلی	Understanding the molecular mechanism of thermal decomposition of methyl benzoylformate using bonding evolution theory
١١٨	۲۳۶	سمیرا پیمانی	Time-dependent properties and major electronic transitions in diphenylbacteriochlorin as a dye in DSSC: A quantum chemistry study
١١٩	۲۴۰	سمیرا پیمانی	A bacteriochlorin-based structure with a good planarity in charge transfer in DSSCs
١٢٠	۵۸۵	فریبا سادات محمدیان ثابت	The prediction of absorption and emission wavelengths in thermally activated delayed fluorescence organic light-emitting diodes(OLEDs)
١٢١	۳۶۸	الهام هدایتی راد	Revealing substituent effects on π-π stacking and halogen bond interactions. A Theoretical study
١٢٢	۱۰۱	نازنین باقری	Synthesis of biodegradable and highly porous conductive hydrogel based on carboxymethyl cellulose and aniline; evaluation of dye removal capability
١٢٣	۱۷۸	فردین گراوند	Electrochemical synthesis of AgO nanoparticles
١٢٤	۲۰۴	حسن رئیسی آهوان	Deep Eutectic Solvent Copper salt as a green catalyst for the acetylation of various alcohols, phenols and amines
١٢٥	۲۱۹	سهیلا نخجیری کامرانی	A highly stable and very active heterogeneous Pd nanocatalyst in the O-arylation of phenol or C-O cross couplings
١٢٦	۶۲۹	سهیلا نخجیری کامرانی	Preparation and characterization of antibiofouling PES nanofiltration membrane

۱۲۷	۲۷۴	سودابه قاسمی	synthesis of glucose optical biosensor nanocomposite based on tragacanth gum biopolymer
۱۲۸	۲۷۸	علیرضا زنهاری	Green synthesis and antibacterial activity of rosemary (Rosmarinus officinalis) assisted superparamagnetic iron oxide nanoparticles
۱۲۹	۳۲۲	آزاده ایزدی	Synthesis and cytotoxic evaluation of poly(ethylene glycol)-coated superparamagnetic nanoparticles
۱۳۰	۳۴۹	زینب رحمانی	Preparation of porous hydrogel beads based on calcium-ion-crosslinked gum tragacanth/graphene oxide: Swelling and drug delivery behavior
۱۳۱	۳۶۲	مهدی قمصری	Fast and highly efficient removal of some cationic dyes from aqueous solutions using Sulfonated-Oxidized activated carbon
۱۳۲	۳۷۶	لیدا مومنی	The interaction of trypsin with one nanoparticle (CuO): Spectroscope identification
۱۳۳	۳۹۶	امید جاوید	A microcrystalline cellulose/manganese schiff base complex as a novel eco-friendly biocomposite for oxidation of alcohols
۱۳٤	۴۷۶	امید جاوید	Supported molybdenum schiff base derivated from 2-aminopyridine on oxidized cellulose by sodium periodate: synthesis, characterization, and catalytic activities
۱۳٥	۴۴۱	الناز سیستانی پور	catechin-conjugated hydroxyapatite nanoparticles increase Osteocalcin and Runx2 proteins in Mesenchymal stem cells
۱۳٦	۴۵۴	نیلوفر ارشادی	Synthesis of Cl-Methylated Carbon Nanotube as a 5-FU Drug Carrier
۱۳۷	۴۲۴	علیرضا بهنام ثانی	Photodynamic Therapy Mediated Cytotoxic Activity of ZnO/HAP Nanocomposites in Human Osteosarcoma Cells under UV Irradiation
۱۳۸	۴۸۰	مصطفی غفوری گوراب	Biological Surfactants, use in Iran, distance to global use
۱۳۹	۴۸۵	سعید نجاتی	A computational study of all di-fluoroazulenes
۱٤۰	۵۳۷	محسن مقیسه	Morphological studies of LDPE prepared using pyridine-imine based catalysts: Effect of catalyst bulkiness and metal
۱٤۱	۵۳۸	محسن مقیسه	Beneficial influence of MWCNT on the pyridine-imine catalyzed ethylene polymerization: effect of type, content and technique

١٤٢	۵۶۳	مولود فلسفین	Benzimidazole based porous organic polymer: synthesis and characterization
١٤٣	۵۷۸	ابوالفضل حیدری	Effect of coupling agent (malic anhydride) on polypropylene compound
١٤٤	۶۳۹	حسین صفدری ترکمان	Synthesis of pressure sensitive adhesive using emulsion polymerization of core-shell technique, effect of acrylic acid monomer on Shear strength
١٤٥	۷۳۱	عاطفه معتمدنیا	A Facile and Low Cost Method for the Synthesis of Magnesium Oxide Nanostructures by Oxidation of Magnesium Metal
١٤٦	۷۶۳	عباسعلی عربی	Photocatalytic degradation of Reactive Black-5 Dye (RB5) from Aqueous Solution by calcium doped lanthanum manganite under visible light irradiation
١٤٧	۸۷۳	کامران مهدوی	Synthesis and Characterization of Nano Structures of $CuFeS_2$ Chalcopyrite by a Simple solvothermal method
١٤٨	۹۳۷	هانیه السادات میران موسوی	Investigation of physically treated recycled cross-linked polyethylene foam waste for automotive insulator
١٤٩	۹۴۶	مریم مهاجرانی	Fatty acid composition and antioxidant activity of Ferula persica Boiss
١٥٠	۹۸۸	فاطمه سالارحسینی	Antibacterial properties of polyethylene containing thymol and silver nanoparticles against Aeromonas hydrophila
١٥١	۹۸۹	فاطمه سالارحسینی	Chitosan / bentonite / ZnO nanoparticles composites: From synthesis to antibacterial properties
١٥٢	۱۰۰۷	فرانک فیضی	Sonochemical Synthesis and Structural Characterization of a New Nanostructured Sm(III) Porous Coordination Polymer
١٥٣	۱۰۱۵	هادی بابایی	Synthesis of pressure-sensitive adhesives based on butyl acrylate, effect of cross-linking agent
١٥٤	۱۰۶۹	محمد منصوری	Synthesis of PE/MgO nanocomposites via in-situ polymerization using Ziegler-Natta catalyst
١٥٥	۱۰۷۴	محمدامین شعبانی	Leaching of low grade sulfide copper ore by ferric sulfate
١٥٦	۱۰۷۶	محمد فانی خشتی	Measurement of pressure drop due to connections in the flow path of water flow in a multipurpose device
١٥٧	۱۰۷۸	عنایت رحیمی پور	Synthesis of PE/graphene nanocomposite via in-situ polymerization using a multinuclear catalyst of late transition metals based on cobalt

١٥٨	۱۰۸۵	رقیه شاهی مریدی	Synthesis of CuFe$_2$O$_4$ hollow sphere and their application in the preparation of 4,4´ -(aryl methylene)bis(3-methyl-1H-perazol-5-ol)s derivatives as catalyst
١٥٩	۱۰۸۷	اعظم سیفی	Synthesizing porous anti-reflection and self-cleaning coatings as a cover for the glass of solar cells
١٦٠	۱۱۰۱	سکینه هرگل زاده	Study of the self-cleaning effect of silver nanoparticles and silver / zinc oxide on the basis of graphene
١٦١	۱۱۳۳	آرزو کسکنی	Cytotoxic evalution of chenopodium botrys essential oil on the cancer cell category of the tumor cervix(Hela)
١٦٢	۱۰۶۸	کبری قاسمی	Effect of cyclic electrodeposition on performances of Lesd flow battery
١٦٣	۱۱۹۸	محمود احمدیان	Selective Deuteration of pyridinecarboxylic acid derivatives by decarboxylation and D$_2$O
١٦٤	۱۱۹۹	حامد پاشا	Deuteration of aniline aromatic ring in the presence of Heterogeneous Platinum Catalyst
١٦٥	۱۲۰۲	حامد پاشا	Metal catalyst Synthesis of methyl-d3-amine hydrochloride by nitro group reduction
١٦٦	۱۲۰۰	سجاد اسد بیگی	Preparation of deuterated methyl iodide through trimethylsulfoxonium iodide intermediate
١٦٧	۱۲۰۱	امیر احمد رضایی	Synthesis and Characterization of Deuterated Glycine d-5: comparison of deuterated and non-deuterated glycine spectra
١٦٨	۵۲۷	اکبر رستمی ورتونی	Green synthesis of Ag nanoparticles on Fe$_3$O$_4$/HZSM-5 and its evaluation as a catalyst for reduction of organic pollutants
١٦٩	۵۲۸	اکبر رستمی ورتونی	Immobilization of Ag nanoparticles on porous carbon prepared via carbonization of red water using Caesalpinia gilliesii flower extract

Contents

Plenary Lectures

Paper code: 270

Ultrasound assisted desulfurization of fuel oil with choline chloride based deep eutectic solvent and magnetic NaY zeolite using artificial neural network

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The increasing trend of respiratory, digestive, and dermatological problems is the result of environmental exposure to sulfur dioxide gases (SO_x), especially sulfur dioxide (SO_2) [1]. These gases are the main source of acid rain and air pollution, result from the conversion of fuels containing sulfur compounds in combustion engines. Therefore, some serious regulations were arranged for the amount of sulphur compound in fuel. The simplest way to decrease the amount of SO_2 emitted into the air is to reduce the amount of sulfur in fuel. Different methods such as hydrodesulfurization (HDS), extractive desulfurization, oxidative desulfurization, adsorptive desulfurization have been used to reduce sulfur content in fuels. Adsorption is an attractive process for desulfurization of transportation fuels due to high efficiency, lower temperature and pressure, simple and easy regeneration of sorbent [2]. In this research study, a combination of magnetic NaY zeolite and choline chloride based deep eutectic solvent (DES) and magnetic NaY zeolite were synthetized and applied for desulfurization of dibenzothiophene in n-hexane. The synthetized DES was characterized with NMR and IR. Magnetic NaY zeolite was also characterized with IR and SEM. The effect of influential parameters of temperature, time, amount of sorbent, and amount of extraction solvent were investigated. Under optimum conditions of 25 °C, 10 min, 50 mg, and 75 µL for temperature, time, amount of sorbent, and amount of extraction solvent respectively, the maximum desulfurization (%) of 94.5 was obtained which showed high potential of the proposed process in desulfurization process.

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Paper code: 413

Synthesis of superparamagnetic nanocomposite of poly(*m*-amino benzenesulfonic acid) and Fe_3O_4 and its high efficiency in solar cell

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This work reports synthesis and characterization of core-shell nanocomposite of poly(*m*-aminobenzenesulfonic acid) with $FeCl_3.6H_2O$ as oxidant for polymerization and precursor of nanoparticles for preparation of nanocomposite in solid-state condition. The synthesized nanocomposite (NCABS-Fe_3O_4) was characterized and its properties such as thermal, photophysical (solar cell), and magnetic were investigated. This nanocomposite was exhibited good thermal stability with 10% weight loss temperatures ($T_{10\%}$) in the 492 °C. It was showed that strong interfacial interaction between inorganic particles and the polymer matrix contributed to the high thermal properties. According to Vibrating sample magnetometry (VSM), it has high saturation magnetization of 40 emu/g at 8000 Oe, and has superparamagnetic properties at room temperature. SEM and TEM were indicated the same results and particles with 42-44 nm average size.

Polymer solar cell was prepared by NCABS-Fe_3O_4 on fluorine doped tin oxide (FTO) and aluminum electrodes. The photovoltaic cell characteristics, i.e. open circuit voltage (V_{OC}), short circuit current density (I_{SC}), fill factor (FF) were measured under simulated solar irradiation and power conversion efficiency (PCE or η) was found to be 4.24% for FTO/NCABS-Fe_3O_4/Al structure [1-3].

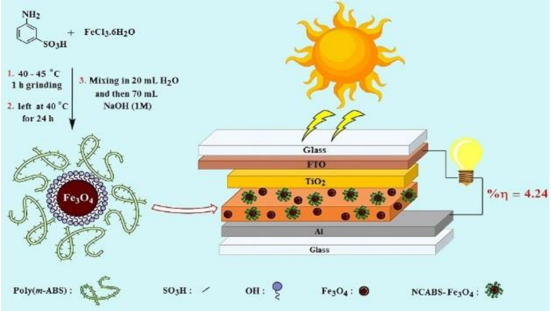

Fig. 1 The Synthesis of NCABS-Fe_3O_4 core-shells and its high efficiency in solar cell.

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Paper code: 747

New Insight in Medicinal Chemistry of Human tyrosinase; Based on a comparative study on Mushroom tyrosinase and Human tyrosinase

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A great deal of our knowledge about tyrosinases comes from the in-vitro studies which were conducted on Agaricus bisporus tyrosinase (AbT) mainly because edible mushroom is a rich, safe and inexpensive source of this enzyme (1) and the other sources including human tyrosinase (HuT) are not easily accessible. Results of these studies gave us insight about important aspects of tyrosinase enzymology including kinetics of both mono-oxygenase and oxidase activities, selectivity, specificity, inhibition, activation, inactivation, functional stability, structural stability, cooperativity and allostery. Consequently, this knowledge increased our expectations for tyrosinase related applications in various fields of medicine, pharmacology, health care, cosmetic, agriculture, sensor technology and environment researches (2).

An important part of this research directly deals with medicinal chemistry of tyrosinase. The structure-reactivity researches on AbT have resulted in discovery of the structural and electronic features needed to design a potent tyrosinase inhibitor. Similar researches have been initiated during past two decades to reveal structural prerequisites for an activator of tyrosinase. However, recent studies indicate that the success of any kind of tyrosinase modulator is preconditioned through the non-Michaelis Menten kinetics of the enzyme (3). What makes the subject even more challengeable is the fact that there is some evidence revealing differences between responses of AbT and HuT to the same modulator.

On the other hand, despite the impressive progress in the studies on melanogenesis at cellular level, there are few suggestions for successful and safe control of HuT activity while public concerns about the side effects of the current medicines has been elevated. It seems the future of medicinal, health care, and cosmetic market of tyrosinase related products is heavily dependent on the efficiency of the modulating substances which modify (control) tyrosinase activities safely.

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Paper code: 1208

Innovative applications Of ionic liquids in Chemistry and chemical engineering

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During past few years, ionic liquids (ILs) have kept attracting much attention as “green and designer” media for chemical reactions. Room-temperature ILs have emerged as a potential replacement for organic solvents in catalytic processes on both laboratory and industrial scales [1, 2]. Effectively, ILs, among a unique set of chemical and physical properties, have no measurable vapor pressure, which lends them as ideal replacements for volatile, conventional organic solvents. The wide and readily accessible range of room-temperature ILs with corresponding variations in physical properties, prepared by simple structural modifications to the cations or changes in anions, offers the opportunity to design an ionic liquid-solvent system optimized for particular processes. Highlights recent advances of ILs are as versatile “green” engineering liquids in a variety of industrial applications including heat transfer fluids, azeotrope-breaking liquids, lubricants, electrolytes, liquid crystals, supported IL membranes, plasticizers, and more. This paper highlights specific examples of ionic liquid Innovative applications in chemistry and chemical engineering.

Fig. ionic liquids

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Paper code: 1209

Nano-pumice hybrid porous materials for catalytic organic & inorganic compounds assembling

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Pumice-like solid materials are unique nanostructures which have a wide range of applications, from catalysis to biology [1]. Among them, microporous and mesoporous hybrid materials are more popular due to its higher stability, higher surface area, and relatively suitable pore size [2]. In this presentation, we reviewed the advancements in these area arrayed nanostructures and their applications including catalysis, H_2 generation, and photoctalysis. It can be concluded that organic and inorganic binded or assembled nanoporous materials can be a powerful tool multidisciplinary fields by having a high potential in all areas.

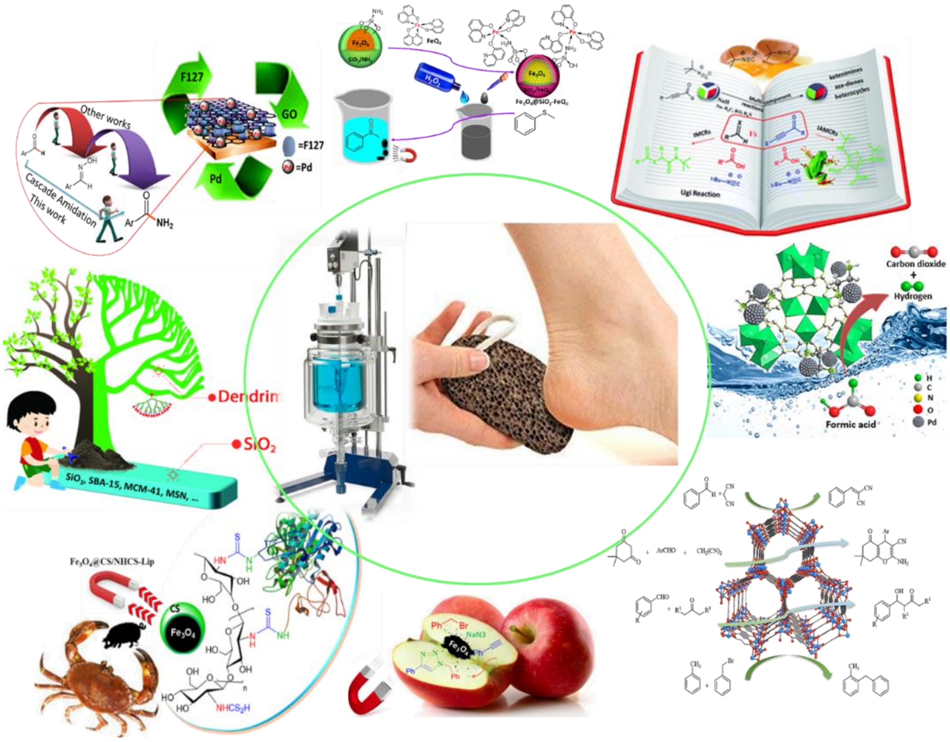

Fig. 1 Recent works by pumice-like mesoporous materials as the catalysis: published by our ONG group.

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Paper code: 1217

The Binuclear Organoplatinum(II) Complexes with Diphosphine Bridging Ligands; Synthesis and Optical Properties

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Cyclometalated organometallic compounds have been extensively investigated by many research groups because of their catalytic reactivity in organic synthesis and diverse medical and industrial applications. However, most applications are restricted to mononuclear cyclometalated organoplatinum(II) complexes, in which different kinds of electronic transitions, such as metal to ligand charge transfer (MLCT), ligand-centered (LC), and ligand to ligand charge transfer (L′LCT), are involved in any related emission operation. Also, the molecular interactions in platinum(II) complexes lead to significantly red-shifted long-wavelength emission, which is of considerable interest in near-infrared (NIR) absorbing and emitting organic materials.

The binuclear platinum complexes have drawn attention because of their particular photophysical properties. Metal−metal to ligand charge transfer (MMLCT) transitions exist in binuclear platinum(II) complexes when the Pt···Pt distance is less than 3.5 Å (the sum of two platinum van der Waals radius), leading to marked red shifts compared to the corresponding emission peaks of mononuclear platinum complexes. Although mononuclear platinum(II) complex units tend to interact with each other in the solid state and in concentrated solutions, Pt···Pt interactions are generally not strong enough to emerge in a diluted solution at room temperature. Moreover, even in the solid state, fine control of the Pt···Pt interactions is rather difficult for self-assembled mononuclear platinum(II) complexes.

From this viewpoint, double-decker platinum(II) complexes with well-defined Pt···Pt distances, built by bridging ligands, are very attractive. Furthermore, Pt···Pt distances can be precisely controlled using the appropriate bridging ligands. The formation of MMLCT transitions is due to charge transfer between a full Pt−Pt dσ* orbital and a partially empty ligand π* orbital on the cyclometalated ligand to accomplish a significantly red-shifted spectrum. In most cases, to design these systems, double bridging ligands with N^N, N^S, and N^O coordinating atoms were used, but the complexes with single P^P bridging ligands, such as bis(diphenylphosphino)methane (dppm), are still rare.

The aim of this presentation is to introduce several new class of emissive cyclometalated platinum(II) complexes with a bridging dppm ligand. The luminescence properties of binuclear complexes with bridging dppm were studied; the influence of bridging dppm on its metal−metal interactions and their emission were explored.

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Paper code: 1224

Pillar-layered MOFs: Functionality, Interpenetration, Flexibility and Applications

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Among the top investigations in solid state chemistry, Metal-Organic Frameworks (MOFs) [1] are the class of promising materials that have attracted tremendous amount of attention in the past two decades. Pillar-layered MOFs are one of the most striking branches of MOF materials. Due to great number of reports related to pillar-layered MOFs, investigating their structure diversity, properties and applicability as multi donor porous frameworks is of great interest. Introducing pillar linkers improve dimensionality as well as ability to tune the obtained frameworks. Detailed modification in pillar-layered architecture as a third building block of pillar-layered MOFs, together with metal nodes and oxygen donor linkers can enhance controlling structure assembly, leading to specific properties and can help us to fabricate novel networks with desirable performance, which is an important goal in recent MOF assembly. Controlling flexibility, interpenetration, chemical stability and functionality through changing pillar backbone or simple conversion in the spacer or functions in pillar bridges are attractive issues, which give opportunity to the scientists to design structures with optimal pore volume and efficiency such as good candidates in different areas as selective adsorption, separation, catalysis, sensing and so on [2].

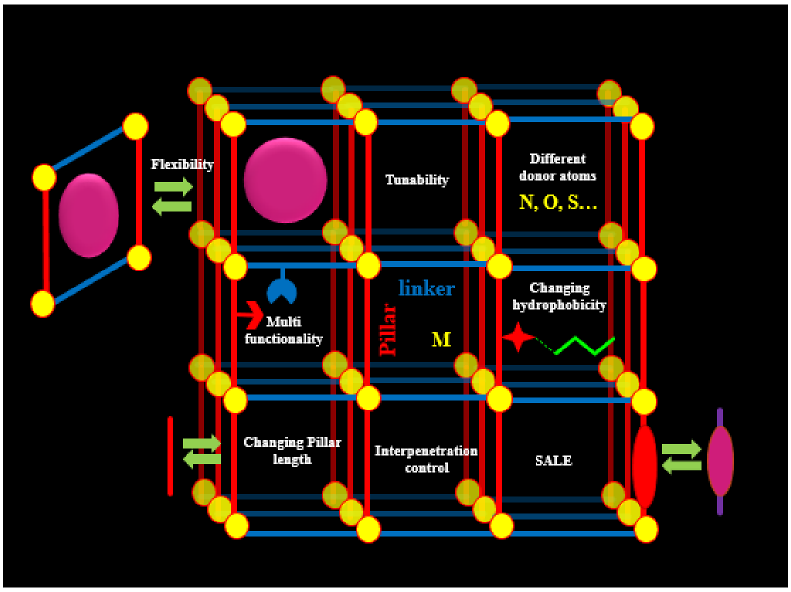

Fig. 1 Representation of pillar-layered MOFs properties.

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Paper code: 1253

Trifluoromethylated Compounds: Synthesis and Evaluation of their Biological Activities

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Fluorine has come to be recognized as a key element in materials science. Furthermore, many fluorine-containing biologically active agents are finding applications as pharmaceuticals and agrochemicals. Heterocycles containing only one trifluoromethyl group directly attached to the ring (trifluoromethylated heterocycles) constitute an extended family of organic compounds with substantial potential for application, most notably in biomedical and agricultural fields [1].

One of common methods for introducing the trifluoromethyl group into organic compounds is the use of building blocks containing CF_3 group such as trifuoroacetimidoyl chloride. Trifuoroacetimidoyl chloride are obtained via refluxing a mixture of trifluroacetic acid and a primary amine in carbon tetrachloride in the presence of triethylamine and triphenylphosphine [2]. In this study a new series of trifluoromethylated compounds have been synthesized using trifuoroacetimidoyl chloride [3]. Also we assessed biological activity of some new synthesized compounds. These compounds displayed good to excellent biological activities such as antimicrobial, antibacterial and anticancer. [4]

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Paper code: 1258

Recent approaches and advancements in energy production, conversion and storage systems using electrochemical methods

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One of the obstacles in human's sustainable development is energy production and storage. Batteries, fuel cells, solar cells and electrochemical supercapacitors have been selected as practical and effective energy production and storage technologies. During the last two decades, the lead acid batteries have been widely used because of their exclusive advantages. However, one of the main problem in lead acid batteries is a breakdown of water into oxygen and hydrogen gases which leads to the loss of electrolyte, increasing of the self-discharge and explosion risk. Modification of Pb electrodes and electrolyte in lead acid batteries were used in order to affect the polarization potentials of hydrogen and oxygen evolution [1]. As well, nanomaterials and structures play an important role in technologies related to energy applications, such as fuel cells and water splitting. Hydrogen evolution reaction (HER) is a reductive half-reaction of water- splitting, and it requires an active catalyst to lower the onset potential and facilitate the hydrogen production. In this case, reduced graphene oxide nanoflakes (RGONF) is synthesized in a new way and modified with metal and metal alloys nanoparticle by a solvothermal method. The obtained results confirm that these hybrids have high HER electrocatalytic activity with low overpotential [2]. Also, Fuel cells, due to their clean exhaust and high-energy efficiency are regarded as promising power sources. But, the high cost of fuel cells' electrocatalysts (especially Pt-based electrocatalysts) is one of the obstacles against becoming economical. Alloying of Pt with less precious metals, like Pd, Au, Ni and Cu are suggested as a practical solution which reduces the cost, mitigate poisoning effect and improve the power output. The nanopores on nanoporous stainless steel (NPSS) can provide confined spaces for the growth and stabilization of noble metal nano-structures in electrochemical energy-conversion systems [3]. Finally, the performance of the dye solar cells as an important green energy source, have been studied. The power efficiency of these systems are critically returned to the rate of electron transfer from the photosensitizer to the semiconductor and electron transport in the semiconductor, compared with the recombination processes. In order to achieve maximum efficiency, modification of semiconductor by noble metal doping, decorating with nanocomposite structures and synthesis of the new morphology of compounds is suggested. On the other hand, solar energy is a good choice for decomposing pollutants. In a new strategy, bifunctionalized NF-TiO_2 film is used. One part of the film is used as a dye-sensitized zone, and the other used as a degradation zone [4].

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Paper code: 1267

A review on some recent topics in quantum studies

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In recent years, quantum systems have been widely studied. Anthony Leggett, the Nobel Prizer in Physics, introduced the macroscopic quantum systems in 2003 for the first time in 1980. In the first part of this seminar, we look at an example of a macroscopic quantum system under dissipative effects. We solve the quantum Langevin equation in the Bohm quantum model and then we compare the results with the standard quanum prediction. Bohm's theory is one of the most famous rival quantum theories, which its contradiction with standard quantum predictions has so far not been observed. Another important research topic in recent years has been the definition and explanation of consciousness using quantum theory. The lecture continues with talking about some of the existing approaches to quantum consciousness, including Penrose-Hemeroff's view.

Paper code: 1270

Designing of Novel Multicomponent Reactions using 3-Formyl Chromone for the Synthesis of Functionalized Heterocyclic Skeletons

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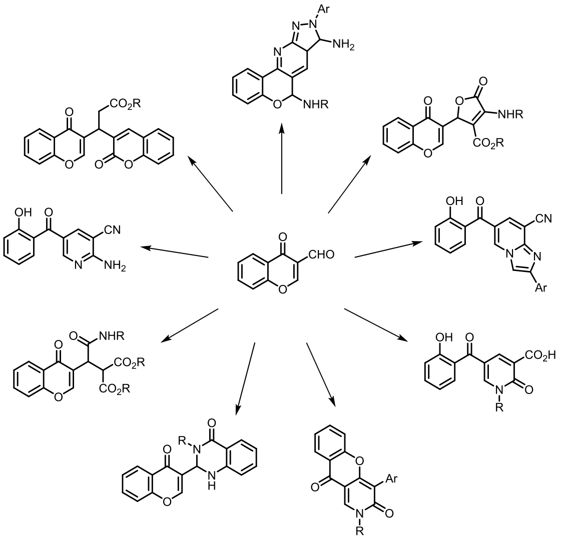
The synthesis of new chemical structures has always been a major challenge in the field of organic synthesis. In this context, multicomponent reactions (MCRs) are a powerful synthetic approach for generating complex molecules and are suitable for exploring substituent diversity.

3-Formyl chromones are used for the construction of different heterocyclic systems through reactions with binucleophiles. Meanwhile, chromonyl Meldrum's acid is suitable substrate as starting material as a source of the chromone scaffold for its insertion into the structure of biologically active compounds.

Here, different multicomponent reactions based on 3-formyl chromone and chromonyl Meldrum's acid present that could be used for the synthesis of different heterocyclic skeletons through the ring opening of chromone or without ring opening and formation of the functionalized chromone. For example, synthesis of chromone hydrazide and its reaction with malononitrile and primary amines in the presence of trimethylamine leading to fused pyrazolopyridines with chromone moiety.

This presentation will focus on the synthesis of chromone derivatives and using them for the synthesis of functionalized heterocyclic skeletons.



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Paper code: 1274

Role of chemistry knowledge in know-how development of industrial catalysis; petroleum refinery case study

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Today, the presence of heterogeneous catalysts in the chemical industry is very extensive and highlighted. The development of technical knowledge of new catalysts to increase the efficiency of industrial units has become the most important competition among the owners of technical knowledge of chemical processes[1]. The catalyst is a chemical solid with an optimal chemical composition for a chemical reaction and contains a structure appropriate to the properties of the physical chemistry suitable for the industrial process. The type and geometry of the industrial reactor is important for the design of the catalyst structure, which is why the reactor and the catalyst are two components that are completely interconnected [2]. The introduction of various chemical challenges, heat and mass transfer, mechanical strength, reactor filling and discharge procedure, contact time with reactor feed, etc., have made the catalyst an interdisciplinary science requiring a wide range of expertise in surface and solid chemistry, chemical engineering, ceramic materials, mechanics and solid state physics. Among them, the role of chemistry as a path initiator is very high. In this paper, the role of solid and solid chemistry on the development of technical knowledge of heterogeneous catalysts has been considered on the basis of refinery catalytic processes [3].

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Paper code: 1276

Interactions of nanoparticles with lipid membrane: simulations and experiments

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In the past decade, nanoparticles (NPs) have emerged as a promising new class of drug and gene delivery vectors as well as agents for targeted destruction of cancer cells. [1] Therefore, an in-depth atomic level understanding of NPs cellular uptake mechanism is still necessary. We report a systematic study of different NPs interacting with model membranes. Transcellular transport of gold nanoparticles (AuNPs) of different surface charge and carbon dots (C-dots) are investigated in the present study (see Fig. 1). The effect of various functional groups on membrane permeability of nanoparticle are explored.

The simulations indicate that AuNPs experiences a free energy barrier to bind with the extracellular leaflet, in agreement with experiments [2]. The corresponding energy barriers for AuNPs entering the bilayer are found to be about 134 kJ/mol. Also, the energy barrier for C-dots piercing into the bilayer are calculated. The simulation results are compared with florescent microscopy investigations.

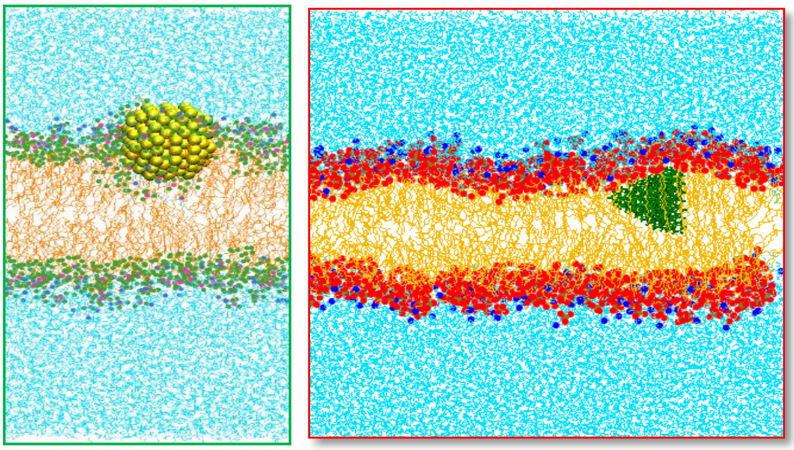

Fig. 1 Visualization of AuNP (left panel) and C-dots (right panel) with DPPC membranes.

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Paper code: 1277

Binding of small molecules to proteins: An old problem with new insights

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In characterization, various aspects of macromolecular phenomena in living systems, reversible binding of small molecules to biological macromolecules such as proteins and DNA is of fundamental importance. This is illustrated by the binding curve that measured experimentally and analyzed by the binding models in order to characterize its physical nature and biological importance. This article represents the results of more than 20-year research and study on experimental, theoretical, and computational aspects of this phenomenon in our group. Accordingly, the novel analyzing models and experimental measuring techniques are introduced and the contribution of these works on improvement of our understanding of the functional chemistry of proteins is discussed.

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Paper code: 1278

Metal-graphene hybrid materials as the heterogeneous catalyst for organic reactions

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Graphene is one of the most promising materials in nanotechnology. From a theoretical point of view, it provides the ultimate two-dimensional model of catalytic support. Its unique physical, chemical, and mechanical properties are outstanding and could allow the preparation of hybrid materials with unique characteristics [1,2]. This study, the thirteen nanohybrids based on graphene as support were designed and synthesized as well as heterogeneous catalysts used in the organic reactions. All nanohybrids were characterized by X-ray diffraction, Raman scattering, transmission electron microscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy.

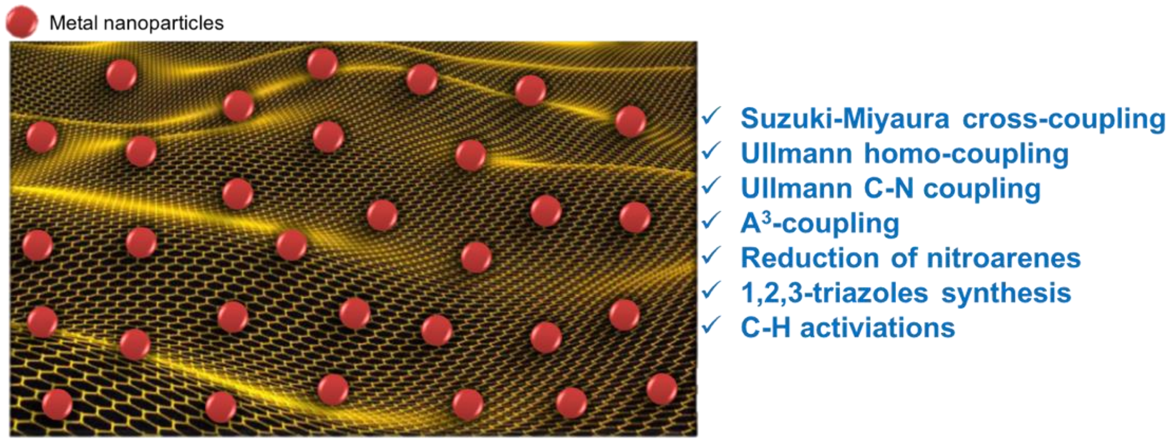

Fig. 1 metal-graphene hybrid materials as the heterogeneous catalyst for organic reactions

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Paper code: 1279

Recent Research on Nanobioinorganic Chemistry

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Nanobioinorganic chemistry is a new field of bioinorganic chemistry, which converges inorganic chemistry and biology at the nanoscale. This field deals with nanomedicine, nanotoxicology, tissue engineering, biotechnology, environmental science, drug nanocarriers, and bioimaging.

Recently, my research group has been focused on several aspects of nanobioinorganic chemistry including bioconjugation of gold and copper nanoparticles to non-steroidal anti-inflammatory drugs (NSAIDs), DNA bases and catecholic amino acid 3,4-dihydroxyphenylalanine (DOPA), immobilization of gold nanoparticles on the folate-conjugated dendritic mesoporous silica-coated reduced graphene oxide nanosheets, and folic acid-conjugated dendritic mesoporous silica nanoparticles for pH-controlled release and targeted delivery of a cyclometallated gold(III) complex as an antitumor agent.

Our recent works can further be extended to various applications and domains in the nanomedicines, targeted drug delivery systems, new bactericidal agents, targeted and photothermal therapies, drugs and biomolecules stabilizers, new anticancer agents, targeted cancer therapies, and nanobiotechnology fields.

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Paper code: 1281

Application of Heteropolyacids in Nanoscience for the Development of Green Catalytic Reactions

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In recent years, green catalysis has become an emerging field of science due to its high activity, selectivity and productivity. Heteropolyacids are promising candidates for green catalysts, as they are harmless to the environment with respect to corrosiveness, safety, quantity of waste, and separability. Other key green aspects of solid heteropolyacids are related to their synthesis in an aqueous process and achievements of successful practical applications. These features have resulted in the development of numerous catalytic protocols for the synthesis of nanostructure materials using heteropolyacids.

Therefore, the field of catalysis using heteropolyacids and their applications in nanoscience and nanotechnology continues to attract significant attention, so the number of publications and patents continues to grow, and new researchers are entering the field. Encouraged by our recent success in work with heteropolyacids as green catalysts in field of nanoscience and nanotechnology, the present work mainly focused on our fundamental investigations on many of the recent catalytic developments in nanoscience using heteropolyacids. This research demonstrates our important findings for the important catalytic role of heteropolyacids in the advances of nanotechnology, especially in synthesis of nanomaterials, nanocomposites, and nanotubes.

Paper code: 1282

Chemical sensors, biosensors and bioprobes

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Todays, the strategic aim in analytical chemistry, is the simplification of the analytical methodology to a level where the measurements of the analytes in real samples become simple with a minimal operator skills. Achievement to this practical goal has resulted in construction of chemical and biochemical sensors. Because of their capability to give continuously, reversibly and selectively and also a fast response to a specific analyte in real samples without perturbing the systems, therefore, they are used in chemical industry, food and pharmaceutical industries, as well as, medicine and environmental control [1]. In this presentation, the characteristics and applications of a new optical sensor (surface plasmon resonance sensor) and some of the electrochemical sensors will be discussed.

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Paper code: 1283

University entrepreneurship, a force for science-based economy

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The President of Khorasan Science and Technology Park

There is no doubt that science today is considered to be the most effective factor in economic development. In these conditions, universities are expected to play a broader role in national and local development as well as education and science production. The process of technology transfer from industry to university in the form of creation and improvement of new products and services can be one of the most effective activities of universities for wealth production and economic growth.

The appearance of entrepreneur university is a respond to the necessity of science and innovation in national and local development.

Historic investigations show that as the word of entrepreneurship was created three decades ago, some American universities began to shift their orientation toward educating and training entrepreneurs rather than science production about entrepreneurship. In other words, entrepreneurship was based on traditional resources such as money, land and other financial resources but in early 1990s, innovation based on science and entrepreneurship based on science and science-based economy have developed interactively. Some successful examples of entrepreneurship are MIT university, Stanford university, SME companies in Silicon Valley and other examples in Europe and southeast Asian countries in which entrepreneur universities became a force for the development of science-based economy and SMEs.

Since the most important feature of entrepreneur universities is the commercialization of science, it is clear that going through such a process needs different sources of income, entrepreneurial activities of academia and creating new strategies for the compatibility of university structures and entrepreneurial activities. For example, Lestra considers university entrepreneurship to be the engagement of university and faculty members in related commercialization activities including the cooperation between university and industry, investment in companies based on university, simultaneous employment of faculty members in university and Spin off companies and preparing new supportive infrastructures for promoting entrepreneurship (such as establishing technology transfer offices, widespread cooperation with science and technology parks and technology incubators)

In other words, inputs in a university entrepreneurial system are professors, students, scientific skills, entrepreneurship educations and etc.

Outputs are graduates with the capability to start business and take adventures.

Developing sustainable entrepreneurship in the absence of a scientific ecosystem seems impossible. Scientific ecosystem and innovation can provide the basis for developing innovative and science-based businesses.

But it is an important question that what percent of our professors and students are engaged in entrepreneurial education and what percent are working in science-based enterprises or institutes of technology?

Paper code: 1284

Electrochemical Energy Storage: A Survey of Our Research Group Activities over the Past Two Decades

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Global consumption of fossil fuels for the generation of energy has come at a cost to the natural environment and a negative impact on human health. Developing efficient energy conversion and storage technologies is thus highly demanding in an era where energy plays an essential role in our everyday lives. The demand for renewable and clean energy from the sun and the other clean energy sources is rapidly increasing. Nevertheless, the intermittent nature of the renewable sources of energy calls for the development of efficient energy storage devices that can deliver energy upon demand. Currently, the dominating energy storage devices are batteries and electrochemical capacitors, also known as supercapacitors.

In this talk, I go through the steps that my research group has taken over the past two decades on the ways of developing advanced electrode active materials for electrochemical energy storage. We started our research activities with developing polymer-based rechargeable batteries [1] and then continued with fabricating dry and wet batteries in a bipolar configuration. We then developed variety of metal-based, conducting polymers and advanced carbon-based nanostructures [2] for supercapacitive energy storage. We also utilized a regenerative mechanism, via a catalytic interaction at the electrode-electrolyte interface, to supply additional charge [3]. In our recent studies, we have utilized advanced materials such as metal-organic frameworks (MOF) and layered-double hydroxides (LDH) for supercapacitive energy storage. It is my hope that these strategies would help us to take a step forward towards the development of advanced energy storage devices for state-of-the-art applications. You can find my research activities via the Google Scholar link [4].

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Paper code: 1285

Quantum computational (QC) study of Supercapacitors and Li-ion batteries

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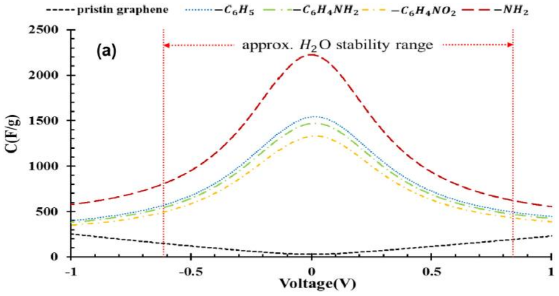
Supercapacitors and ion-lithium batteries are some of the most important electric storage devices due to their high specific Power density, high cycling life and high specific capacity. Therefore, the quantum computational study of the electrodic materials of this devices is also increasing.

Despite the expectation the experimental results showed that graphene did not have significant capacity as a supercapacitor electrode, which was attributed to its hydrophobicity. In 2013 Peak et al showed that the major problem of graphene is its low quantum capacity which is the ability of the electrode to store electrical charge. The differential quantum capacitance (C_q^{dif}) and the integrated quantum capacitance $C_q^{int}(V)$ are obtained as$C_q^{dif} = e^2 \int_{-\infty}^{+\infty} D(E)\, F_T(E-\mu)\, dE$ and $C_q^{int}(V) = \frac{1}{Ve} \int_0^V C_q(V')\, dV'$ where $D(E)$ is the density of states and $F_T(E-\mu)$is thermal broadening. In 2015, our research team showed that the addition of functional groups significantly increases the quantum capacity of graphene especially at low voltages (see the figure). Also, the results showed that adding functional groups to the two adjacent atoms or the divalent functional groups has lower effect in increasing capacity [1]. Experimental study in 2017 confirmed our computational results. Also, in the same year, we showed that the codoping of graphene with P atom and one of the Si, N, S, and ... atoms has more effect on the increase of quantum capacity than each of these atoms [2]. Our studies continued and resulted in the publication of several articles.

In the QC study Li/Na-Ion Batteries, we can calculate the voltage and the theoretical specific capacitance and estimate the theoretical specific power. The voltage can be defined as $V = E_{coh} - E_b$ where E_{coh} is cohesive energy of Li/Na and E_b defined as $E_b = (E_{nX/sys} - E_{sys} - nE_X)/n$.The theoretical specific capacity in $mAh\ g^{-1}$can be defined as $C_t = 26,801 \times n/M_W$ where n is the transferred electron number in considered structural unit. In 2017 functionalized graphene efficiency was studied as an organic anode electrode materials in Na-Ion battery. The results showed that the Al doped graphene that functionalized with organic compounds, showed a significant increase in the capacity and can absorb more than 12 Na atoms before cohesive energy Per a functional group. To find the potential energy curve for Li/Na diffusion in the Electrodic Materials, all possible paths were examined using reliable nudged elastic band (NEB) method and specific power of them was estimated.



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Paper code: 1286

Mesoporous templated films in dye sensitized and perovskite solar cells

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Using photovoltaic solar cells for direct conversion of light energy to electrical energy has been the human goals for exploitation of the sun as a clean and renewable energy source. Dye sensitized and Perovskite solar cells are a new generation of the photovoltaic cells which have attracted much attention in recent years, due to their simple construction method and economical cost.

In the first section of this study, ordered and disordered mesoporous templated films were prepared by using dip and spin coating methods. To obtain these types of films with high thickness and without any cracking, a stabilization step after each coating and a calcination step after every five layers were used and finally their performance in solar cells was investigated. A maximum efficiency of 8.33% was achieved for dye sensitized solar cells made of the ordered mesoporous films prepared by dip coating method [1].

In the second section, solar cells based on mesoporous films with four different morphologies of hexagonal, cubic, wormlike and gridlike were prepared and maximum efficiency of 8.73%, open circuit voltage of 743 mV, short circuit photocurrent density of 16.35 mA/cm^2, and fill factor of 0.72 was recorded for dye sensitized solar cell made of photoelectrode with cubic morphology [2].

In the third section, interfacial blocking layers were synthesized using four types of copolymers including PSA, Brij58, P123 and F127 and their impact was examined and compared with traditional dense blocking layers on performance of dye sensitized and perovskite solar cells. Our results showed that, through replacing the blocking layer templated by P123 copolymer with dense film, the short circuit density significantly improved from 15.89 to 21.23 $mA\ cm^{-2}$ for dye sensitized solar cell and from 18.72 to 24.09 $mA\ cm^{-2}$ for perovskite solar cell due to striking increase in light transmittance. Also, introduction of the P123 templated interfacial layer presents conversion efficiency enhancement by 33% and 16% in dye sensitized solar cell and perovskite solar cell, respectively [3].

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Paper code: 1287

Thermo-pH-Dual-Responsive Smart Polymersomes for Controlled Release of Doxorubicin

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Recently, design and development of effective drug delivery systems (DDSs), with a special attention to new strategies to control drug release and tumor targeting have attracted considerable attention.

In one of our study, thermoresponsive poly(N-isopropylacrylamide)-doxorubicin (PNIPAM-DOX) hydrogel was synthesized and loaded into pH-responsive poly ethylene glycol)-2,4,6- trimethoxybenzylidenepentaerythritol carbonate (PEG-PTMBPEC) polymersomes in order to fabricate a smart thermo-pH stimuli responsive drug delivery system. The *in vivo* release evaluation demonstrated that the DOX release from polymersomal formulation was pH-dependent, i.e. significantly faster drug release at pH 5.5 compared to physiological pH. On the other hand, the drug release rate was significantly decreased at 37^{O}C due to the gelation of PNIPAM-DOX conjugate in the interior compartment of the pH-responsive polymersomes. The *in vivo* anti-tumor efficiency of the prepared polymersomal formulation of DOX was evaluated implementing C26 tumor-bearing mice after either intravenous (i.v.) or intratumoral (i.t.) single dose injection. The obtained result demonstrated that the prepared system significantly inhibited tumor growth rate in mice receiving single dose *via* either intravenous or intratumoral injection in comparison with free DOX-treatment group. Furthermore, treatment with polymersomal formulation did not cause any systematic toxicity in terms of pathological alteration of vital organs, survival rate and body weight loss.

The prepared smart hydrosomal formulation significantly increased the blood half life time of drug and modified the biodistribution and pharmacokinetic parameters of formulated DOX.

In this regard, thermo-pH-dual-stimuli responsive hydrosomal formulation represent a novel approach in nanomedicine development for effective cancer therapy.

Paper code: 1288

Smart silica-based nanoparticles for targeted drug delivery

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Amongst various nanocarriers used for drug delivery applications, silica nanoparticles have received emerging interest. Also they have gained FDA investigational new drug approval for their human use in clinical trial. Mesoporous silica nanoparticles (MSN) are used extensively as drug delivery vehicles due to their excellent properties such as tunable nanoparticle size, large pore volume, highly ordered channels, convenient surface functionalization and large surface area.

We synthesized various types of silica NPs in our laboratory comprising MSN, hollow mesoporous silica nanoparticles (HMSNs), rod silica NPs and dendritic silica NPs.

Our research provides and important avenue for development of hybrid silica-based nanomedicines.

In one of our study, to efficiently deliver the chemotherapeutics to the tumor tissue and minimize the associated adverse effects, nucleolin-targeted hybrid nanostructure based on HMSNs were fabricated. To provide the controlled, sustained drug release and enhance blood circulation, the surface of doxorubicin-encapsulated HMSNs were coated with acetylated carboxymethyl cellulose (Ac-CMC) and then covalently conjugated to AS1411 aptamer for guided drug delivery to nucleolin overexpressed cancerous cells. In vitro cellular uptake and cytotoxicity studies confirmed that AS1411 aptamer specifically targets nucleolin overexpressing MCF-7 and C26 cells. Moreover, the in vivo tumor inhibitory effect of AS1411 aptamer conjugated formulation demonstrated a superior therapeutic efficiency over non-targeted formulation and free doxorubicin. The obtained results might open a new insight to the development of targeted intelligent hybrid materials based on AcCMC-coated HMSNs with high loading capacity, smart characteristics and desirable anticancer potential.

Analytical Chemistry

Paper code: 4

Simultaneous detection of L-cysteine and tryptophan as two important amino acids using a MgO nanostructure-based electrochemical sensor

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Modified electro-analytical sensors showed many advantages for the analysis of food, drug, and biological and environmental electro-active compounds [1]. The application of electro-catalytic mechanism to electrochemical analysis sensors can be increased the selectivity of system [2]. In this work, the synergic effect of MgO nanoparticle (MgO-NPs) and acetylferrocene (AFc) was studied for modification of carbon paste electrode (CPE) as a highly sensitive electrochemical sensor for electro-catalytic determination of L-cysteine in the aqueous solution. A calibration curve showed a linear relation in the range of 0.1-700.0 µM. The detection limit 30.0 nM was obtained for analysis of L-cysteine at a surface of AF/MgO-NPs/CPE. Figure 1 showed differential pulse voltammograms of L-cysteine in the presence of tryptophan with different concentration of two amino acids. The AF/MgO-NPs/CPE showed two separated oxidation signals with ΔE~170 mV in the solution containing L-cysteine and tryptophan that was sufficient for simulation determination of these amino acids. The modified electrode was successfully used for the determination of L- cysteine in real samples.

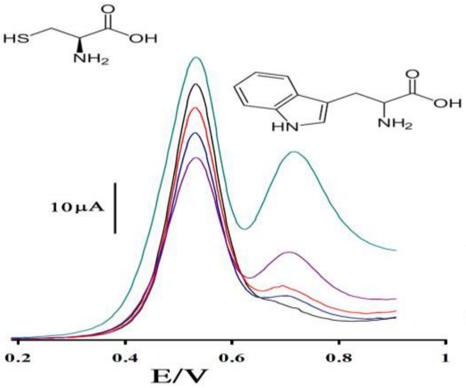

Fig. 1 Differential pulse voltammograms of AF/MgO-NPs/CPE in 0.1 M PBS (pH =7.0) containing different concentrations of L-cysteine and tryptophan

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Paper code: 15

Determination of tetracycline by adsorptive differential pulse cathodic stripping voltammetry

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A novel type of Pb-polyaminophenol filmed glassy carbon electrode for adsorptive cathodic stripping analysis of trace amounts of tetracycline was developed. The Pb-polymer electrode was fabricated in situ by simultaneous electrodeposition of Pb and cathodic electropolymerization of 4-nitrophenol in a sodium acetate medium at -1.5 volts. The outputs of some experiments showed that tetracycline can be adsorbed on the surface of this Pb-polymer filmed electrode in an open circuit condition. Therefore, it was used in adsorptive cathodic stripping analysis of tetracycline. Among new kinds of environmental contaminants, tetracyclines (TCs) are referred to as modern pollutants, since they have been found in soil and aquatic media [1]. These compounds are routinely used for human therapy and in the livestock industry [2]. The response of the electrode was enhanced in the presence of cetyltrimethylammonium bromide. Some parameters affecting the performance of the electrode were studied and optimized. The response of the electrode was linear in the range of 5×10^{-8} - 1×10^{-5} mol L^{-1} of tetracycline with a correlation coefficient of 0.9981. The relative standard deviation for 5×10^{-7} mol L^{-1} of tetracycline was 1.8 % (n=5). The L.O.D and L.O.Q were 4×10^{-9} and 1.3×10^{-8} mol L^{-1} of tetracycline, respectively. The introduced electrode was used for determination of tetracycline residues in some samples and the obtained results were in good agreement with the results of HPLC.

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Paper code: 19

Designing and fabrication of electrochemical aptasensor based on a novel MWCNTs@Au nanocomposite for bisphenol A detection

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Bisphenol A (BPA) is a harmful endocrine disruption which is extensively used in production of beverage bottles, baby bottles, children's toys, and also the inner surface coating of cans used for food and the like [1]. Because of the negative effects of BPA on the environment and human health, the detection of BPA is urgently needed both for food safety concerns, and environmental monitoring. In recent years, the proposed sensing techniques based on electrochemical transducer especially, aptasensors have made the BPA detection simpler, faster, and more economic [2].

In this study, we provided an electrochemical aptasensor using anti-BPA aptamer as the recognition probe and MWCNTs@Au nanocomposite as an immobilization platform for BPA detection. The anti-BPA aptamer was immobilized on a glassy carbon electrode modified with MWCNTs@Au nanocomposite. The interaction between the aptamer and the BPA molecules was monitored by cyclic voltammetry (CV) in the electrochemical probe. The conformation of aptamer showed a change after BPA binding, triggering a decrease in the electron transfer of $Fe(CN)_6^{3-}/^{4-}$ on the electrode surface. The observed decline was detectable as a function of the presence of BPA. The calibration graph was obtained in the concentration range of 0.1-8 nM with limit of detection 0.03 nM for BPA.

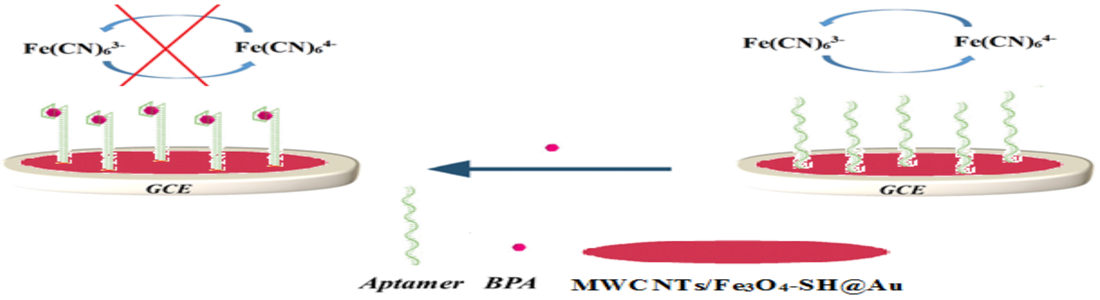

Fig. 1 Schematic of proposed aptasensor for the sensing of BPA molecules.

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Paper code: 20

Design of an electrochemical bisphenol A sensor based upon magnetic nanoparticles modified with Au

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Production and consumption of plastics have been grown globally from 1950. Bisphenol A (BPA) can be migrate from its containers (polycarbonate plastic and epoxy resins) into a variety of foods and drinks [1]. Estrogenicity of BPA in vitro is similar to the 17β-estradiol which can mimic hormons and disrupt endocrine function. Therefore, BPA display an adverse effect in humanimmune function [2]. Therefore, it is quite logical that detection of BPA with the various used analytical methods. Among them, electrochemical techniques are the one of acceptable and extensible methods, due to advantages such as: fast operation, sensitive detection, low detection limit and no needs to (pre)treatment of samples [3].

The objective of this study is to develop a sensitive and selective electrochemical method for detection of BPA. Therefore, a novel magnetic nanoparticle-supported triethoxypropylthiole gold nanocomposite was successfully prepared by attaching Au NPs to functionalized Fe_3O_4 nanoparticles (Fe_3O_4@Au). The prepared nanocomposite was applied in fabrication of an electrochemical sensor (GCE/Fe_3O_4@Au). It was found the synthesized nanocomposite be highly efficient for the electrooxidation of BPA. Good linear range (0.005-120 μM) and low detection limit 1.62 nM (S/N=3) in determination of BPA were obtained. Moreover, the sensor was used at detection of BPA in some real samples.

Fig. 1 Schematic of electrochemical bisphenol A sensor.

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Paper code: 21

Electrochemical synthesis of $CuCo_2O_4$ nanosheets on Ni foam as a binder-free electrode for supercapacitors

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In recent years, supercapacitors have attracted great attention as high-power energy sources due to their fast charge-discharge rate, high power density, long cycle lifetime and high reliability [1]. Recently binary metal oxides such as spinels are emerging as new electrode materials owning to their rich redox reactions [2]. In this study, for the first time, we developed a facile electrodeposition method combined with post-annealing to grow ultrathin $CuCo_2O_4$ nanosheets on Ni foam substrate as a binder-free electrode for supercapacitors. In a typical synthesis, 0.2 mmol of copper nitrate and 0.4 mmol of cobalt nitrate were dissolved in 25 mL of DI water and a potential of −1.0 V (vs. Ag/AgCl) was applied to deposit Cu–Co hydroxide precursor. After electrodeposition for 10 min, the as prepared electrode was rinsed several times with deionized water. Finally, in order to get crystallized $CuCo_2O_4$ nanosheets, the sample was annealed in air at 300 ℃ for 2 h. The FESEM image (Fig. 1) confirms the preparation of $CuCo_2O_4$ nanosheets. The results of electrochemical measurements revealed that the $CuCo_2O_4$ electrode has a high specific capacitance of 1330 F g^{-1} at a current density of 2 A g^{-1} with 93.6 % specific capacitance retention after 5000 cycles. Owing to the unique structural features, the as obtained $CuCo_2O_4$ nanosheet is considered as an effective electrode for the next generation energy storage device.

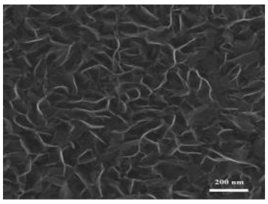

Fig. 1 FESEM image of $CuCo_2O_4$ nanosheets

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Paper code: 39

Electrochemical synthesis of S-doped cobalt–copper layered double hydroxide for energy storage systems

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Electrochemical capacitors, also called supercapacitors, have attracted increasing interest over the past few years due to their potential to deliver high power density in a very short time, their excellent cyclability [1], Recently, transition metal sulfides including binary cobalt sulfides, nickel sulfides, copper sulfides, and ternary copper cobalt sulfides have been investigated as novel supercapacitor electrode materials with improved electrochemical performance [2], In this study, two-layered copper-cobalt hydroxide and nanostructure of copper-cobalt-sulfide were synthesized on nickle foam: The electrochemical behavior of nanostructured compounds obtained as supercapacitor electrode materials were studied. In addition to the proper conductivity and durability of the nanoscale, the materials are fixed in the foam pores and provide a high effective surface, which leads to increased electrochemical reaction and the capacity. In this Synthesis 0.01 M of)$Co(NO_3)_2.6H_2O$), 0.005 M of ($Cu(NO_3)_2.3H_2O$) and 0.75 M Tu were solved in 30ml DI water and a potential of -0.1 V (Ag/AgCl) by simple method of electrochemical was done. The FESEM image explain the $CuCo_2S_4$ nanosheets (Fig. 1) In the next step, electrochemical performance of the synthesized compounds on nickle foam as the supercapacitor electrode material were investigated by using cyclic voltammetry (CV) and charge-discharge (CD) in a 1 M KOH. Finally, the maximum capacitance 255 and 1565 F g^{-1} were obtained at a current density of 1 A g^{-1} for the nanostructure of copper-cobalt and copper-cobalt-sulfide in a three-electrode system, respectively. Also, the energy density 65.75 wh Kg^{-1} and power density 0.252 Kw kg^{-1} were obtained for copper-cobalt-sulfide nanostructure.

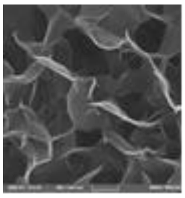

Fig. 1 FESEM image of $CuCo_2S_4$ nanosheets

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Paper code: 46

Investigation of Ion-Pair Association for KCl Electrolyte in Methanol Based on Conductance Method

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The conductometry is the analytical method used both in research laboratories as well as in industry. The electric conductivity is one of the most important properties of electrolyte solution [1]. The theoretical assumption of this method is the fact that the electrolytic conductivity is the result of the motion of anions and cations [2].

In this research, using the Debye-Huckel limiting law and by calculating the appropriate amount of parameter, $A_{D\text{-}H}$, in the methanol and water solvent, the values of the mean activity coefficients for KCl at each concentration were calculated. Then, based on the Fuoss Approximation, the dissociation constant, and using the law of mass action and activities, the association constant, all as a function of concentration, along with the limiting conduction for KCl electrolyte in methanol were determined by conductimetric method, and compared with their corresponding values in aqueous solvent.

KCl in	K_d (mol)	K_a (mol^{-1})	K_a(G.B) (mol^{-1})	K_a(Fuoss) (mol^{-1})
MeOH	0.07	13.6	12 ± 3	13.7
H_2O	4.2E+06	2.4E-07	-	-

According to the results, it was found that the formation of ion-pair for KCl in water is essentially zero, but with decrease of Dielectric constant of solvent, the degree of ion-pair formation also increases with concentration.

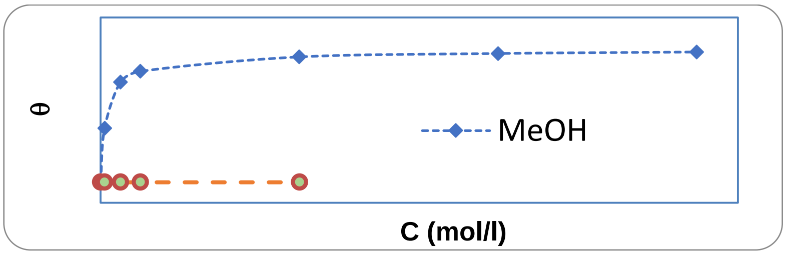

Fig1. Graph of formation ion-pair vs. concentration for KCl electrolyte in water and methanol solvents.

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Paper code: 66

Developing a modified bipolar electrode for selective measurement of nitrate ion based on palladium nanoparticles deposited on a cathode pole

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In a bipolar electrochemistry (BPE), an isolated conductor substrate which called "bipolar electrode", is placed in the electrolyte solution and an external electric field is applied to it [1]. Also, there is no physical connection between the bipolar electrode and the power supply [2]. Here we report a modern type of sensing platform that relies on the electrodissolution of a metallic layer on a bipolar electrode (BPel). In this study, we designed a modified bipolar electrode that makes it possible to measure nitrate ion (Fig. 1). In the proposed method, the silver layer deposited on a recordable digital versatile disc (DVD-R) has the role of an anode pole of a bipolar electrode. The nitrate ion is reduced on the cathodic pole which has been modified by copper and palladium nanoparticles, and at the same time dissolution of the silver layer in the anodic pole takes place. Length of the silver layer dissolution was considered as the analytical signal. Through the BPE method, the linear range and the detection limit of nitrate were found to be 0.5 - 3500.0 µM and a detection limit of 0.16 µM respectively. Moreover, the proposed method was used to determine of nitrate ion in industrial samples and the results indicated that this modified bipolar electrode has great potential for practical applications.

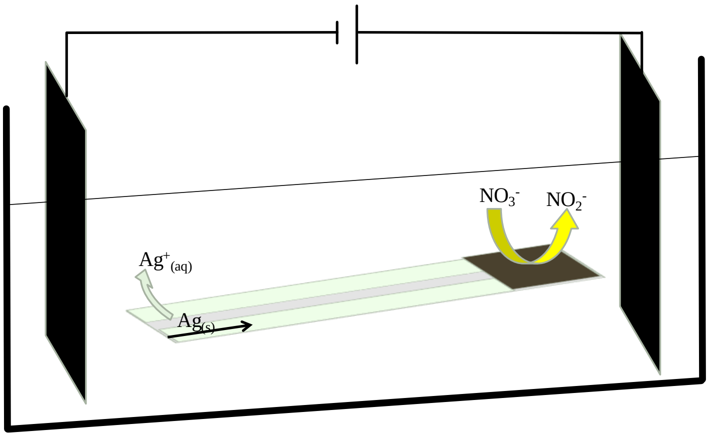

Fig. 1 scheme of nitrate measurement based on the bipolar electrochemistry

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Paper code: 67

Method Validation for the Quantitative Analysis of Aflatoxins (B1, B2, G1, and G2) in Rice by HPLC with Fluorescence Detection

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Aflatoxins are a group of toxic metabolites produced by species of Aspergillus, which were found worldwide in air and soil. Aflatoxins commonly found are aflatoxin B1 (AFB1), B2 (AFB2), G1 (AFG1), and G2 (AFG2). AFB1 is the most potent of all aflatoxins known to date and is generally found in the highest concentration in food and animal feeds. Aflatoxins occur naturally in food substances and can colonize these substances either during the growth period or in storage. Worldwide, rice is one of the most important staple food for more than half of the world's population. Usually, rice cultivation is conducted in subtropical/tropical environments, which are characteristically warm and humid. Furthermore, rice is generally dried after harvesting and under inappropriate storage conditions, rice can be an ideal substrate for mycotoxin-producing fungi [1].

After a deep research, the author has concluded that few studies about the Iranian rice have provided a fully validated method of analysis. Analytical methods used by enforcement laboratories in order to implementation of legislation, must be subject to validate procedures. In order to ensure the results of the testing method, these methods need to provide accurate and reproducible results both within and between laboratories. This is especially important in view of legal actions and trade specifications, as well as monitoring and risk-assessment studies. This study aimed to validate a methodology for the determination of aflatoxins B1, B2, G1 and G2 in rice, using A KOBRA® Cell derivatization system and quantification by HPLC with fluorescence detection [2].

The extraction of AFs from rice were performed by this method: blending 50g of sample rice with 200ml of methanol: water (80:20, v:v) in 5 min.Then the extract was filtered and 20 ml of that were transferred to a flask and diluted to 130 mL with PBS buffer (pH 7.4 ± 0.1). The diluted extract was passed through an AflaTest immunoaffinity column at a flow rate of 2-3 ml/min. Subsequently, 1.5 mL of methanol were applied to the column and finally samples were eluted by gravity into a glass vial. 1.5 milliliter of water was added, 50 µL were injected into the HPLC system.

The modified methods were validated by measuring the specificity, selectivity, linearity, sensitivity, accuracy, repeatability, reproducibility, recovery, LOD, and LOQ parameters.

High linearity was obtained over a dynamic range of 0.4–7.2 µg/kg for each aflatoxin. Recoveries varied from 92.21 to 108.28 %, with reproducibility standard deviations lower than 8.63% and repeatability standard deviations lower than 5.16 % Limits of quantification (LOQ) were 0.4 µg/kg for B1, B2, G1 and G2. Limits of detection (LOD) were 0.13 µg/kg.

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Paper code: 91

Simultaneous determination of β-sitosterol and cholesterol in food samples by using solid phase microextraction fibers based on monolithic moleculary imprinted polymer followed by HPLC–UV

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In this paper, an efficient and sensitive analytical method monolithic solid phase microextraction (SPME) fiber on the basis of moleculary imprinted polymer coupled to reverse phase high performance liquid chromatography (RP-HPLC) - UV detection analysis was developed for extraction and determination of β-sitosterol and cholesterol in food samples. Monolithic fiber is provided as follows: Template molecule (β-sitosterol) (2mmol) was dissolved in 30 mL acetonitrile (porogen) and functional monomer (MAA) (30 mmol), cross-linking monomer (EGME) (120 mmol) and intionar (AIBN) (280 mg) were added respectively. Then, 1mL of the mixture was transferred into small glass tube and was deoxygenized for 10 min with nitrogen gas. In order to prepare monolithic fibers, capillary home-made glass tubes as mold were treated according to the following recipe before preparation of monolithic fibers: In order to cut capillaries approximately, 30cm long pieces and windows of about 1 cm were prepared by burning the protecting polymer layer. Then, the capillary was filled with the polymerization mixture and both capillary ends were closed with two small pieces of rubber. The filled capillaries were inserted in an oven and polymerization took place typically at temperature 60 °C for 12 hours. Then polymeric monolith was withdrawn from mold by immersed capillaries in solution 40 % hydrofluoric acid for 2 hours. To obtain optimum extraction performance, several extraction parameters including extraction and desorption solvent, starring rate, extraction and desorption time were investigated and discussed. Under the optimized extraction conditions, the limits of detection (S/N = 3) of the proposed method were 0.03 and 0.05μg L^{-1}, for of β-sitosterol and cholesterol respectively. Satisfactory linearity was achieved in the range of 0.1–20μg $L^{-1}$for analytes with the correlation coefficients (r) above 0.9975. A method precision was performed by Intra-day and inter-day precisions taste which was achieved for the analysis of β-sitosterol and cholesterol in the range of 1.1–1.9%. This procedure was successfully applied with satisfactory results to the determination β-sitosterol and cholesterol in spiked milk, egg yolk and olive oil samples. The relative mean recoveries of oil samples ranged from 92.0% to 101.0%.

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Paper code: 97

Preparation of Fe_3O_4@silica sulfuric acid/MWCNT-modified electrode for detection of acetaminophen in the presence of ascorbic acid

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Acetaminophen (AC) and Ascorbic acid (AA) plays an important role in human health. At traditional electrodes, AC is oxidized at potentials close to that of AA, resulting in an overlapping voltammetric response. In this work, a carbon paste electrode (CPE) is modified by incorporating Fe_3O_4@silica sulfuric acid/multi-walled carbon nanotubes (MWCNT). The resulted modified electrode is used as a sensitive voltammetric sensor for simultaneous determination AA and AC. The electrode showed efficient electrocatalytic activity in lowering the anodic overpotentials and enhancement of the anodic currents. This electrode is able to completely resolve the voltammetric responses of AA and AC. The effects of potential sweep rate and pH of the buffer solution on the response of the electrode, toward AA and AC, and the peak resolution is thoroughly investigated by cyclic and differential pulse voltammetry (CV and DPV). The best peak resolution for these compounds using the modified electrode is obtained in solutions with pH 4.0. Peak potential separation nearly 350 mV is resulted for two compounds. The modified electrode showed good sensitivity and selectivity. The electrode has very good reproducibility (R.S.D.≤3%), high stability in its voltammetric response (more than two months without any considerable change in response) and low detection limit (0.8 μM) for both AA and AC. The prepared electrode is successfully applied for the voltammetric detection of AA and AC in pharmaceutical preparations.

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Paper code: 107

pH assisted homogeneous liquid-liquid microextraction followed by electrochemical detection on MWCNTs modified electrode for the determination of 4-nitrobenzaldehyde in water samples

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The analysis of nitroaromatic compounds such as nitrobenzene, nitrobenzaldehyde and nitrophenols in natural waters and its effluents has a major reputation for environmental control due to their appearance from a wide range of activities [1]. Recently, so-called switchable hydrophilicity solvents (SHS) have been proposed as possible extraction solvents in liquid-liquid microextraction [2]. Ahmar et al. investigated the behavior of the SHS [3] for the determination of nitroaromatic compounds. In this work, a novel approach is presented to determine 4-nitrobenzaldehyde in water samples. The procedure is based on pH assisted homogeneous liquid-liquid microextraction using a solvent having switchable hydrophilicity and then determination by differential pulse voltammetry at the surface of multi-walled carbon nanotubes (MWCNTs) modified glassy carbon electrode. The extraction technique is based on the use of a water-immiscible solvent (N,N-Dipropylamine) that can be miscible upon the changes of pH of aqueous sample solution. Afterwards, phases separation is induced by the addition of sodium hydroxide. 4-nitrobenzaldehyde as a model compound was extracted from water samples into the N,N-Dipropylamine. Subsequently, the electrochemical behavior of 4-nitrobenzaldehyde has been studied on the MWCNTs modified glassy carbon electrode. Experimental parameters were optimized using a one-factor-at-a-time strategy. Under optimized conditions, a linear range was obtained between 1.5 and 350 μgL^{-1} Also, limits of detection and quantification (at S/N=3) were 0.45 μgL^{-1} and 1.5 μgL^{-1}, respectively. Finally, the performance of the proposed method was evaluated in river water as a real sample.

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Paper code: 117

Ultra-trace determination of thallium (I) in water using TiO_2 nanoparticles prior to its quantitation by ICP-MS

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Nowadays heavy metals such as thallium have received considerable attention owing to their effects in the pollution of the environment [1]. A new method has been developed for the determination of trace amounts of Tl(I) from aqueous solution based on simultaneous sorption and preconcentration with TiO_2 nanoparticles as sorbent prior to its determination by Inductively coupled plasma mass spectrometry (ICP-MS). In this research we use self-made PTFE microcolumn packed with TiO_2 nanoparticles with high specific surface area were prepared using sonochemical synthesis method at high frequency, low intensity and relatively low temperature (75˚C)[2]. The retained metal ions on the microcolumn were eluted with small amounts of a suitable eluent solvent. The optimum experimental parameters for preconcentration of Tl(I), such as pH, volume and flow rate of sample solution, eluent and interfering ions, have been investigated. Under the optimal conditions, the linear range, detection limit and precision (R.S.D., n=5) for Tl (I) were (35 -720 ng L^{-1}), 5.0 ng L^{-1} and 2.3 % respectively. The adsorption capacity of TiO_2 nanoparticles for Tl(I) was found to be 25 mg g^{-1}. The method has been also applied for determination of trace of this element in some environmental water samples and standard reference material with satisfactory results.

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Paper code: 118

Process analysis of chabahar maritime university reverse osmosis desalination plant

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Desalination processes make freshwater from the separation of salt from seawater or brackish water. Seawater (about 97.5% of the total available water), in abundance, constitutes a reliable sustainable source of freshwater, with high potential to fulfil the continuously increasing freshwater demand of the future [1]. Today, main types of desalination processes are used worldwide, Multiple Effect Distillation (MED) and Multi Stage Flash (MSF), Reverse Osmosis (RO) and Electro Dialyses for this porous [2]. Reverse Osmosis is the most widely adopted. It achieves the separation of freshwater through the use of a semi-permeable membrane which allows the passage of water whilst preventing the passage of salts into the permeate stream. Recently Ashkelon seawater reverse osmosis (SWRO) Plant is now featured as a successful model in this filed [3]. The chabahar maritime university desalination plant which its prototype was launched in 1994, currently with two set reverse osmosis membranes (recovery ratio of 50%) is producing fresh water with a capacity of 432±20 m^3/h with TDS of 500±50. In the present work, it is attempting to draw the unit design and to product technical documents of its constituent parts. Also process specifications such as feed water quality and quantity, the amount and quality of the outlet water, pre-preparation and post-preparation processes, etc. are investigated and recorded. Finally, while estimating cost and technical analysis of the process, the strengths and weaknesses of the RO system are compared with the updated RO system, we will have suggestions for increasing the efficiency and quality of producing freshwater. The results indicate that intake seawater with TDS of 28000-34000 is of variable quality and inadequate quantity. The site requires structural and technical improvements to keep up-to-date and work by high efficiency. For post treatment, adding some important minerals, especially magnesium and calcium, is recommended for drinking purposes. And like most plant, sometimes the water consumption increases than the amount of site production. This causes tension in the work of the site, especially the reverse osmosis membrane modules.

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Paper code: 121

Development of a novel Polyacrylonitrile/ metal-organicframework-199 electrospunnanofiber adsorbent for thin film microextraction of Heptachlor and Endosulfan in vegetables and fruits samples

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In this work, electrospun polyacrylonitrile/metal-organic frameworks-199 (PAN/MOF-199) nanofiber film was synthesized and investigated as a novel adsorbent for thin film microextraction (TFME) of heptachlor and endosulfan in vegetables and fruits samples. Some properties of the prepared PAN/MOF-199 nanofiber film, including morphology, structure, wettability, solvent stability and extraction performance were studied systematically. Porous fibrous structure, large surface area, good stability, strong hydrophobicity and excellent extraction efficiency were obtained for the film. Based on the PAN/MOF-199 film, a thin film microextraction-gas chromatography-flam ionization (TFME-GC-FID) method was developed, and the experimental parameters that affected the extraction and desorption were optimized. Under the optimal conditions, the limits of detection (LODs) were in the range of 0.02-17.3 μL^{-1} for the analysis of six aldehydes. Good linearity was achieved with correlation coefficients (R^{2}) being lager than 0.9943. Satisfactory recovery (92 % to 112%) and acceptable reproducibility (relative standard deviation: 2.1 % to 4.3%) were also obtained for the method. The developed TFME-GC-FID method has been successfully applied to the analysis of heptachlor and endosulfanin the in vegetables and fruits samples of lung cancer patients and healthy people.The method possesses the advantages of simplicity, rapidity, cost-effective, sensitivity and non-invasion, it provides an alternative tool for the determination of heptachlor and endosulfan in vegetables and fruits.

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Paper code: 123

Co_3O_4 nanoparticles and multiwalled carbon nanotubes modified carbon paste electrode for determination of gallic acid using electrochemical techniques

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Gallic acid, GA, is one of the main phenolic components found in black tea, grapes, and several other plants [1]. Recently, polyphenols, especially those naturally present in foods, have been a subject of increasing interest due to their biological properties, including anti-inflammatory, antihistaminic, and antitumor activities, scavenging of free radicals, and protecting against cardiovascular diseases [2]. On the other hand, GA is final product of basic hydrolysis of tannic acid present toxic effluents which cause environmental pollution [3]. Therefore, the objective of the work was to develop and apply an efficient simple sensor for rapid adsorptive stripping voltammetric determination of GA at low concentration. For this purpose, Co_3O_4 nanoparticles and multiwalled carbon nanotubes (MWCNTs) modified carbon paste electrode (CPE) was used as a fast and sensitive tool for the investigation of electrochemical oxidation of gallic acid. The study was carried out by using cyclic voltammetry (CV) and differential pulse voltammetry (DPV) techniques. In fact, the electrochemical behavior of Co_3O_4/MWCNTs /CPE was explored utilizing cyclic voltammetry and electroactive surface area (ESA) calculations. Gallic acid was detected over a linear concentration range of 0.05-20 µM by differential pulse voltammetry with correlation coefficient of 0.992. In addition, the values of LOD and LOQ for this method were derived 0.012 and 0.039 µM, respectively. It is interesting to note that the suggested sensor showed an acceptable selectivity toward gallic acid in the presence of some interferent substances, repeatability and long-term stability. Finally, the electrochemical oxidation of gallic acid at the surface of Co_3O_4/MWCNTs/CPE employed efficiently for the voltammetric determination of gallic acid in green and black tea and orange juice.

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Paper code: 126

Introducing a new pH assisted homogeneous liquid-liquid microextraction method based on switchable-hydrophilicity solvents followed by GC-MS for the determination of PAHs in water samples

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Recently, a new group of compounds, namely switchable hydrophilicity solvents (SHSs), has been introduced into the extraction field [1]. In this study, a new pH assisted homogeneous liquid-liquid microextraction method based on SHSs followed by GC-MS detection has been developed for preconcentration and determination of polycyclic aromatic hydrocarbons (PAHs) in water samples. PAHs are important compounds because of their prevalence in the environment [2]. The extraction technique makes use of 150 µL of a water-immiscible solvent (Dipropylamine) that can be solubilized in the aqueous phase (6 mL) using HCl as a reagent. Afterwards, phases separation is induced by the addition of sodium hydroxide. The effects of operational parameters of the extraction were investigated and optimized. Under the optimum conditions, proposed method provided good linearity (1–1000 µg L^{-1}), low limits of detection (0.3 µg L^{-1}) and acceptable extraction repeatabilities (RSD% = 4.3-6.8). Finally, the proposed method allows the determination of the target analytes in different types of natural water samples and acceptable recoveries were obtained.

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Paper code: 128

Study of supported liquid membrane transport of 2,4-Dichlorophenoxyacetic acid (2,4 D) using Nano material as new support

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Dichlorophenoxyacetic acid (2,4D) is one of the most widely used pesticides in agriculture for weeds elimination [1]. This carcinogenic contaminant is very toxic and has hazardous effects on the environment and ecosystem. Recently, supported liquid membrane transport has been applied for determining and treatment of organic pollutants in aqueous samples [2]. The benefits of this approach include availability, low cost, use of conventional solvents, and simple operation [3]. In this work, transport of 2,4 D from aqueous media was investigated using supported liquid membrane and the efficiency of nano materials polyacrylonitrile (PAN) has been studied as a preservative instead of conventional membranes. Optimum feed, membrane and received phase were included of pH = 1 and NaCl 2M, dichloromethane wet nano polymer, pH = 14 and NaCl 2M, respectively. Other transport conditions, such as stirring speed, time, temperature, etc., were optimized and the interference effect has been investigated. Under same working conditions, the transport of 2.4 D showed a significant increase in Nano support compared to the polysulfone.

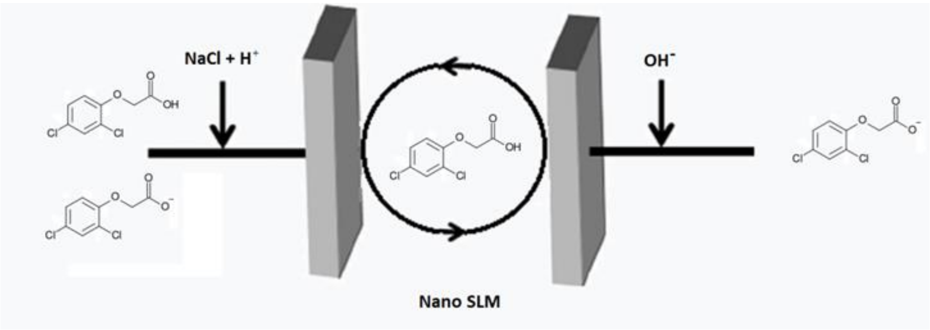

Fig. 1 transport mechanism

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Paper code: 131

Study of facilitated bulk liquid membrane transport of lithium ion from seawater and use of carbon nanotube as additive in membrane

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In this century, lithium and its compounds as most important trace element find many applications such in making ceramics, lubricants, atomic energy, aerospace, pharmaceuticals, and lithium battery [1]. But we must find other potential sources of lithium to compensate for the increasing demand and in the meantime, seawater with estimating amount of 231.2 billion tons of lithium has attracted as suitable alternative source of this element [2,3].

Here, Transport of lithium ion as a valuable and useful metal in major industries was done through a facilitated bulk liquid membrane using 12 crown 4 as carrier. Procedure affecting parameters such pH of the feed and receiving, type of membrane solvent, concentration of carrier, stripping solution conditions, time, temperature were investigated. On the other hand, effect of carbon nanotube as additive of liquid membrane was studied which shown a noticeable increase in the lithium transport process. In the optimum work conditions and after 2 hr, %12 (±0.06) of Li+ from feed phase (containing Li+ = 0.0057 M, NaCl = 0.1 M, pH = 6.2) across a dicholoromethane membrane (12C4 = 0.005 M) was transported into the receiving phase (containing $(NH_4)_2SO_4$ 0.001 M and pH = 6.1). The selectivity of method was evaluated by performing the competitive transport experiments on the seawater simulated mixtures containing Na^+, K^+, $Ca^{2+}$and Mg^{2+} ions with their conservative concentration in seawater.

$$Li^+(sp) \xrightarrow{K_e} Li^+L(mp + CNT) \xrightarrow{K_s} Li^+(sp)$$

Fig. 1 transport mechanism

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Paper code: 150

Magnetic Fe_3O_4/SiO_2 Nanoparticles for Ciprofloxacin Detection in Biological Samples

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Ciprofloxacin, chemically 1,4-dihydro-1-cyclopropyl-6-fluoro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic acid (Fig. 1), is a quinolone antibiotic drug with a broad spectrum of activity against a variety of gram positive and gram-negative bacteria. Several methods have been reported for the quantitative analysis of the ciprofloxacin, such as titrimetry[1], HPLC[2] and AAS[3] methods.

The present work aims to develop a highly sensitive, simple and rapid UV-Vis spectrometric method for application in quality control analysis. This study has been offered a solid phase extraction method based on functionalized magnetic nanoparticles. This method is simple, fast and affordable to extract ciprofloxacin from aqueous solution. Synthesis of functionalized magnetic nanoparticles of iron and sodium hexafluorosilicate is done with the help of co-precipitation method. Detection was performed at 275 nm, the maximum wavelength of ciprofloxacin. In this condition, linear range was achieved in two areas. For low concentrations of 0.1 to 1 and 1-20 (mg/L) for high concentrations were evaluated. The method limits of detection and limits of qualification were 0.0472 and 0.157 (mg/L) for low concentrations and 0.458, 1.52 (mg/L) for high concentrations, respectively. Also in optimal conditions, the concentration of ciprofloxacin in real samples of blood were determined and relative recoveries for real samples were evaluated too.

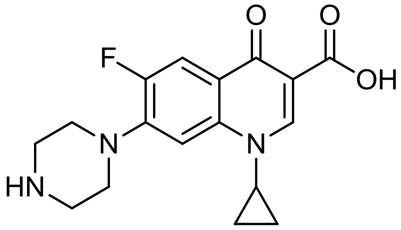

Fig. 1 Molecular structures of ciprofloxacin

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Paper code: 160

Sensitive determination of imatinib in human biological samples by differential pulse voltammetry based on carbon paste electrode modified by MMWCNTs/PAN NFs

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In the present work, the electrochemical oxidation of new generation of anti-cancer drug, imatinib, using by differential pulse voltammetry based on carbon paste electrode modified by MMWCNTs/PAN NFs (MMWCNTs/PAN NFs/CPE) has been reported. The results of a study showed that imatinib provided well-shaped oxidation peak at positive potential of +0.8 V (vs. $E_{Ag/AgCl}$) in the phosphate buffer solution at pH 6.0. The experimental conditions, i.e. pH, modulation amplitude, a modulation time, a step potential, and a scan rate, were optimized, A simple, rapid, selective and sensitive DPV procedure for the determination of imatinib was performed in the concentration range of 1.69×10^{-9} - 4.24×10^{-7} mol/L with the limit of detection (LOD) and the limit of quantification (LOQ) of 3.2×10^{-10} and 1.8×10^{-9}, respectively.

The proposed method with using anodic signal of imatinib at MWCNT/CPE shown comparable detection limit as for boron-doped diamond electrode and hanging mercury drop electrode in the determination of this anticancer drug [1, 2].

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Paper code: 217

Kidney cancer cells monitoring using a novel CNTs-based biosensor

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A facile metal- and enzyme-free nanobiosensor using a glassy carbon electrode (GCE) modified with multiwall carbon nanotubes and zein bio-nanoparticles (GC/ZBN/MWCNTs) has been constructed at low cost. The electrochemical studies were carried out by using cyclic voltammetry (CV), amperometry and linear sweep voltammetry. The results demonstrated improvements in both electrical conductivity and catalytic activity of CNTs as was expected [1] when zein protein was wrapped around them. The sensor provided attractive electrocatalytic performances for sensitive and selective detection of hydrogen peroxide (H_2O_2) within a linear concentration range of 0.049-29.36 µM H_2O_2 with a detection limit of 35 nM H_2O_2 in 0.10 M phosphate buffer (pH 7.2). Moreover, the cytocompatibility of the constructed electrode made it an appropriate nanobiosensor for monitoring the living cancer cells through nanomolar level detection of H_2O_2 [2] as it released from both human dermal fibroblasts (HDF) and renal cell carcinoma (RCC; kidney cancer cell).

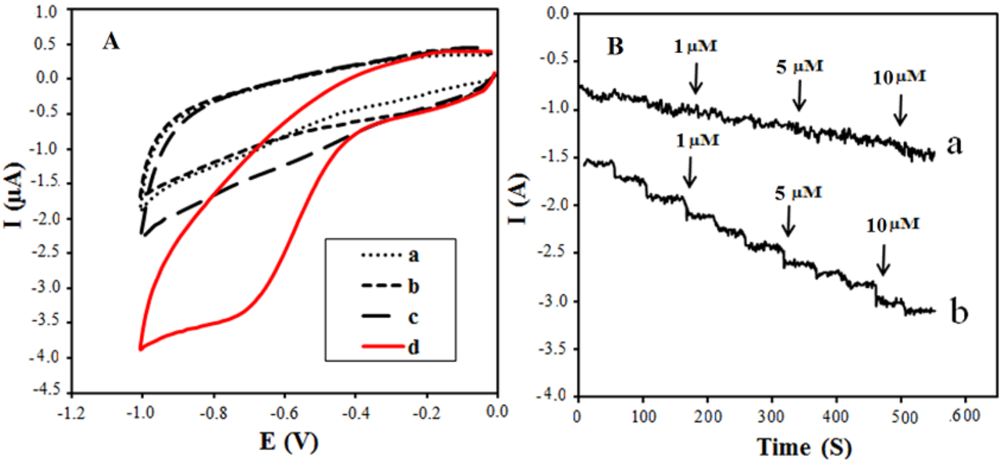

Fig. 1 (**A**), The CVs of a bare GCE (**a**) and the GC/ZBN/MWCNTs (**b**) in the absence of H_2O_2 as well as in the presence (**c** and **d**, respectively) of 5.0 µM H_2O_2. (**B**), The amperometric responses of 1.0-10.0 µM H_2O_2 (pH 7.2) at the surface of (**a**) bare GCE and (**b**) GC/ZBN/MWCNTs.

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Paper code: 221

Study of the electrochemical behavior of Gabapentin at surface of glassy carbon electrode modified by Prussian blue and carbon nanotube

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Gabapentin is a useful drug used to treat seizures and neuropathic pain. It is also can be used for treatment of anxiety disorders insomnia, and bipolar disorder . electrochemical techniques have been proven to be very sensitive to the determination of drugs and related molecules [1]. In this work, Prussian blue (PB)and carbon nanotubes (CN) used as intermediate for electron transfer modified glassy carbon (GC) electrode [2]. Electrochemical properties of the modified electrode showed that electrocatalytic oxidation of Gabapentin were evaluated in comparison with unmodified electrode, the electrode catalytic activity for oxidation of Gabapentin revealed that the (PB-GCM) and(CN-GCM), a large anodic peak appears, indicating that the anodic oxidation of Gabapentin could be catalyzed at (PB-GCM) and (CN-GCM) electrodes. The anodic peak, 110mV for (PB) and 180mV for (CN) displaced to more negative potentials.

The kinetic parameters such as the electron transfer coefficient (α) and the number of electrons involved in the rate-determining step (n_α) for the oxidation of Gabapentin were determined utilizing cyclic voltammetry (CV). Also, diffusion coefficient was estimated used chronoamprommetry.

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Paper code: 243

An electrochemical method for the detection of hydrogen peroxide using glassy carbon electrode modified with Cu/Fe layered double hydroxide@Fe_3O_4 nanoparticles

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Hydrogen peroxide (H_2O_2) is widely used in food, medicine, cosmetics, industry, and water treatment applications [1-2]. It can be toxic at higher concentration because of the oxidizing and corrosive nature. In this work, a novel electrochemical sensor based on Cu/Fe layered double hydroxide@Fe_3O_4 nanoparticles has been successfully fabricated and used to H_2O_2 detection.

The prepared LDH nanocomposite was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), cyclic voltammetry (CV), and differential pulse voltammetry (DPV). Then, the LDH nanocomposite was immobilized on glassy carbon electrode and its electrocatalytic activity for H_2O_2 reduction was studied. Factors which affect the electrocatalytic activity (modifier amount, pH of solution, and analysis time) have been investigated. Under the optimized conditions, the H_2O_2 reduction current was linear to its concentration within the range of 10 – 400 µM, and the detection limit was found to be 3 µM (S/N = 3). Finally, the prepared sensor has been successfully applied to determine the H_2O_2 content in human urine samples.

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Paper code: 261

Electrochemical determination of bisphenol A using a cobalt oxide sensor

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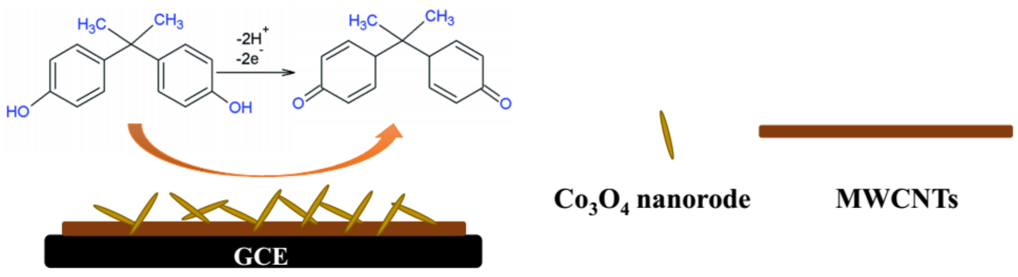
Bisphenol A (BPA), one of the important organic compounds, is widely used in the industrial production such as plastic bottles, baby bottles, children's toys, and also the inner surface coating of cans used for food. BPA exhibits weak estrogenic transcriptional activities and potentially interferes with the endocrine system of both the wildlife and humans. Several analytical methods, have been employed for determination of BPA such as high-performance liquid chromatography, fluorescence, gas chromatography, liquid chromatography-mass spectrometry and electrochemical detection. Among them, electrochemical methods were regarded because fast response, portability, simplicity for operators and low cost.

In this work, we used a laminate nanocomposite based on multiwall carbon nanotubes (MWCNTs) and Co_3O_4 nanorode at the surface of a glassy carbon electrode for BPA detection. The electrooxidation of BPA molecules was monitored by cyclic voltammetry (CV) and differential pulse voltammetry (DPV), It was found that the proposed sensor improves the oxidation of BPA at the modified electrode surface compared to the bare electrode more than ten times. The results of the analyses showed that the fabricated sensor had a good linear range (0.01–100 µM) and a low detection limit (3.1 nM). The obtained results revealed high selectivity of the method which provides determination of BPA in a wide variety of real samples.



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Paper code: 264

Ultrasonic-assisted liquid-liquid microextraction linked deep eutectic solvent for determination of lead using flame atomic absorption spectrometry in water and soil samples

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One of the most important environmental challenges is heavy metals contamination of soil and water sources. Lead is one of the toxic heavy metals and its accumulation in human body even in trace levels leads to serious diseases and disorders such as respiratory and digestive problems, cancer, and cardiovascular failure [1]. Different analytical techniques have been reported for separation/preconcentration of lead. Among them liquid-liquid microextraction techniques have been in the centre of attention due to the short extraction time, low amount of extraction solvent [2]. Green solvents such as deep eutectic solvents are widely applied in recent years. In this study, choline chloride-Urea deep eutectic solvent was synthetized. To this aim, choline chloride and Urea with the mole ratio of (1:2.5) were stirred at 100 °C for 60 min. The synthetized DES was used for extraction of trace amount of lead using Ultrasonic-assisted liquid-liquid microextraction and determined with flame atomic absorption spectrometry. Linear range of 25-500 µg L^{-1} was achieved. The detection and quantification limits were 12.8 and 34.2 µg L^{-1}. The proposed method was successfully applied in water and soil samples.

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Paper code: 265

Modeling the retention behavior of some drugs in high performance affinity chromatography

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The major goal of the present study is to predict retention behavior for a series of drugs such as warfarin, diazepam and ect. in high performance affinity chromatography [1,2]. Multiple linear regression (MLR) was used as variable selection method to investigate the relationship between the selected descriptors and the retention times of the studied drugs.

The molecular descriptors were generated from the molecular structure of drugs and calculated by the DRAGON software. Besides DRAGON descriptors, additional quantum mechanical descriptors were obtained using density functional theory/B3LYP/6-31G method in Gaussian 09 software. By excluding some descriptors with ignorable contributions, components of the QSRR models were simplified. The data set was divided into two groups including training set (21 molecules) and test set (7 molecules). The theoretical modeling of the retention time of studied compounds was established as a function of molecular descriptors by using linear regression method.

The predictive ability of the models was evaluated using cross-validation, Y-randomization and an external test set. The results showed that MLR is a good method for predicting retention times of studied drugs.

The best model is:

$$ret=6.948+(12.656*RNCG)+(1.392*c\text{-}028)-(80.797*R6e)-(1.255*IDDE)$$

Correlation coefficients of the selected model were R=0.982 and R= 0.99 for training and test sets, respectively.

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Paper code: 306

Fabrication of Covalent Organic Framework-based Composite as Advanced Adsorbent for Removal of Cationic and Anionic Dyes from Water

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Many industries give rise to dye-bearing effluents in their production processes. Textile industries, particularly, are major consumers of water and release a fair amount of color in their effluents. Adsorption techniques have been widely applied to the treatment of industrial wastewater [1]. In this work, the porous covalent organic framework-based (COF) composite which its structure was shown in Fig. 1 with superiorchemical stability and large surface area was synthesized. It was used as sorbents for simultaneous removal of harmful anionic and cationic dyes (tartrazine (Tart) and methylene blue (MB)) from aqueous solutions. The adsorption efficiency was followed by UV-Vis spectroscopy. Some methods such as scanning electron microscopy, transmission electron microscopy, X-ray diffraction, FT-IR, dynamic light scattering and zeta potential were used for characterization the adsorbent. The effects of pH and composition of composite on removal efficiency were examined. Higher removal efficiency was obtained at pH=10 for MB and pH=4 for Tart. Fifty percent of COF was selected as optimum composition of the composite. Adsorption kinetics and isotherm parameters were determined from the experimental data.

Two models of first order, second order were used for kinetic and four models of Lungmuir, Freundlich, Temkin and D-R were fitted for isotherms. Based on experimental data removal of Tart was followed by second order and Freundlich model. Also, removal of MB was followed by second order and Lungmuir model. This advanced composite can remove both of cationic and anionic dyes at pH=7 with removal efficiency higher than 99.7% for MB with q_m=151.5 mg/g and 80% for Tart with K_F=24.7 ((mg/g)(L/mg)$^{1/n}$).

The results indicate that this composite adsorbs both MB and Tart efficiently and could be employed as effective adsorbent in wastewater treatment for the removal of cationic and anionic dyes.

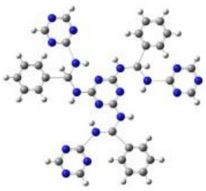

Fig. 1 Structure of covalent organic framework

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Paper code: 324

Simultaneous Voltammetric Measurement of Dopamine, Acetaminophene and Xanthine at a Glassy Carbon Electrode Modified with reduced graphene oxide

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In current work highly sensitive and stable electrochemical sensor for simultaneous detection of dopamine (DA), acetaminophene (AC) and xanthine (XA) is constructed based on the modified GCE with reduced graphene oxide (rGO) [1]. A facile electrochemical method was applied to prepare electrochemically reduced graphene oxide(rGO). The morphology and structure of rGO were characterized by Field-emission Scanning Electron Microscope (FESEM), and X-ray diffraction (XRD).
Cyclic voltammetry (CV), different pulse voltammetry (DPV) and electrochemical impedance spectroscopy (EIS) were used to study the electrochemical properties of the modified electrode. The results indicate that the rGO has excellent electrocatalytic activity for the oxidation ofdopamine (DA), acetaminophene (AC) and xanthine (XA) [2]. Com-pared with the bare glassy carbon electrode (GCE), rGO modified GCE (rGO/GCE) exhibits much higherelectrocatalytic activities toward the oxidation of dopamine (DA), acetaminophene (AC) and xanthine (XA) with increasing of peak currents and decreasing of oxidation overpotentials. Differential pulse voltam-metry results show that, two concentration ranges of 0.1-4.9 and 4.9-150.0 µM for DA, two concentration ranges of 0.4-7 and 7-150.0 µM for AC and two concentration ranges of 0.1-12 and 12-150.0 for XN. The calculated detection limits of the analytes were calculated as 20, 44 and 43 nM for DA, AC and XN, respectively. The proposed modified electrode was successfully used for simultaneous determination of in DA, AC and XN in the human serum and urine samples.
This work provides a simple and green route to construct graphene-basedelectrochemical sensor, which is promising for the simultaneous determination of DA, AC and XA.

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Paper code: 338

Fabrication of nanostructure electrochemical sensor for simultaneous determination of sulfite and nitrite in real samples

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Since nitrite and sulfite have been extensively used and coexist in the ecosystem, resulting in threatening human health and disquieting pollution to the environment, the development of a selective and sensitive method for simultaneous determination of nitrite and sulfite is highly desirable for analytical application [1,2]. In this work, we describe a high sensitive electrochemical sensor for determination of sulfite with present of nitrite using a carbon paste electrode (CPE) modified by NiO nano particles (NiO -NPs) and acetylferrocene (AF). The AF/NiO-NPs/CPE showed good electro-catalytic activity for analysis of sulfite in the range of 5.0 nM-500.0 µM with limit of detection 1.0 nM using differential pulse voltammetric method (DPV). Figure 1 insert show differential pulse voltammograms of sulfite in the presence of nitrite with different concentration of two pollutants. The AF/NiO-NPs/CPE showed two separated oxidation signals with ΔE~310 mV in the solution containing sulfite and nitrite that is sufficient for simulations determination of these pollutants. The present method was successfully applied to the determination of sulfite and nitrite in water samples.

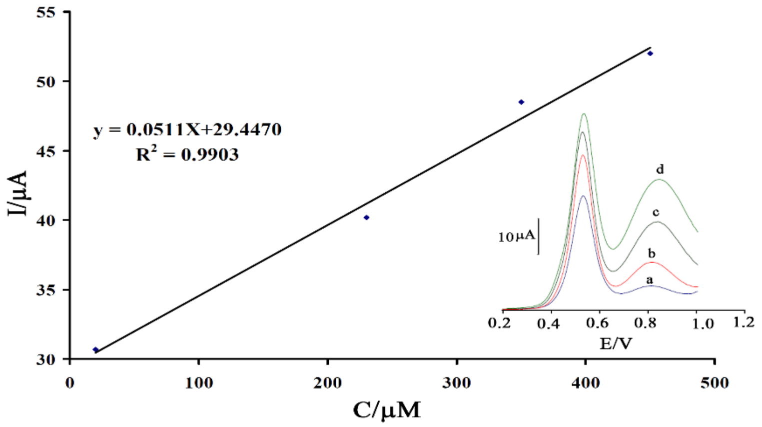

Fig. 1 Differential pulse voltammograms of CPE/NiO-NPs/AF in 0.1 M PBS (pH= 7.0) containing different concentrations of sulfite and nitrite

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Paper code: 372

Synthesis of magnetic MIL-53(Fe) as an efficient sorbent for coextraction and determination of acidic, basic and amphiprotic pollutants

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Phenol, aniline and their derivatives are some of the most important pollutants present in the environment, have become more and more significant due to their high toxicity to natural environments and humans [1]. Owing to their high toxicity, it is crucial to develop a reliable, sensitive, and environmentally friendly method for determination of these pollutants. Nowadays different analytical techniques have been developed for the determination of these compounds by high-performance liquid chromatography (HPLC) [2]. Sample pretreatment and preconcentration step is always necessary prior to mentioned techniques for determination, due to the low concentration of these compounds in real samples [3].

In this study, an easy and fast dispersive micro-solid phase extraction (D-µ-SPE) method was developed for coextraction of target analytes. Magnetic MIL-53(Fe) was synthesized and used as an efficient sorbent in D-µ-SPE method. The synthesis of MOF was confirmed by Fourier transform infrared spectroscopy, X-ray dispersive spectroscopy, thermogravimetry analysis, scanning electron microscopy, transition electron microscopy, vibrating sample magnetometry and X-ray diffraction. The method is easily operated, benefits from good reproducibility values, low detection limit with wide dynamic linear range, and acceptable extraction recovery. Due to the magnetic property, the phase separation was convenient and rapid for D-µ-SPE procedure.

The opted conditions were: pH of the sample, 5; MOF amount, 20 mg; sorption time, 8 min; salt concentration, 15% w/v; sample volume, 20 mL; type and volume of the eluent, acetonitrile, 130 µL; elution time; 2 min. Under the optimum conditions detection limits and linear dynamic ranges were obtained in the range of 0.03-0.2 µg L^{-1} and 0.1-2000 µg L^{-1}, respectively. The percent of extraction recovery and relative standard deviations (n = 5) were in the range of 39.5-93.34 and 3.5-12.6, respectively. Eventually, the synthesized magnetic MOF was successfully applied for the coextraction and determination of target analytes in various water samples with satisfactory results.

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Paper code: 390

Multivariate optimization approach for Cu(II) ions selective extraction from a mixture of six metal cations via benzyl bis(thiosemicarbazone)

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Copper(II) ion is an environmental contamination, which has been tested and assessed over the past few years from both the toxicological and human health viewpoints [1]. It has been well reported that the accumulation of copper in human body causes brain, skin, pancreas and heart diseases [2]. Therefore, various methods for the recovery of Cu(II) ions from the aqueous solutions have been used.

The main aim of this work is to investigate the competitive extraction of Cu(II) ion from an aqueous solution containing Mn(II), Co(II), Ni(II), Cu(II), Zn(II) and Pb(II) metal cations using benzylbis(thiosemicarbazone) **(I)** as carrier. Taguchi design approach for screening and central composite design (CCD) for optimization was carried out and optimum conditions were determined. Under the optimal conditions, Cu(II) ions were extracted of 93.35% from the mixture of six metal cations solution, and other cations remained in source aqueous phase (Fig. 1).

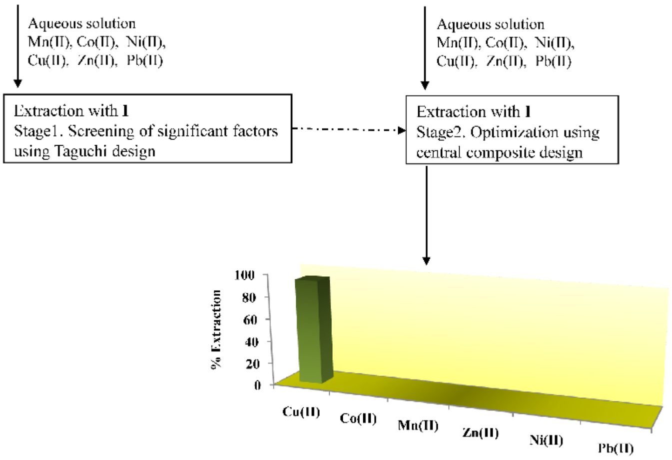

Fig. 1 The result of competitive extraction of six-metal cations in optimum condition.

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Paper code: 391

Preparation of polypyrrole/TiO2 nanocomposite via surface molecular imprinting technique and its photocatalytic activity under UV irradiation

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In this work a novel nanocomposite photocatalyst using molecularly imprinted polymer (MIP) technique for the detection of chloroquine phosphate was developed. The chloroquine phosphate imprinted polymer / TiO2 photocatalyst was prepared under the optimal conditions. Polypyrrole was synthesized chemically using ferric chloride (III) as oxidant. A Plackett-Burman design (PBD) was chosen as a screening method to estimate the relative influence of the factors that could have an influence on the analytical response (absorbance). The significant variables were optimized using central composition design (CCD). Under the optimized conditions, the calibration curve demonstrated linearity over a concentration range of 1×10^{-7} to 1×10^{-4} M of chloroquine phosphate with $R^2=0.9950$. The detection limit of chloroquine phosphate was obtained 3.8×10^{-8} M ($3s_b$, n=6) with a highly reproducible response (RSD 3.24%, n=4).

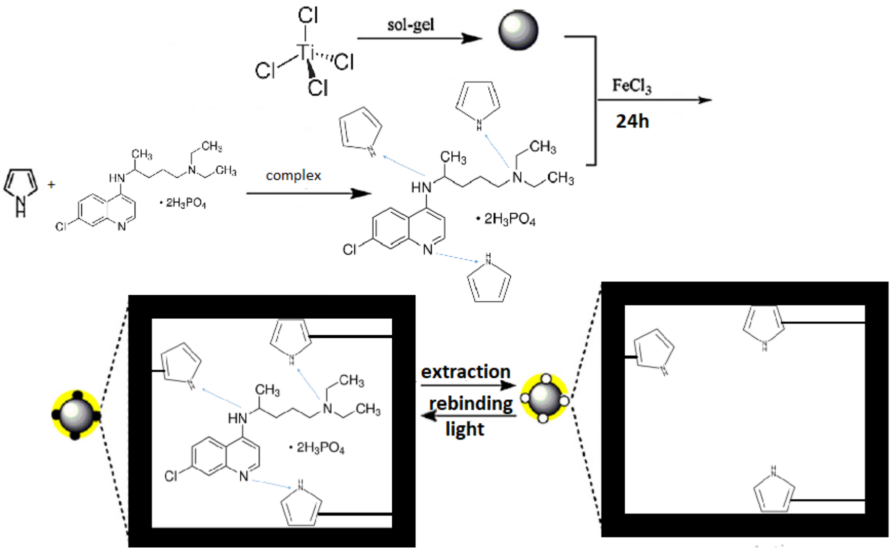

Fig. 1 The route for preparation of MIP-PPy/TiO2 photocatalysts.

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Paper code: 398

Computational design of a molecularly imprinted electrochemical sensor for determination of amlodipine via multivariate optimization technique

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This study reports the design and evaluation of a new electrochemical sensor based on the molecular imprinting technique to overcome the amlodipine (AML) quantification problems in complex real matrix. In this regard, density functional theory (DFT) calculations [1] were employed to select the most suitable imprinting system for AML quantification technique, which encompassed pyrrol (PY) as functional monomer and water as polymerization solvent. The molecularly imprinted polypyrrole film capable of selectively recognizing AML was successfully synthesized by electropolymerization technique on the pencil graphite electrode (PGE) modified by multi-walled carbon nano-tubes (MWCNTs) [2]. The molecularly imprinted polymer (MIP) film was tested for AML rebinding and differential pulse voltammetry (DPV) was utilized to record the oxidative current signal of AML. Multivariate optimization methods such as Plackett–Burman design (PBD) and central composite design (CCD) were employed to predict the optimum conditions controlling the performance of the MIP sensor. Under optimized conditions (Fig. 1), the MIP electrochemical sensor showed high sensitivity with a linear response from 5 nmol L^{-1} to 0.2 mmol L^{-1} of AML and a limit of detection of 1.5 nmol L^{-1}. Moreover, the designed sensor exhibited long-term stability (36 days), good repeatability (RSD 5.3%), reproducibility (RSD 3.4%), and sensitivity toward AML determination in pharmaceutical and human serum samples.

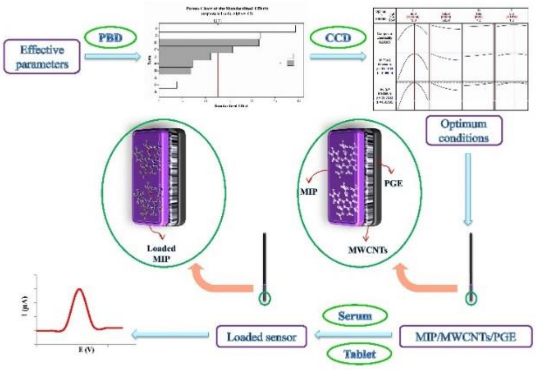

Fig. 1 Synthetic protocol for MIP development at the surface of MWCNTs-COOH modified PGE under optimized conditions for AML quantification in pharmaceutical and serum samples.

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Paper code: 400

Development of new nanocomposite based on Polyoxomolibdate nanoclusters/Graphene oxide as an efficient sorbent for solid-phase microextraction: Application in MDMA screening

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The 3,4-Methylenedioxymethamphetamine (MDMA) is a commonly used recreational drug known as “ecstasy”, which is frequently encountered in postmortem toxicology laboratories [1]. In contrast to methamphetamine, it has a methylenedioxy substituent on the phenyl ring, which results in distinctive psychoactive properties. MDMA, itself a popular drug of abuse in the 1960s [2]. A highly porous nanocomposite of chitosan/ polyoxomolibdate nanocluster/Graphene oxide was prepared for use in headspace solid-phase microextraction (HS-SPME) of MDMA as a model of abused drug. The highly porous chitosan/ polyoxomolibdate nanocluster/Graphene oxide nanocomposite is found to be capable of efficiently extracting MDMA from biological complicated sample. The nanomaterial was immobilized on a stainless-steel wire for fabrication of the SPME fiber. Following thermal desorption, the MDMA were quantified by IMS. The new nanocomposite coating offers good mechanical and thermal stability and high extraction efficiency due to its large specific surface. The SPME conditions such as temperature, pH, and concentration of NaCl and extraction time were optimized with the aid of central composite design through response surface methodology. The limits of detections range from 0.12 ng mL^{-1}, and the calibration plots are linear within the 0.27–400 ng mL^{-1} concentration range. The method was successfully applied to the extraction and determination of MDMA in plasma, urine and hair samples. Under optimized conditions, the repeatability for one fiber (n=3), expressed as the relative standard deviation, is 5.2 %. The method is simple, rapid, and inexpensive. The thermal stability of the fiber and the high relative recovery make this method superior to conventional methods of extraction.

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Paper code: 406

Urea-based porous organic polymer/graphene oxide hybrid as a highly efficient sorbent for bovine serum albumin

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In this work, a porous organic polymer (POP) was prepared via the reaction of *tetrakis*(4-aminophenyl)methane and 1,4-Phenylene diisocyanate [1]. The polymer was then combined with graphene oxide (GO) [2], to prepare POP/GO as a novel and highly efficient sorbent for pre-concentration and extraction of serum albumin samples, the most abundant protein in plasma [3], prior to spectrophotometric determination.
Parameters which influence the extraction efficiency such as the amount of the adsorbent, pH of sample solution, ionic strength, adsorption and desorption time were investigated and optimized. Detection limit of the method 0.068 mg L^{-1} and determination coefficients (R^2) of 0.9991 were obtained. The intra- and inter-day was calculated with five replicates in the same day and seven consecutive days, respectively. Intra-day and inter-day precisions were 1.7% and 5.9%, respectively. The maximum sorption capacity was 357.1 mg g^{-1}. The proposed method was demonstrated to be sensitive enough for determination of serum albumin from bio-samples.

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Paper code: 423

Synthesis of graphitic carbon nitride nanosheet and its application for determination of 2-Mercapto benzo thiazole by resonance riley scattering technique

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In this study (research), nanosheets of graphite carbon nitride are synthesized by thermal method and optical properties and fluorescence intensity are investigated. In the following, these nanosheets are analyzed with a transmittance electron microscopy(TEM). After that, the fluorescence intensity of synthesized nano plates in the presence of 2-mercaptobenzotiazole is examined and the combination is expected to increase the floristic intensity of the nanoplated due to the presence of a sulfur substrate. In the following, various variables affecting the interaction of 2-mercaptobenzotiazole and nanoplates are investigated. So, by finding optimal values, the best fluorescence sensor response range is plotted relative to the amount of 2-mercapto benzotiazole.

At the end, a system designed to accurately measure the amount of 2-mercaptobenzotiazole in real samples such as tab water and ... is being tested.

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Paper code: 425

Colorimetric determination of Formaldehyde based on localized surface plasmon resonance of gold nanoparticles

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The development of sensitive colorimetric sensors has become widely popular, due in part to their simplicity, rapidity; precision and common availability of the basic equipment in laboratory and field uses [1]. In this area, noble metal nanoparticles (NPs) have fascinated scientists because of their physico-chemical properties and potential applications in different areas such as catalysis, electronics, plasmonics, biotechnology, and so on. Among these nanoparticles, gold and silver nanoparticles have drawn much research attention because of their various promising properties [2]. These properties of nano particles, which give rise to localized surface plasmon resonance (LSPR) absorption and scattering, can be used in the development of analytical methods such as optical sensing and detection [1-3].

Formaldehyde (CH_2O) is the most common aldehyde in the environment and its application covers a wide range. Formaldehyde (FRD) is considered one of the most significant industrial hazards and air pollutants. So, determination of FRD is very important [4].

In this work a new simple and sensitive method for the determination of FRD is proposed. The method is based on the reaction of FRD with an oxidizing agent (gold ion) and preparation of gold nanoparticles (Au NPs). The intensity of LSPR of Au NPs was monitored spectro photometrically at the maximum wavelength of 530 nm vs. time. With the increase of FRD concentration, the LSPR spectrum intensity of formed Au NPs was increased, and the enhanced intensity of LSPR was linearly proportional to the FRD concentration. There is a linear relationship between absorbance intensity of AuNPs and the concentration of FRD over the range of 0.01-0.40 µg mL^{-1}(n=16) at 530 nm. The detection limit was 0.003 µg mL^{-1}. Finally, the proposed method has been successfully applied for the determination of FRD in different water samples.

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Paper code: 428

Removal of Brilliant green dye from aqueous solution using Au-Fe_3O_4, B cyclodextrin nanocomposite as a novel sorbent

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Removal of polluting dyes from the effluents of dyeing industries before their discharge into environment is a recommended step to reduce their hazardous effect [1]. Several techniques were applied for the treatment of industrial wastewaters. One of the most effective techniques is adsorption since it is easy, inexpensive can treat concentrated dyes and the spent sorbent can be regenerated for further use [2].

In this work reports preparation Au-Fe_3O_4, β cyclodextrin nanocomposite as a sorbent and their application for a cationic dye (Brilliant green) removal from aqueous solutions. The composition, morphology and structure of Au-Fe_3O_4, β cyclodextrin nanocomposite were characterized by FTIR, SEM and EDX. Adsorption experiment was carried out under various conditions. Analysis of the adsorption data was performed using Langmuir, Freundlich and Temkin models. The results indicated that the adsorption system showed excellent correlation with the Langmuir isotherm model R^2(0.9999).

Adsorption of brilliant green onto the nanocomposite follows pseudo-second order rate kinetics. The thermodynamic parameters ΔH°, ΔS° and ΔG° calculated from the temperature-dependent adsorption isotherms suggested that the adsorption isotherms process of brilliant green on synthesis nanocomposite was spontaneous and endothermic. The maximum adsorption capacity of the nanocomposite for BG dye were determined 111.1 mg/g. Overall, the simple synthesis, low cost, highly-effective and stability in aqueous phase features enable prepared nanocomposite as excellent candidates to adsorptive removal process. The results of regeneration experiments confirmed that excellent recyclability of the nanocomposite has excellent potential application in BG adsorption.

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Paper code: 432

Colorimetric determination of fexofenadine by citrate-capped silver nanoparticles after extraction by molecularly imprinted polymer

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In this work, we describe a selective and sensitive colorimetric method for the extraction and determination of fexofenadine (FEXO) in biological samples. The proposed method combines the benefits of a molecularly imprinted polymer (MIP) for selective sample clean-up and preconcentration with a sensitive colorimetric assay based on citrate -capped silver nanoparticles (AgNPs) probes. The MIP was successfully synthesized by a chemical method using pyrrole (PY) as monomer and FEXO as a template. The template molecules were removed by ethanol /water solution (3:1, v/v) and this solution was selected as the extraction solvent .In this two-step the analyte (FEXO) was isolated from the matrix by MIP .The extraction solvent containing the FEXO molecule is then transferred to aqueous dispersion of citrate-capped AgNPs.The interaction between amino groups of FEXO and citrate-capped AgNPs induces rapid aggregation of AgNPs accompanied by a naked-eye visible color change,resulting in precise quantification of FEXO that can be detected by a UV-visible spectrophotometer. This aggregation decreases original absorbance of Ag NPs at 392 nm and appear a new absorption band above 522 nm. Several significant parameters controlling the performance of the MIP and colorimetric method were examined and optimized using multivariate optimization method. Plackett–Burman design (PBD) and central composite design (CCD) were used for optimization step. Under the selected optimal conditions, the absorbance intensity ratio (A_{522nm}/A_{392nm}) is correlated with the FEXO concentrations over the range of 0.05-5 μM and the detection limit is 25nM.

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Paper code: 456

Application of dispersive liquid phase microextraction followed by corona discharge-ion mobility spectrometry for determination of pramipexole

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Pramipexole is a medication using in treatment of Parkinson's disease and restless legs syndrome. High performance liquid chromatography (HPLC) is frequently used for determination of pramipexole in different real samples [1,2]. Ion mobility spectrometry (IMS) is a fast, sensitive and inexpensive technique used in pharmaceutical analysis [3]. This method can be applied as an alternative method for HPLC.

Analysis of pramipexole in the complex real samples need to a proper sample-preparation method. Microextraction methods can be considered as convenient and reliable methods for reaching this goal. This communication intends to describe a dispersive liquid phase microextraction method, assisted with a homogenizer, for extraction-preconcentartion of pramipexole from aqueous samples followed by its determination by ion mobility spectrometry (IMS). Figure 1 shows an ion mobility spectrum of pramipexole. Different parameters affecting the efficiency of the method like solvent type, stirring rate, ionic strength and stirring time have been evaluated and optimized. Analytical performances of the method were evaluated under optimized conditions. The linearity range of the method was found to be 50-1000 ng/mL with a limit of detection of 18 ng/mL. The method demonstrated adequate precision with relative standard deviations (RSDs) lower than 7.1%. Finally, method was successfully used for determination of spiked pramipexole in different real samples including urine, plasma and pharmaceutical samples. The relative recoveries of pramipexole ranged from 82 to 107 %.

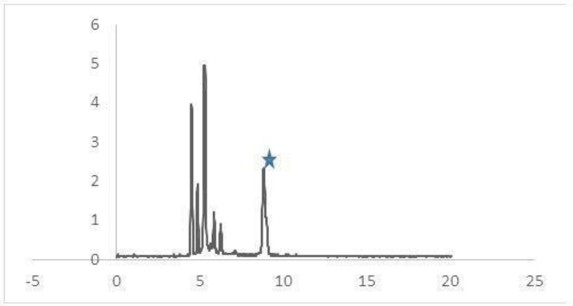

Fig. 1 Ion mobility spectrum of pramipexole.

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Paper code: 458

Lactose intercalated layered double hydroxide as a green sorbent for efficient and selective removal of heavy metals from aqueous solution

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In recent years, layered double hydroxides (LDHs) have shown a remarkable potential for effective removal of heavy metals owing to their large surface area, high anion exchange capacity and good thermal stability [1]. This study represents the efficient removal of heavy metals from aqueous solution by layered double hydroxide intercalated with biomolecule as a green and economical sorbent. The Lactose (LA) was intercalated into copper-aluminium layered double hydroxide (CuAl-LA-LDH) to produce an adsorbent which indicates highly selective and extremely efficient removal of heavy metal such as Hg^{+2} and Pb^{+2}. LA-LDH was prepared using the co-precipitation method. The structure of sorbent was investigated using X-ray diffraction, scanning electron microscopy, Fourier transform infrared, Brunauer-Emmett-Teller, Barret-Joyner-Halenderm and transmission electron microscopy. To extract the analytes, 20 mg of sorbent was added into 20 mL of the solution containing certain concentrations of heavy metals. The mixture was stirred for 1 h at a constant temperature of 25 °C. After extraction of the ions at equilibrium time, the sorbent was setteled by centrifugation. The metal ions concentrations in the supernatant solutions were determined using ICP-AES. Sorption isotherm for Hg^{+2} and Pb^{+2} agrees with the Langmuir model suggesting a monolayer adsorption and maximum adsorption capacity was 303.0 mg g^{-1} for Hg^{+2} and 322.6 mg g^{-1} for Pb^{+2}. The sorption kinetics for mentioned ions follows a pseudo-second-order model, suggesting a chemisorption process. The results were shown that the sorbent has high capability to remove heavy metals from aqueous solutions.

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Paper code: 479

Development of magnetic solid phase microextraction method for the determination of Diclofenac drug

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In this research, magnetic solid phase microextraction is used as a sample preparation method for separation and preconcentration of diclofenac drug which was finally analyzed by UV-Vis spectrophotometry. By covalently linking dialdehyde starch and amine functionalized Fe3O4 nanoparticle, and modifying with arginine amino acid functional group, the novel monodisperse nano-composite has been successfully synthesized without any toxic crosslinking agent.

The effective parameters, such as sample volume, salting effect, pH, surfactant amount and sorbent amount, desorption and extraction time were optimized with the aid of response surface methodology (RSM) and experimental design. [1,2]. Factors including; pH, sample volume and salting effect had the greatest effect on the process. The optimum conditions for these parameters were 2.20,13 mL and 7.42% respectively. The limits of detection was 0.039 mgL^{-1} Under the optimized conditions, the pre-concentration factors are 148.

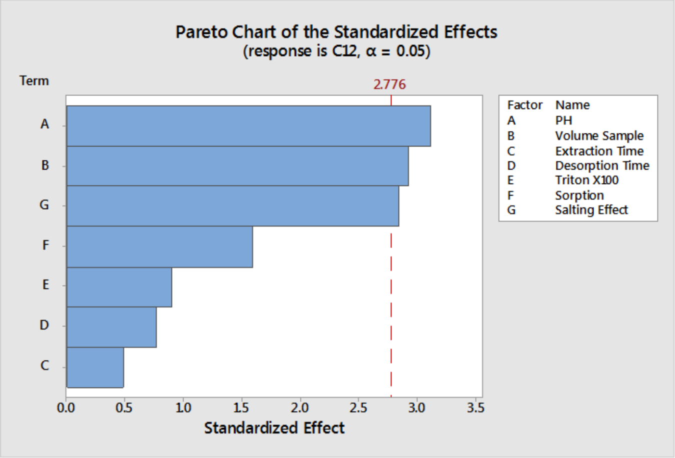

Fig. 1 The standardized main effects Pareto chart for experimental design

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Paper code: 506

New glassy carbon modified electrode with MXene/ZnO for electrochemical measurement of bilirubin

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Bilirubin is the yellow-orange bile pigment found in blood, mostly bound to the plasma protein albumin. Bilirubin is an important serum biomarker used in clinical medicine for assessing hemolysis, hepatic function and cardiovascular risk [1]. This molecule originates from the degradation of the heme moiety in hemoglobin, other hemoproteins, such as cytochromes, catalase, peroxidase and tryptophan pyrrolase, and free heme. Higher and lower concentrations of bilirubin are associated with certain diseases. For instance, jaundice, caused by high bilirubin levels in the blood, is associated with gallbladder and liver diseases (e.g., cirrhosis, hepatitis), blood infection, transfusion reaction or haemolytic diseases of the newborn (cell destruction). Conversely, low levels of bilirubin are associated with anaemia and coronary artery diseases [2]. Therefore, to know the treatment and study of the mechanism of these disease determinations of bilirubin in biological fluids can be of analytical interest. Among many techniques, electrochemical techniques as alternative methods have also received much interest due to their higher selectivity, faster and simple operation, lower cost, quick response, and therefore, have become of considerable importance for determination of analytes. Carbon electrodes such as glassy carbon electrode (GCE) and carbon paste electrode (CPE) possess many advantages including low fabrication cost, wide accessible potential window, chemical and electrochemical stability so that, in many cases, these electrodes are superior with respect to other electrodes [3]. In order to improve their electrochemical performance, glassy carbon electrodes have been modified with nanosized materials. In this paper, MXene/ZnO nanocomposite based electrochemical sensor was fabricated for the determination of bilirubin. Electrochemical studies were carried out by using cyclic voltammetry (CV), Differential pulse voltammetry (DPV) and chronoamperometry (CHA). The DPV data showed that the obtained anodic peak currents were linearly dependent on the bilirubin concentrations in the range of 0.1–600.0 µM, with the detection limit of 0.05 µM. The prepared electrode was successfully applied for the determination of bilirubin in real samples. Moreover, the modified electrode exhibited excellent stability and reproducibility.

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Paper code: 507

A novel MXene(Ti_3AlC_2)/ZnO nanocomposite modified glassy carbon electrode for rapid voltammetric detection of bisphenol A

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Bisphenol A (2,2-bis (4-hydroxyphenyl) propane, BPA) is an organic compound that widely used in the plastic industry as a monomer for producing epoxy resins and polycarbonate. BPA is ubiquitous since it can be released into the environment from bottles, packaging, and landfill leachates as well as plastics plants. BPA was non-biodegradable and highly resistant to chemical degradation, so that the concentration of BPA in the environmental is frequently high [1]. BPA is postulated to cause reproductive disorders including decrease of sperm quality in humans, birth defects due to its fetal exposure and various kinds of cancers, such as breast, testicular, and prostate cancer [2]. Therefore, a method with high sensitivity, short analysis time, low energy consumption and low-cost equipment is required to detection BPA [3]. Glassy carbon electrode (GCE) possess many advantages including higher electron rate transfer, wide accessible potential window, low fabrication cost. That for improve sensor electrochemical performance, glassy carbon electrodes have been modified with nanosized materials. In this paper, MXene(Ti_3AlC_2)/ZnO nanocomposite based electrochemical sensor was fabricated for the determination of BPA, which is very important in the clinical diagnosis. Electrochemical studies were carried out by using cyclic voltammetry (CV), differential pulse voltammetry (DPV) and chronoamperometry (CHA). The results demonstrated an enhancement of the corresponding anodic currents measured after modification of the GCE. These results are beneficial for real sample analysis. The sensor worked linearly in the range of 0.1-50.0 μM and had a detection limit of 0.07 μM. The experiments illustrate that MXene(Ti_3AlC_2)/ZnO nanocomposite is a worthy electrode material which offers a large surface-to-volume ratio and improves the sensitivity.

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Paper code: 508

Application of dispersive liquid phase microextraction followed by corona discharge-ion mobility spectrometry for determination of pramipexole

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Pramipexole is a medication using in treatment of Parkinson's disease and restless legs syndrome. High performance liquid chromatography (HPLC) is frequently used for determination of pramipexole in different real samples [1,2]. Ion mobility spectrometry (IMS) is a fast, sensitive and inexpensive technique used in pharmaceutical analysis [3]. This method can be applied as an alternative method for HPLC.

Analysis of pramipexole in the complex real samples need to a proper sample-preparation method. Microextraction methods can be considered as convenient and reliable methods for reaching this goal. This communication intends to describe a dispersive liquid phase microextraction method, assisted with a homogenizer, for extraction-preconcentartion of pramipexole from aqueous samples followed by its determination by ion mobility spectrometry (IMS). Figure 1 shows an ion mobility spectrum of pramipexole. Different parameters affecting the efficiency of the method like solvent type, stirring rate, ionic strength and stirring time have been evaluated and optimized. Analytical performances of the method were evaluated under optimized conditions. The linearity range of the method was found to be 50-1000 ng/mL with a limit of detection of 18 ng/mL. The method demonstrated adequate precision with relative standard deviations (RSDs) lower than 7.1%. Finally, method was successfully used for determination of spiked pramipexole in different real samples including urine, plasma and pharmaceutical samples. The relative recoveries of pramipexole ranged from 82 to 107 %.

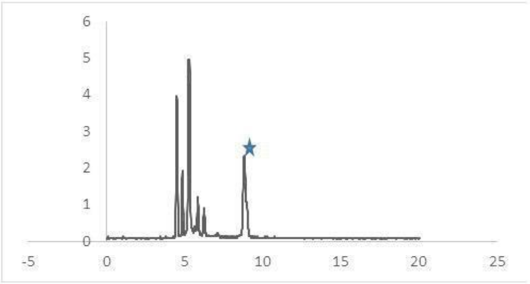

Fig. 1 Ion mobility spectrum of pramipexole.

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Paper code: 513

Electrodeposition of carbon nitride nanosheets on the graphanized pencil lead as an effective SPME fiber for extraction of PAHs in edible samples

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This study introduces a green, cheap, easy to prepare and powerful SPME sorbent for environmental monitoring applications. Here, graphitic carbon nitride (g-C_3N_4) nanosheet has been prepared on graphenized pencil lead (GPL) as a sorbent by one-step electrochemical reduction for the first time. Carbon nitride (CN) is a kind of metal-free polymer with many advantages, such as non-toxic nature, high stability, low cost, suitable band structure and easy preparation [1]. Graphitic carbon nitride (g-C_3N_4: as an analogue of graphene) has attracted many interests recently. It can be as the best candidate to complement carbon materials [2]. It had been reported as a new sorbent for the extraction or removal of metal ions and aromatic compounds with high sorption capacity [3]. GPL not only serves as fiber platform for g-C_3N_4, but also significantly enhances the immobilization of g-C_3N_4 by π-π interaction, also significantly enhances the adsorption ability of g-C_3N_4 (~2 times); additionally. Moreover, due to the study of adsorption capacity of g-C_3N_4, the PAHs as model analytes were chosen. After SPME procedure, the extraction phase was injected to HPLC-UV for determination of PAHs. The prepared fiber with g-C_3N_4 green sorbent has been showed the ultrasensitive and rapid detection of with a wide linear range. In addition to, the real samples analysis showed satisfactory recovery.

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Paper code: 514

Fabrication and characterization of polyaniline nanotubes/silver composite for the electrochemical sensing of anticancer drug, 5-Fluorouracil

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A polyaniline nanotubes/silver composite (PANINTs@AgNPs) was prepared through a simple one-step method without using any extra acid, reducing agent, and template [1]. The as−prepared nanocomposite characterized by Field Emission Scanning Electron Microscopy (FESEM), size distribution diagrams and X−ray diffraction. The resultant nanocomposite not only possessed high specific surface area but also exhibited good stability and durability. The study was explored using the Taguchi experimental design method and the results were confirmed by the ANOVA [2]. We weigh 0.002 mg of the silver-polyaniline nanotube composite added with HCl (10 ml). The solution was sonicated for 10 min to achieve homogeneous suspension. We select the potential range of (-0.2 to 0.10 V), and the number of cycles of 20. The nanoscale is reduced by the electrode surface. The designed sensor could detect 5- Fluorouracil (5-FU) in the dynamic linear range from 20 µM to 380 µM, with a low detection limit of 0.06 µM (S/N=3). Additionally, the fabricated sensor showed excellent selectivity and acceptable sensitivity. The satisfactory results in analysis of human serum samples indicated that it had potential application in clinical monitoring of 5-FU.

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Paper code: 522

Electrochemical Oxidation of 3,4-Dihydroxycinnamic acid in the Presence of Barbituric Acids Derivatives

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Electrochemistry provides a versatile means for the selective reduction and oxidation of organic compounds. The importance of an electrochemical synthesis lies not only in the selectivity of the reaction but also in the formation of electrons at the electrode surface. Since the electrons are reagent-free, pollution of the environment by spent reagents can be avoided [1]. Recently, we have dealt with the electrochemical oxidation of catechols and 1-(4-(4-hydroxyphenyl)piperazin-1-yl)ethanone in the presence of nucleophiles in aqueous solution. Our previous studies show that the electrochemically generated *o*-quinone and *p*-quinone imines are reactive intermediates and as a Michael acceptor, participate in different types of reactions [2,3]. On the other hand, barbituric acid derivatives are well known to possess antibacterial, sedatives, herbicides, fungicides and antiviral agents [3]. However, until now, no report has been published about the electrooxidation of 3,4-Dihydroxycinnamic acid **(1)** in the presence of barbituric acid derivatives. In this work electrochemical oxidation of 3,4-Dihydroxycinnamic acid (**1**) has been studied in the presence of barbituric acid (**3a**) 1,3-dimethylbarbituric acid (**3b**) and 2-thiobarbituric acid (**3c**) as nucleophiles (Fig. 1).

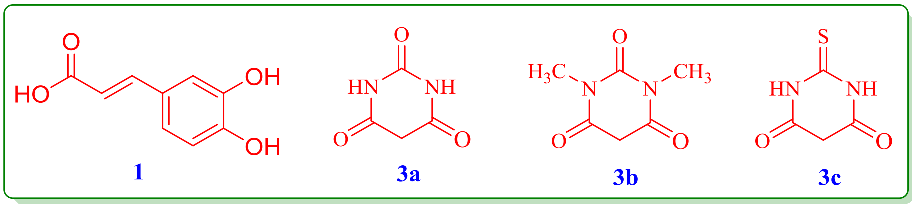

***Fig. 1**.*

Some electrochemical techniques such as: cyclic voltammetry using diagnostic criteria derived by Nicholson and Shain for various electrode mechanisms and controlled-potential coulometry were used. The results indicate that the electrochemically generated *o*-quinone participate in Michael-type addition reaction with barbituric acids (**3a–c**) *via* ECECE mechanism and convert to the different barbituric acid derivatives with good yield under controlled potential conditions, at carbon electrode.

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Paper code: 523

Electrochemical evidences in Drug-Drug interaction of acetaminophen with the Duloxetine and Fluvoxamine

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Acetaminophen (**1**) is used worldwide for its analgesic and antipyretic properties. It is widely available and present in many prescription and non-prescription medications. It is an attractively alternative drug for children and people who are sensitive to aspirin [1]. Recently, we have dealt with the electrochemical oxidation of acetaminophen and 4-(Piperazin-1-yl)phenols in aqueous solution [2,3]. The oxidation of these compounds is followed by many chemical reactions such as hydrolysis, hydroxylation, and/or dimerization reaction [2, 3]. In this work with the aim of obtaining information about drug-drug interaction (DDI) we studied the electrochemical oxidation of acetaminophen (paracetamol) in the presence of Duloxetine and Fluvoxamine (**3a,3b**) (Figure 1) by means of cyclic voltammetry and Controlled-potential coulometry.

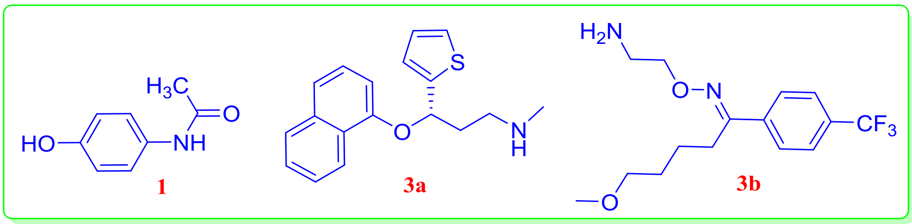

Fig. 1.

Our results indicate the participation of electrochemically generated *p*-quinone imine (NAPQI) produced from electrooxidation of acetaminophen in Michael-type addition reaction with **3a,b**. This reaction cause to reduce the concentration of NAPQI and decreases the effective concentration of these drugs. We would like to report a simple electrochemical procedure on the drug-drug interaction between acetaminophen and **3a,b** and synthesis a new product of electrooxidation of acetaminophen in the presence of Fluvoxamine (**3b**) *via* ECECE mechanism under controlled potential conditions at biological pH and carbon electrode.

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Paper code: 524

Inhibition activity modeling of CINPA1 analogs as novel inverse agonists of constitutive androstane receptor

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In biological research, increasing the effectiveness of anticancer drugs and attenuating multi drug resistance are of prime importance. In this study, a combination of docking-quantitative structure activity relationship (QSAR) methods is implemented for modeling and predicting inhibition activity of CINPA1 analogs as novel inverse agonists of constitutive androstane receptor (CAR). We also proposed novel agents for inhibiting the CAR activity considering the QSAR results. The optimal ligands conformation as well as their position and orientation within active site were obtained from docking and were used for calculating molecular descriptors and investigation of different interactions in CAR ligand binding domain.

The data set containing 50 molecules with known pIC_{50} was divided into training and test sets, each including 40 and 10 molecules, respectively. Binary version of gravitational search algorithm (GSA) and bayesian regularization based neural networks (BRANN) were applied to develop a predictive model using the most informative descriptors regarding the ligand binding positions. This analysis revealed that hydrophobic interactions, number of nitrogen atoms and cation-π interactions play important roles in the CAR inhibition activity of the agents.

The results of external validation and internal cross-validation tests in conjunction with Y-randomization confirm the predictive ability, robustness and effectiveness of the generated model. This study shows that a combination of molecular docking and QSAR modeling are effective tool for characterization and synthesis of the potent inhibitors.

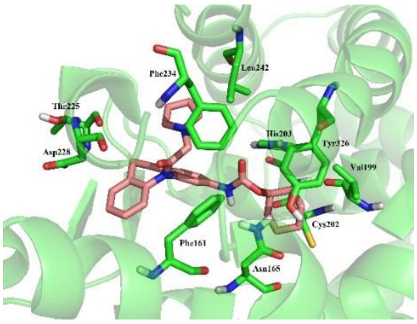

Fig. 1 Residues involved in the interaction of the most potent inverse agonist of dataset with CAR.

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Paper code: 525

An electrochemical sensor for the determination of Cd(II) using a modified gold electrode with organic-inorganic hybrid polyoxotungstate

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Currently, environmental pollution by heavy metals is a global problem. Therefore, it is crucial to develop effective detection techniques to determine the levels of heavy metal contamination in various mediums [1]. Voltammetry is a highly sensitive electrochemical method used for the detection of heavy metal ions [1-3]. In this study is developed an electrochemical sensor based on a gold electrode modified with a kind of inorganic– organic hybrid polyoxometalate (POM) and used for the determination of Cd^{2+} by square wave voltammetry (SWV). $[(L\text{-}Cys)_3PW_{12}O_{40}]$ has been prepared by solvent free reaction at room temperature and structurally characterized by an elemental analysis, FT-IR spectroscopy and UV-Vis absorption spectroscopy. The conditions for the prepared electrode were optimized. Under optimal conditions, the SWV peak currents showed good linear relationships with Cd^{2+} concentrations in the range of 1.0– 200.0 µM with detection limits of 800 nM (S/N = 3) (Fig.1).

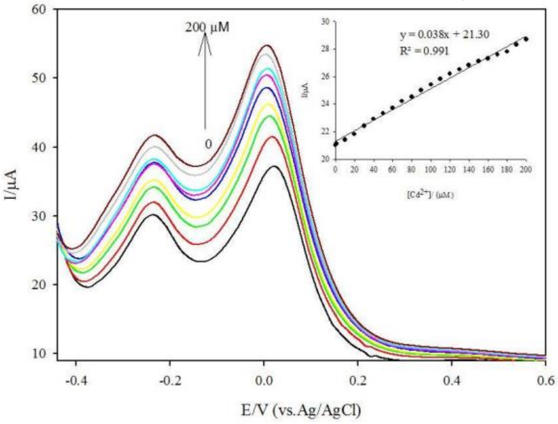

Fig.1 Square wave voltammetry of Au-(Cys)PW SAM modified electrode in the absence and after injection of different concentrations of $CdCl_2$ in 0.1 M $HClO_4$. Inset shows the corresponding calibration curves.

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Paper code: 526

Electrochemical determination of lead (II) on modified gold electrode by square wave voltammetry

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Toxic heavy metals pose a great threat to living organisms due to their non-biodegradability and persistence [1, 2]. Over the past few decades, there has been an increasing interest in the development of highly sensitive analytical methods for the detection of trace amounts of toxic heavy metals. Electrochemical detection of heavy metals offers several advantages such as simplicity, accurateness, low-cost, remarkable sensitivity and high stability. Square-wave voltammetry (SWV) has been widely recognized as a powerful technique for the determination of trace metal ions. In this study, A sensitive method for the electrochemical determination of Pb(II) in acidic aqueous solution has been developed based on a gold electrode modified with $[(L\text{-}Cys)_3PW_{12}O_{40}]$ using SWV. $[(L\text{-}Cys)_3PW_{12}O_{40}]$ has been prepared by solvent free reaction at room temperature and structurally characterized by an elemental analysis, FT-IR spectroscopy and UV-Vis absorption spectroscopy. The conditions for the prepared electrode were optimized. Under the optimum conditions, a linear relationship existed between the current and the concentration of Pb(II) in the range between 1.0– 200.0 µM with the detection limits of 760 nM, based on a signal-to-noise ratio equal to 3 (S/N = 3).

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Paper code: 535

Electrochemical sensor based on graphene oxide/chitosan/ZnO/Au nanocomposite for the determination of losartan

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Detection and measurement of biological species and drug molecules are important, so that they have a significant part of the research not only in the field of diagnosis of diseases, but also in various therapeutic areas [1]. Undoubtedly, one of the prominent approaches at the scientific-research level is to use nanotechnology to design and manufacture a variety of biological and chemical sensors in order to increase the sensitivity and improve their specific performance. Graphene has been used for the sensitive determination of various drugs molecules, due to their excellent conductivity because of π-π staking and synergetic effects with other materials [2]. Chitosan as a natural polymer is a suitable material with promising characteristics to be used for biosensors. Metal nanoparticles (MNPs) based electrochemical sensors and biosensors are playing important role in diagnostic device [3].

In this study, a highly sensitive electrochemical sensor based on glassy carbon electrode modified by graphene oxide, chitosan, gold metal nanoparticles, and zinc oxide with a constant potential method for measuring losartan drug. The morphology and structure of the nanocomposite were characterized by the Field emission scanning electron microscopy (FE-SEM), Energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy. Electrochemical and electro catalytic behavior of this modified electrode for identification and measurement of losartan were carried out in pH 7.0 PBS, by Cyclic voltammetry (CV) and Differential pulse voltammetry (DPV). Under optimum conditions, DPV indicated linear relationship between oxidation peak current and losartan concentration in the range of 0.5-18.0 µM with detection limit of 0.073 µM. The sensor was successfully applied for the highly sensitive determination of losartan in pharmaceutical products and urine samples with satisfactory results.

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Paper code: 536

Electrochemical sensor for simultaneous determination of dopamine and epinephrine based on reduced graphene oxide/TiO_2 nanocomposite

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Measuring the insignificant amounts of catecholamines in biological samples is of particular importance due to the very important biological role that the human body plays in preventing diseases such as Parkinson's, and many ways to improve sensitivity and the reliability of these measurements has been developed. One of the best practices is the use of electrochemical sensors. Graphene, as a carbon material, has special properties that make it an ideal choice for generating graphene-based composite materials. Graphene properties increase with the combination of nanoscale materials and the formation of unique composites. Today, the presence of nanoparticles in composite materials has unique properties [1-3].

In this study, reduced graphene oxide/titanium dioxide nanocomposite (RGO/TiO_2) was synthesized by using a chemically method and used for simultaneously determination of dopamine and epinephrine. The morphology and structure of the nanocomposite was characterized by the field emission scanning electron microscopy (FE-SEM), Energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy. Electrochemical and electrocatalytic behavior of this modified electrode for simultaneous determination of these species were carried out in pH 7.0 PBS, by cyclic voltammetry (CV) and Differential pulse voltammetry (DPV). Under optimum conditions, the calibration curve is plotted for each of the desired compounds. The dopamine shows three linear regions of 5.0-15.0 μM, 15.0-180.0 μM and 180.0-1000.0 μM and. Epinephrine also shows two linear regions from 5.0-20.0 μM and 20.0-1000.0 μM. The detection limit based on (S/N = 3) for simultaneous determination of dopamine and epinephrine was 0.23 μM and 0.18 μM, respectively. The nanocomposite film sensor was successfully used to accurately detect the content of EP in practical samples, and the recoveries for the standards added are 97%–103%.

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Paper code: 539

Voltammetry determination of Tramadol and Dopamine by using of glassy carbon electrode modified with Alizarine Red S

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A novel and easy method for the determination of Tramadol (TRA) is investigated using a glassy carbon electrode (GCE) modified with thin film of Alizarin Red S (ARS) by electro-polymerization. The electrochemical results showed that ARS/GCE displayed excellent increases in the peak currents and a decrease in over potential of TRA in comparison to bare GCE. The measurements were carried out by using differential pulse voltammetry (DPV), cyclic voltammetry (CV) and chrono-amperometry (CA) methods. Application of the DPV method showed that there was a linear relationship between the oxidation peak current and the concentration of TRA over the range of 200-2450 μM with detection limit of 1.64 μM in phosphate buffer (0.1 M, pH=7). The effects of intromitting substances on the definition of TRA were also investigated and it was found that proposed sensor is very selective. The sensor was applied to the determination of TRA in human plasma serum preparations with satisfactory results [1,2].

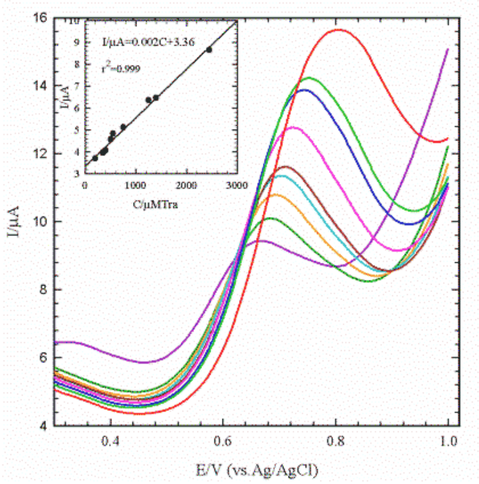

Fig. 1 DPVs of different concentrations of TRA at the ARS/GCE (pH 7). The inset shows the peak current linear dependence on the TRA concentrations at 200-2450 μM

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Paper code: 541

Using the CPE-scanometry method for the simultaneous preconcentration and determination of the Rhodamine B and Nile blue

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In this work CPE-Scanometry as a fast, facile, cheap and sensitive method was used for simultaneous separation, preconcentration and determination of Rhodamine B and Nile blue in aqueous samples. Nile blue (or Nile blue A) is a fluorescent dye and a stain that used in biology and histology. It may be used with live or fixed cells, and imparts a blue color to cell nuclei [1]. Rhodamine B is a chemical compound and a dye. It is often used as a tracer dye within water to determine the rate and direction of flow and transport. Rhodamine B is used in biology as a staining fluorescent dye, sometimes in combination with auramine O, as the auramine-rhodamine stain to demonstrate acid-fast organisms, notably Mycobacterium. Since the rhodamine B cause to cancer and birth defect due to skin contact, so determination and preconcentration of these indicator dyes are important [2]. In this research we was measured the amount of the Rhodamine B and Nile blue simultaneously. Recently scanometry method has been noticed for the measurement of various analytes [3]. To improve the detection limit, this method coupled with preconcentration methods. In the study, was used triton X-114 as surfactant. Furthermore, experimental variables, such as, volumes of extraction and disperser solvents, pH, centrifuge time and round per minutes and salt addition were assessed and optimized with the aid of one variable at a time optimization methods.

Analyte	Main parameter	Minor parameter	Calibration equation after CPE	R^2	RSD% (n=6)	Linear range (mg L^{-1})	DL (mg L^{-1})
NB	R	G	Y=0.1454C+0.0067	0.9964	0.39	0.03-1.30	0.04
RB	G	R	Y=0.385 C + 0.0086	0.9955	0.41	0.01-1.50	0.01

The method is based on the CPE of analytes from aqueous solution, diluting the extracted surfactant-rich phase with ethanol, transfer to Plexiglas® cell and scanning of the cells containing the analyte solution with a scanner and measuring the RGB parameters with software written in visual basic (VB 6) media.

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Paper code: 547

Ionic liquid-based supramolecular solvent microextraction for extraction of synthetic food dyes in foodstuff samples

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Synthetic food dyes are a very important class of food additives. These compounds are widely used to compensate for the loss of natural colors of food, which are destroyed during processing and storage, and to provide the desired colored appearance. However, some of these substances pose a potential risk to the human health, especially if they are excessively consumed [1]. Accordingly, these food additives fall under the strict legislative control as regards their permitted usage, the enforcement of which necessitates the development of a rapid and robust analytical methodology [2]. In the present research, for the first time a new supramolecular solvent (SUPRAs) made up of aggregations of C_{12}minBr ionic liquid was introduced. The extraction was done with micelle formation by dissolving C_{12}minBr surfactant in appropriate water. This method, based on IL-SUPRAs-ME followed with high performance liquid chromatography with ultraviolet detection (HPLC-UV), was applied for rapid extraction and determination of three synthetic food dyes as model analytes in Gummi candy, Candy, fizzy drinks, and jelly powders samples. Effective parameters on the model analytes (i.e., pH, centrifugation time and rate, THF volume, and extraction time) were investigated and optimized by one-variable-at-a-time method. Under optimized conditions, the preconcentration factors of 68.7, 73.6, and 86.5 were obtained for Carmoisine, Ponceau 4R, and Erythrosine, respectively. The calibration curves were linear in the range of 0.2-500 µg L-1 with coefficient of determination (R2) more than 0.9970 for Every 3 analytes, detection limit (S/N=3) of 0.05-0.1 µg L−1, and the relative standard deviations (RSD %) were less than 6.5% based on three replicate measurements. Finally, the proposed method (IL-SUPRAs-ME microextraction) with Good relative recoveries in the range of 85.5–108.0% has been successfully applied for the extraction of three model analytes in different foodstuff samples.

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Paper code: 549

Termodynamics of Ag^+ Cation complexation With N,N′-bis (salicylidene)-1,3-propane diamine in Some Binary Mixed Non-aqueous Solvents

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The complexation reaction between Ag^+ cation and the N,N′-bis (salicylidene)-1,3-propane diamine (SB- SalPr) ligand (Fig. 1) in the binary mixtures: acetonitrile-methanol (AN-MeOH), acetonitrile-ethanol (AN-EtOH), acetonitrile-dimethylsulfoxide (AN-DMSO) and acetonitrile-dimethylformamide (AN-DMF), was investigated using a conductometric method at different temperatures of (288.15, 298.15, 308.15 and 318.15) K. In most of the studied solvent systems, SB- SalPr forms a 1:1 [M: L] complex with the Ag^+ cation. But in some cases, 1:2 [M: L_2] complexes are formed in solutions. The best estimate of stability constant (log k_f=3.74) for the [SB-SalPr. Ag]$^+$ complex, was observed for the AN-MeOH (25:75 mol %) binary mixture at 308.15 K using GENPLOT computer program. The values of the standard thermodynamic parameters (i.e., ΔG_c°, ΔH_c° and ΔS_c°) for formation of the 1:1 complexes of [SB-SalPr. Ag]$^+$ were obtained from temperature dependence of the stability constants of the complexes using the van' t Hoff plots. The results show that, in most cases, the [SB-SalPr. Ag]$^+$ complexes are enthalpy destabilized but entropy stabilized. The values and signs of the thermodynamic parameters are affected by the nature and composition of the mixed solvents [1, 2].

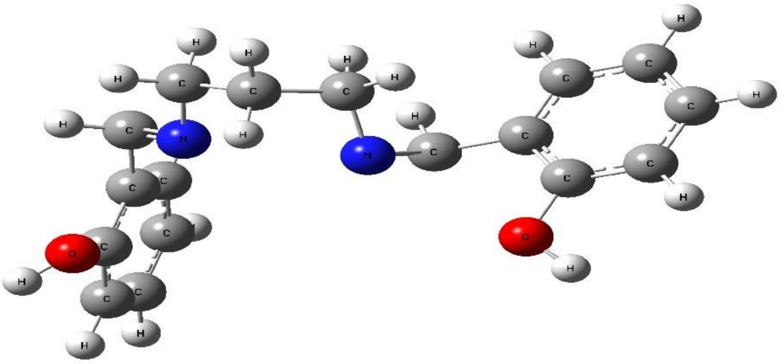

Fig. 1 N,N′-bis (salicylidene)-1,3-propane diamine (SB- SalPr)

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Paper code: 550

Separation study of seven heavy metal cations through a bulk liquid membrane containing N,N',N" -Tri-(4-ethyl benzene) phosphoric triamide

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The competitive seven metal ion transports of Co^{2+}, Cd^{2+}, Ag^{+}, Pb^{2+}, Ni^{2+}, Cu^{2+} and Zn^{2+} from an aqueous phase contained equimolar concentrations of metal ions (at pH=4/9) into an aqueous receiving phase (at pH=3) through an organic phase facilitated by N, N', N" -Tri-(4-ethyl benzene) phosphoric triamide as a carrier was used in organic membrane phase. The following solvents were examined as membrane phase: chloroform ($CHCl_3$), nitrobenzene (NB), 1, 2-dichloroethane (1, 2-DCE), dichloromethane (DCM). The obtained results show that the selectivity and efficiency of transport for these heavy metal ions change with the nature of the organic solvents which were used as liquid membrane in these experiments [1, 2]. A good selectivity was observed for Cu^{2+} cation by this ligand in most solvent systems, but in the case of 1, 2-DCE that was selective to Zn^{2+}. Moreover, the selectivity of metal cations in DCM is higher than the other solvents. The percent of total Cu^{2+} metal cations in the receiving phase (%Receiving), percent of total metal cations in the membrane phase (%Membrane) and rate of the Cu^{2+} ion transport (J (mol per 24 h)) were 0/47, 1/03 and $0/59\times10^{-7}$ respectively after 24 h in DCM solvent. The influence of several factors such as the nature of carboxylic acids: stearic acid (S.A), palmitic acid (P.A), therphetalic acid (T.A) and fumaric acid (F.A) as surfactant in the membrane phase and the time of transport of Cu^{2+} cation were investigated. According to obtained results, the %Membrane of Cu^{2+} ion transport increases in presence of these fatty acids (no acid:1/68, S.A: 21/15, P.A: 3/28, T.A: 15.57 and F.A: 12/41). The maximum transport rate for Cu^{2+} cation from the source phase into the receiving phase concludes, over a period 24 h.

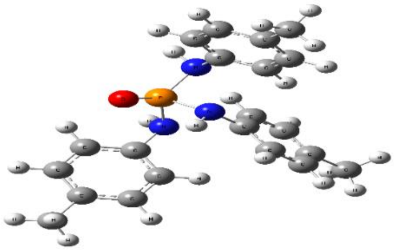

Fig. 1 N, N',N" -Tri-(4-ethyl benzene) phosphoric triamide

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Paper code: 552

Determination of the acid dissociation constant of Nile blue and metanil yellow by the solution scanometric method and comparison with spectrophotometric results

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Correctly determination of the acidity constant of acidity constants cause to perception and quantitative analysis of chemical phenomena such as reaction time, activity, absorption and bio transmissions [1]. Determination of the acidity constant was studied by different methods such as spectrophotometry, potentiometric titration, Proton magnetic resonance spectroscopy, Fluorescence spectrophotometry and chromatography [2, 3]. In this study was applied scanometric method for the determination of the acid dissociation constant of the two indicator dyes (Nile blue (NB) and metanil yellow (MW)). The method is based on the RGB color model, which specifies how much of each color is formed of red, green, and blue colors. Metanil yellow is one of the non-permitted dyes used for food coloring in India. Metanil yellow is a monoazo dye, the sodium salt of m-[(p-anilinophenyl) azo] benzenesulphonic acid. Its toxicity and mutagenicity have been assessed. Nile blue (or Nile blue A) is a fluorescent dye and a stain that used in biology and histology. Electrochemical polymerization of the Nile blue is used for the amperometric measurement of hemoglobin.

The comparison between the current traditional UV-Vis spectrophotometry methods was studied and the results revealed similar trends in both methods. For evaluation acidity constant of the cited indicators, using spectrophotometric data, the Hypspec program was employed. The calculated pKa values of the cited indicators by solution scanometry and spectrophotometric methods are in agreement. The corresponding distribution diagrams were depicted by Hyss 2009.

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Paper code: 559

Electrochemical investigation of acetaminophen/amlodipine interactions

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In this research, electrochemical oxidation of acetaminophen was investigated in the presence of amlodipine, an amine-containing drug. The electrochemical techniques used include cyclic voltammetry and controlled-potential coulometry. The results indicated that *N*-acetyl-*p*-benzoquinone-imine (NAPQI) produced from electrooxidation of acetaminophen can react with amlodipine, based on the Michael addition reaction [1,2]. Corresponding product was synthesized in aqueous solutions by means of electrosynthesis, using a carbon electrode in an undivided cell. It was an environmentally friendly method because in which the application of toxic reagents has been eliminated. Synthesized product was identified by FT-IR, ^{1}H-NMR and ^{13}CNMR spectroscopies.

The cyclic voltammograms were analyzed by digital simulation to measure the homogeneous parameters for the suggested electrode mechanism [3]. The observed rate constant (k_{obs}) for the reaction of electrochemically generated *N*-acetyl-*p* benzoquinn-imine with amlodipine were calculated in various pH (e.g. k_{obs}=652±32.6 ($M^{-1}s^{-1}$)).

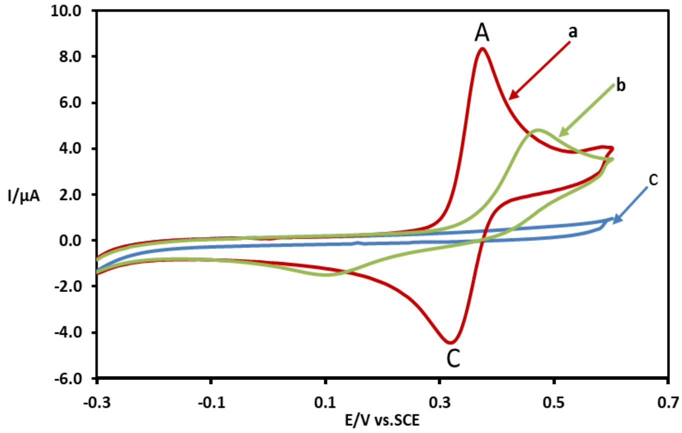

Fig. 1. (I) Cyclic voltammograms of 0.5 mM acetaminophen: (a) in the absence, (b) in the presence of 0.5 mM amlodipine and (c) 0.5 mM amlodipine in the absence of acetaminophen at a glassy carbon electrode in phosphate buffer (pH = 7.0, 0.2 M). Scan rate: 50 mVs^{-1}, t = 25 ± 1ºC

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Paper code: 561

Adsorptive stripping voltammetry determination of methyldopa at a pencil graphite electrode modified with Fe_3O_4 nanoparticle/reduced graphene oxide-chitosan in biological and pharmaceutical samples

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Methyldopa (MD) is a catechol derivative (catecholamine) and an old antihypertensive agent which is used in the treatment of mild to moderate hypertension. It affects nerve centers which control blood vessels in the brain. As blood vessels relax, MD relieves high blood pressure [1]. Several types of analytical procedures have been employed for the analysis of catechol derivatives in pharmaceutical formulations and or biological samples. Among techniques used in several procedures most are based on spectrofluorimetric [2], kinetic measurements [3], nuclear magnetic resonance spectroscopy [4], gas chromatography [5], high performance liquid chromatography [6], chemiluminescence [7], but electrochemical methods have attracted great interests because of their simplicity, rapidness and high sensitivity in determination of MD without any tedious pre-treatments [8]. Electrochemical techniques in the field of pharmaceutical analysis have developed due to their simplicity, reasonable accuracy and precision, low cost, and rapidity. There is no need for derivatization or time-consuming extraction steps in comparison with other techniques because of less sensitivity of electroanalytical methods to the matrix effects [9]. In this study a new, simple and disposable electrochemical sensor for the determination of MD was developed on pencil graphite electrode (PGE) via differential pulse voltammetry (DPV). We report a facile approach to synthesize nanocomposites with Fe_3O_4 nanopaticles (NPs) attached to reduced graphene oxide (rGO), which combines the growth of Fe_3O_4 NPs and the reduction of GOs in one single step. The PGEs were coated with Fe_3O_4 NPs/rGO-CHIT tri-component. Accumulation of MD was found to be optimized in 0.1 M phosphate buffer solution (PBS, pH=2) as an electrochemical probe. Under the optimized condition calibration curve of the MD has three linear concentration ranges from 0.001 to 0.01 µM, 0.01 to 0.1 and 0.1 to 10.0 µM with the limit of detection (LOD) of 0.2 nM. Finally, the modified electrode was successfully employed to determine MD in human urine samples.

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Paper code: 567

A novel nonosized molten salt catalyst for the preparation of dihydropyrano[2,3-*c*]pyrazole derivatives

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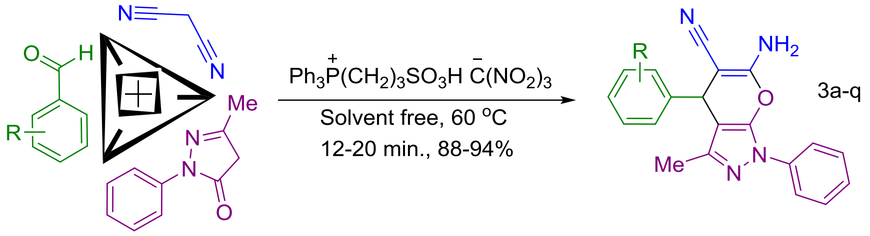
Heterocyclic structural kernels have found their prominent position among the therapeutic active molecules. These compounds play a critical role in molecular form of life like for example nucleotides, carbohydrates, hemes and amino acids. Specifically, nitrogen-rich heterocyclic molecules containing pyrazole moieties due to their privilege applications as biological and pharmacological active species, occupy a distinguished location in the domain of medicinal chemistry [1].

Among fused nitrogen-containing heterocyclic molecules, dihydropyrano[2,3-*c*]pyrazole derivatives which established significant precursors for the drug compounds, exhibit a broad scope of vital medicinal and pharmaceutical applications. They can be used as inhibitors of human Chk1 kinase, anti- inflammatory, anticancer, antimicrobial agents. Therefore, because of the high biological importance of these compounds, it is not surprising that several protocols have been reported for their preparation [2-3] (Scheme 1).



R = 4-Cl, 2-Cl, 2,4-Cl_2, 4-Br, 4-F, 2,6-F_2, 3,4-F_2, 3,5-F_2, 4-CF_3, 3,5-$(CF_3)_2$, 4-CN, 3-NO_2, 4-NO_2, H, 4-Me, 4-OMe, 4-OH-3-OEt,

Scheme 1: Catalytic synthesis of dihydropyrano[2,3-c]pyrazole derivatives

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Paper code: 569

Determination of nortriptyline in aqueous sample by dispersive liquid phase microextraction followed by ion mobility spectrometry

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Nortriptyline is a tricyclic antidepressant which is frequently used for treating clinical depression. Determination of nortriptyline in the different real samples can be very important, particularly in pharmacokinetic and environmental studies [1,2]. Therefore, a fast and sensitive analytical method can be very helpful. Ion mobility spectrometry (IMS) has almost all features for this purpose [3]. On the other hand, a fast and efficient microextraction method can obtain the lower detection limit and better clean-up for real sample analysis. Consequently, in this study, a dispersive liquid phase microextraction (assisted by a homogenizer) combined with ion mobility spectrometry has been applied for determination of nortriptyline. Figure 1 reveals the ion mobility spectrum of nortriptyline. Effective factors such as solvent type, salt addition, stirring rate and extraction time have been investigated and optimized. Analytical features of the method were evaluated under optimized conditions. Limit of detection was achieved 7 μg/L and relative standard deviations were less than 11%. The calibration curve was obtained in the range of 20–500 μg/L with a good linearity ($R^2 > 0.9946$). Human urine, plasma and river water samples were studied as real samples for the evaluation of the method and average relative recoveries were found 87%, 74% and 103% respectively.

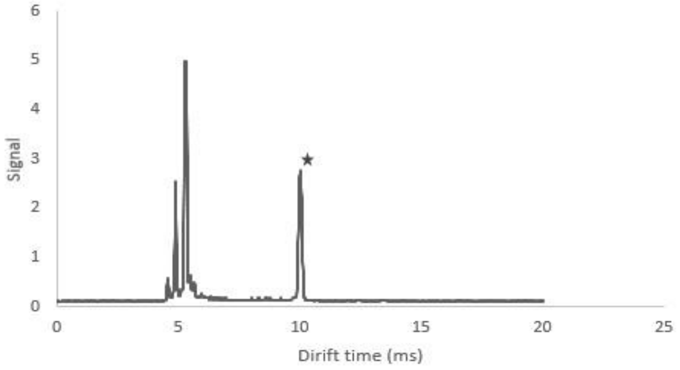

Fig. 1 Ion mobility spectrum of nortriptyline.

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Paper code: 597

Preparation of gC_3N_4–Pt photoelectrocatalyst for electrooxidation of ethanol

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Fuel cells (FCs) featuring high efficiency and low emission to the environment have attracted intensive research interest for over three decades, because of their important roles in the future clean energy solutions [1]. Among several alcohols, which can be used in direct alcohol fuel cells (DAFCs), ethanol is the most promising one due to considerable energy capacity, non-toxicity, biological renewability, easy handling and storing unlike hydrogen fuel [2-4]. In this research work, a fluorine doped tin oxide (FTO) electrode was modified with Pt nanoparticles and graphite carbon nitride (gC_3N_4) photoelectrocatalyst and it was used as an anode in a fuell cell. The gC_3N_4 was drop casted onto the electrode surface, and Pt nanoparticles were deposited on the surface of the electrode using chronoamperometric technique. The microscopic structure, morphology and electrochemical performance of the modified electrode were studied by scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), cyclic voltammetry and chronoamperometry. Moreover, the effects of various parameters such as ethanol concentration, amount of the Pt nanoparticles and gC_3N_4 photo electrocatalyst on the electrooxidation of ethanol were investigated. The results show that the proposed electrode has a high electrocatalytic activity towards the ethanol electrooxidation reaction and it can be used as a suitable anode for electrooxidation of ethanol in fuel cells.

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Paper code: 648

Development of a new liquid phase microextraction method using a switchable solvent for the determination of polychlorinated bi-phenyls (PCBs)

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Polychlorinated biphenyls (PCBs) are a class of synthetic organic compounds that are hazardous due to their chemical and thermal stability, hydrophobicity and toxic properties [1-2]. PCBs often exist at trace levels of concentration in the environment, so an effective pretreatment step is necessary for their preconcentration before quantification. In this study, a new method was successfully developed for the simultaneous determination of seven polychlorinated biphenyls in aqueous samples with switchable hydrophilicity solvent based liquid phase microextraction coupled to GC-MS detection. Triethylamine (TEA) was used as extraction solvent with switchable polarity, which can be miscible/immiscible upon the changes of pH of sample solution. The factors influencing the extraction efficiency, including type and volume of extraction solvent, pH and volume of aqueous sample, extraction time, and salt addition were investigated and optimized. Under the optimized conditions, good linearity (0.5-150 µg/L) and limits of detection (0.15 µg/L) were obtained for the PCBs by the proposed method. Also, the relative standard deviations (RSDs) were calculated between 5.2 and 6.4 %. In addition, enrichment factors (EFs) and extraction recoveries (ERs) were obtained in the ranges of 30.46-32.10 and 76.15-80.25 respectively. Finally, the proposed method was successfully applied for the analysis of PCBs in various water samples with excellent relative recoveries (RRs, 96.30-102.60).

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Paper code: 650

Paper-based colorimetric sensor array for detection of trinitrotoluene using chemometric methods

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The analysis of chemical contaminants in environmental matrices has attracted attention of many scientists in last decade. Trinitrotoluene (TNT) is one the significant, global environmental pollutant. Contamination of soil and groundwater with TNT is the major concern because of its biological persistence, toxicity and mutagenicity [1]. On-site analysis methods can be used to assess the nature and extent of contamination as well as to monitor remediation progress. Current on-site methods often involve multiple steps and are time consuming [2]. In this study we report a new visual colorimetric sensor array for detection of TNT.

TNT has been identified based on its electron acceptance property. Accordingly, the color conversion of TNT in reaction with electron donors (ammines) has been considered according to the Meisenheimer complex reaction.

In order to design a reproducible and cost-efficient sensor array a set of 27 sensing elements were fabricated by using standard filter paper as a sensor substrate. The color conversion has been captured by a photographic camera. Here, based on color changes observable with the naked eye, the concentrations of up to 5 ppm are detectable. Then, nitrobenzene-based materials have been studied as interferences. Finally, captured images were converted to the analytical data by statistical analysis methods. Multivariate statistical methods like PCA and HCA were applied for analyzing the collected data. The use of colorimetric sensor array has proven to be a fast, inexpensive and versatile method for TNT analysis compared to the other techniques.

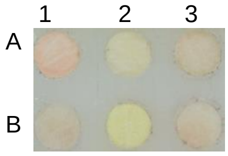

Fig. 1 The result of reaction between 0.5 mg TNT with different indicators in 1.13 cm^2 circle area, A1) Butylamine A2) Triethly amine A3) Ethanol amine B1) 2-(2amino ethyl amino)ethanol B2) Ethylene diamine B3) aminoacetaldehyde dimethyl acetal.

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Paper code: 655

Application of poly-Alizarin red s/ Multi-Walled Carbon Nanotubes-Modified electrode for detection of tramadol and dopamine

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A new electrochemical sensor for the fast and simultaneous determination of tramadol (TRA) and dopamine (DA) was developed based on modification of carbon glassy electrode (GCE) with alizarin red s (ARS) and multi-walled carbon nanotubes (MWCNTs) was developed. Electrochemical methods including cyclic voltammetry (CV) and choronoamperometry (CA), differential pulse voltammetry (DPV) were used to characterize the processes of electro polymerization and electrochemical determination. Under the optimized experimental conditions, TRA and DA have linear responses in the ranges of 10-2250 μM and 0.1-200 μM, respectively, and the detection limits is 0.64 μM and 0.056 μM respectively. In addition, the modified electrode was employed for simultaneous detection of TRA and DA. The analytical efficiency of this sensor has been measured for the detection of TRA and DA in human serum with good results [1,2].

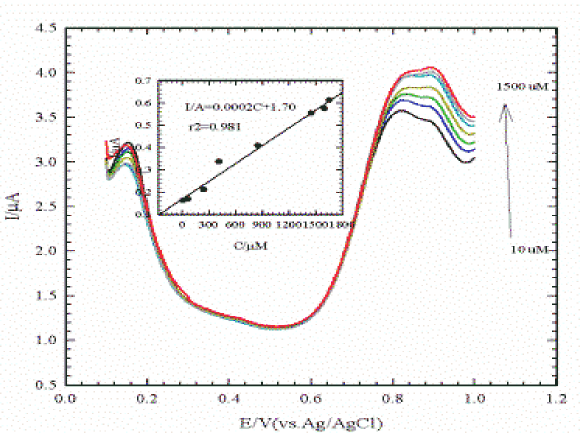

Fig. 1 DPVs of mixture of various concentrations of DA and TRA in PBS (0.1 M, pH=7.0)

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Paper code: 662

Methyl red-functionalized silver nanoparticles as a probe for colorimetric detection of arsenic (III) in water samples

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Arsenic (As) is a high toxic element found in food and drinking water [1]. Arsenic can exist as As(III) and As(V) species in natural waters and its direct exposure is harmful to humans due to its carcinogenic effects on the hematopoietic system, liver, and central nervous system [2]. Thus, there is a growing need for the development of a sensitive and reliable analytical method for the determination of as in water samples.

In this work a simple and rapid colorimetric method for determination of As (III) was developed. The method is based on reduction of As (III) to arsine (AsH_3) in acidic media with sodium borohydride and on the subsequent reaction of AsH_3 with methyl red-functionalized silver nanoparticles (MR-AgNPs). By increasing the concentration of arsenic, the absorbance of the colored solution was reduced fig1. The parameters affecting the arsine generation were optimized. Under the optimum conditions, the calibration graph was linear over the range of 10-100 µg L^{-1} with the limit of detection of 5 µg L^{-1}. The percent of relative standard deviation (%RSD, n = 5) was lower than 3%. The method was successfully applied to the determination of As (III) in water samples.

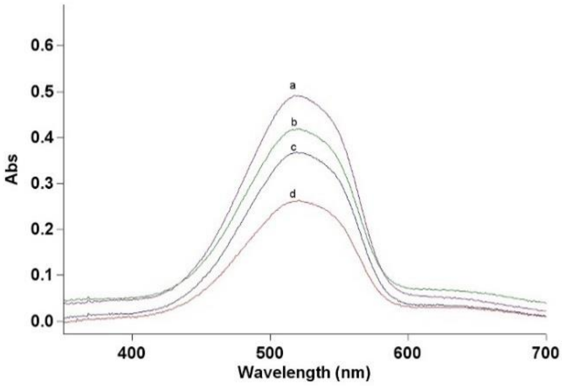

Fig. 1 UV–vis absorption spectra of a) MR-AgNPs, b) MR-AgNPs + 10 µg L^{-1} As(III), c) MR-AgNPs + 20 µg L^{-1} As(III), d) MR-AgNPs + 60 µg L^{-1} As(III)

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Paper code: 663

Electrooxidation of methanol using *lanthanum cobalt oxide*/platinum photoelectrocatalyst

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Direct methanol fuel cells (DMFCs) have recently received great attention as a sustainable power source for dealing with energy shortage and environmental pollution due to their fairly high energy density, low operating temperature and very low environmental intrusion [1-3]. Pt-based electrocatalysts in DMFCs, have shown high activity for methanol electrooxidation reactions at anode of a fuell cell. However, pure Pt as anode is easily poisoned by carbon monoxide (CO) [4]. Therefore, considerable efforts have been recently focused on fabrication of easily available and high active electrocatalysts for the DMFCs. In the present work, *lanthanum cobalt oxide* ($LaCoO_3$) as a photoelectrocatalyst was synthesized for electrooxidation of methanol and it was characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM). At first, the photoelectrocatalyst was dropped onto the surface of the fluorine doped tin oxide (FTO) electrode. Then, the surface of the electrode was potentiostatically coated with Pt nanoparticles at constant potential of -0.2 V. The surface of the modified electrode was characterized by scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX) techniques. The electrooxidation of methanol molecules on the surface of the modified electrode was studied using cyclic voltammetry and chronoamperometry. The results show that the *lanthanum cobalt oxide*/platinum photoelectrocatalyst show a high electrocatalytic activity towards the methanol electrooxidation reaction as compared to Pt catalyst.

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Paper code: 668

Use of switchable hydrophilicity solvents based liquid phase microextraction (SPs-LPME) followed by HPLC-UV for the determination of 17 amino acids in different samples

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In the present study, switchable hydrophilicity solvents based liquid phase microextraction (SPs-LPME) followed by HPLC-UV was applied for the simultaneous determination of 17 free amino acids in different samples. Chromatographic procedure for the determination of amino acids as phenylthiocarbamyl derivatives (PTC) is performed. Several variables relating to chromatographic aspects were studied such as the pH and temperature of the mobile phase, buffer and modifier (triethylamine) concentrations in mobile phase and the stability of PTC-derivatives in solution. Dipropylamine was used as extraction solvent with switchable hydrophilicity that can be miscible or immiscible upon the addition or removal of CO_2 as a reagent. The major benefits of this technique is mainly the very large surface area between the fine droplets of the extraction solvent and the aqueous sample, and the accordingly fast extraction kinetics that result in the rapid achieving of a state of equilibrium and the high enrichment factors (300–430) usually obtained. Under the optimum conditions, proposed method provided low limits of detection (0.18–0.97 $\mu g\,L^{-1}$) and acceptable extraction repeatabilities (RSD%= 3.4-5.7). It was linear over two orders of magnitude. Finally, the developed methods were successfully used in determination of the concentrations of 17 free amino acids in different samples and acceptable recoveries (>80%) were obtained.

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Paper code: 669

Determination of glyphosate residues in wheat samples with switchable hydrophilicity solvents based liquid phase microextraction (SPs-LPME)

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In the present study, switchable hydrophilicity solvents based liquid phase microextraction (SPs-LPME) [1] followed by HPLC-UV was applied for determination of glyphosate residues in wheat samples. Chromatographic procedure for the determination of glyphosate is performed [2]. Several variables relating to chromatographic aspects were studied such as the pH and temperature of the mobile phase, buffer and modifier concentrations in mobile phase and the stability of derivative in solution. Dipropylamine was used as extraction solvent with switchable hydrophilicity that can be miscible or immiscible upon the addition or removal of CO2 as a reagent. The major benefits of this technique are mainly the very large surface area between the fine droplets of the extraction solvent and the aqueous sample, and the accordingly fast extraction kinetics that result in the rapid achieving of a state of equilibrium and the high enrichment factor (200) usually obtained. Under the optimum conditions, proposed method provided low limits of detection (0.2 $\mu g\,L^{-1}$) and acceptable extraction repeatabilities (RSD%= 2.5-5). It was linear over two orders of magnitude. Finally, the developed methods were successfully used in determination of the concentrations of glyphosate in different wheat samples and acceptable recoveries (>86%) were obtained. In conclusion it could be stated that the developed method is efficient and appropriate for determing glyphosate in wheat with HPLC-UV method.

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Paper code: 673

Determination of D-penicillamine at the sonogel-carbon electrode modified with cerium oxide nanoparticles

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D-penicillamine (D-PA) is a medicine that has been used for many years in the treatment of various rheumatic diseases, most commonly rheumatoid arthritis. Increased amounts of D-PA can cause rashes early in treatment. Rashes may be associated with itching, which can often be controlled by simply adding antihistamine medication [1]. CeO_2 Nanoparticles have aroused much interest for development of implantable sensor due to their high mechanical strength, oxygen ion conductivity, biocompatibility, oxygen storage capacity, nontoxicity, high chemical stability and high electron transfers. In the present work, D-PA sensor was prepared by modification of a sonogel-carbon electrode (SNGC) with cerium oxide nanoparticles. The mentioned sensor can act as a suitable platform for oxidation of D-PA due to good conductivity, enhanced electron transfer kinetics and high catalytic activity [2, 3]. The suggested sensor enhanced electrical current compared with bare SNGC for the oxidation of D-PA. The synthesized cerium oxide nanoparticles were characterized by electron scanning microscopy (SEM) imaging and UV-Visible spectroscopy. The methods such as cyclic voltammetry, and linear sweep voltammetry were carried out in this work. Based on the linear sweep voltammetry, the linear range were obtained 0.1-300.0 µM and detection limit was calculated 0.033 µM. The applicability of the designed electrode modified with CeO_2 nanoparticles was investigated in real samples of D-penicillamine tablet and blood serum solutions.

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Paper code: 674

Fluorescent determination of alprazolam via molecularly imprinted polymer embedded CdTe quantum dots sensor

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Acting as a fluorescence sensing material, the molecularly imprinted polymer (MIP) [1] embedded CdTe quantum dots (QDs) [2] was constructed through sol-gel process for highly efficient optosensing of alprazolam. The approach combined the merits of molecular imprinting technology and the fluorescent property of the CdTe QDs. When alprazolam is added to the medium that has a MIP@CdTe QDs composite, fluorescence quenching of this analyte is happened which is related to the concentration of the alprazolam. This fluorescence behavior is used for well testing of alprazolam with the detection limit and linear range of µM. Beside, the prepared sensors could well against the interferences from various biomolecules and be successfully used for the assay of alprazolam in human biological samples, exhibiting excellent specificity. On the other hand, in this work, microwave irradiation was utilized for the synthesis of water-soluble CdTe QDs. As it has been proven, that uniform nucleation and growth rate are critical for the synthesis of nanomaterials with high quality, the conventional hydrothermal synthetic route suffers from a main hindrance since it utilizes convective heating which can cause thermal gradient effects throughout the bulk solution [3]. The resulting composites were verified by X-ray diffraction and Fourier transform infrared spectroscopy (FT-IR). The morphology of MIP-embedded QDs was observed by transmission electron microscopy (TEM).

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Paper code: 678

Electrochemical oxidation of acetaminophen in the presence of clonazepam

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Electrochemical oxidation of acetaminophen has been studied in the presence of clonazepam in aqueous solutions, using cyclic voltammetry and controlled-potential coulometry methods. The obtained results indicated that *N*-acetyl-*p*-benzoquinone-imine (NAPQI) derived from acetaminophen participates in Michael addition reaction with clonazepam, via an EC reaction mechanism [1]. The product has been derived with a good yield based on electrochemical oxidation under controlled potential conditions in aqueous solutions. The procedure was realized with an environmentally friendly method, without using any toxic reagents and solvents at a carbon electrode in an undivided cell [2].

Furthermore, the homogeneous rate constant of the chemical reaction between NAPQI and clonazepam was estimated in various pH (e.g. k_{obs}=782±39.7 ($M^{-1}s^{-1}$)), by comparing the experimental cyclic voltammetric responses with those obtained by digital simulation [2].

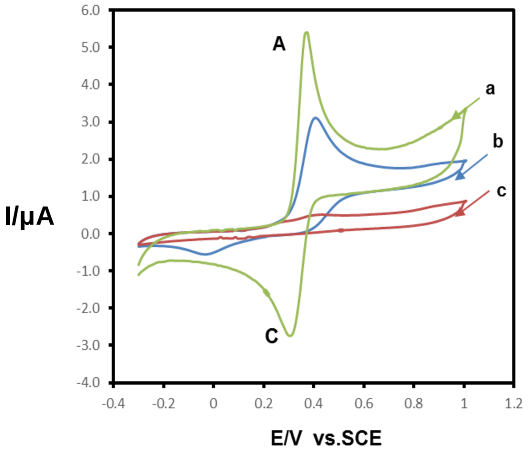

Fig. 1. Cyclic voltammograms of 0.5 mM acetaminophen: (a) in the absence, (b) in the presence of 0.5 mM clonazepam and (c) 0.5 mM clonazepam in the absence of acetaminophen at a glassy carbon electrode in phosphate buffer (pH = 7.0, c=0.2 M). Scan rate: 25 mVs^{-1}, T = 25 ± 1ºC

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Paper code: 681

Epitope imprinted polymer embedded CdTe quantum dots as a highly selective fluorescent receptor for recognition of cytochrome c in biological samples

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In this work, to improve the sensitivity and selectivity of the molecular imprinting sensor [1] detection of protein, fluorescence nanoparticles [2] and epitope approach [3] was utilized. Nanopeptide, separated from cytochrome c (Cyt C), was selected as a template molecule to prepare the molecularly imprinted polymer (MIP) film, and it could bind with the cavities of the MIP. High sensitivity of MIP@CdTe QDs toward Cyt C molecules were observed based on the fluorescence quenching of QDs. The fluorescence of MIP-coated QDs was stronger quenched by the template versus that of non-imprinted polymer (NIP)-coated QDs, which indicated the composites could recognize the corresponding template. Besides, the prepared sensors could well against the interferences from various biomolecules and be successfully used for the assay of Cyt C in human biological samples, exhibiting excellent specificity. This fluorescence behavior is used for well testing of Cyt C with the detection limit and linear range of µM. The recoveries of the material to Cyt C in real samples were obtained in the range of 98.0–102.0%. In brief, this fluorescent artificial receptor functioned as a simple and selective sensing system for Cyt C recognition.

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Paper code: 682

Electrochemical synthesis of hollow gold nanoparticles on the pencil graphite electrode surface as high efficient cathode for hydrogen production

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The worry that always have been existed in using the fossil fuels such as; scarce resources and air pollutant problems, makes the human being to revise about his life style. The idea of using hydrogen as a clean energy is considered to be the best way to prevent the appearance of fossil fuel usage outcomes. Although it is the most common element in the world, hydrogen is found in impure form on our planet combined with oxygen as water and combined with carbon and other elements in fossil fuels and innumerable hydrocarbon compounds [1]. A fuel cell is an accessible device to produce hydrogen green energy and we are interested to apply procedures in order to decrease the overvoltage of hydrogen evolution reaction (HER) which occur during the electrochemical process in the cell. Up to now, much attention has been focused on exploiting transition metal alloys, carbides, nitrides, phosphides, sulphides and so on for catalysis the HER [2]. Platinum is one of the best catalysts for HER but the drawbacks that limited it's practical application is it's high costs and rare resources so the researcher's interest is focused on other earth-abundant noble metals.

In this work reduced graphene oxide (rGO) was deposited electrochemically on the surface of a single-use pencil graphite electrode (PGE). The main reason for choosing the disposable PGE is the ease of preparation, commercial availability, and low costs [3]. Then cobalt nanoparticles (CoNPs) which they act as a sacrificial template, were placed on the rGO surface by the use of electrochemically deposition method after that hollow Au nanoparticles (HAuNPs) were produced using a galvanic replacement reaction between Au^{3+} ions with CoNPs. The advantages of using HAuNPs instead of AuNPs are magnitude surface active area and subsequently lower consumption of gold. In this study the overvoltage of hydrogen evolution reaction in acidic medium on modified electrode was decreased. Exchange current density and electron transfer coefficient were obtained as 6.01×10^{-5} (mA/cm^2) and 0.4, respectively.

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Paper code: 684

Multiwall carbon nanotube- zirconium oxide nanocomposite hollow fiber solid phase microextraction for determination of polyaromatic hydrocarbons in water, coffee and tea samples

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The purpose of this study was to evaluate the application of hollow fiber solid-phase microextraction (HF-SPME) followed by HPLC-UV to determine the ultra-trace amounts of polycyclic aromatic hydrocarbons (PAHs) as model analytes in complex coffee and tea samples. HF-SPME can be effectively used as an alternative to the direct immersion SPME (DI- SPME) method in complex matrices. The HF-SPME method has high clean-up and selectivity due to the high porosity of hollow fiber that can pick out analyte from complicated matrices. As a hollow fiber sorbent, a novel multiwall carbon nanotube/zirconium oxide nanocomposite (MWCNT/ZrO_2) was fabricated [1,2]. The excellent adsorption of PAHs on the sorbent was attributed to the dominant roles of π–π stacking interaction and hydrophobic interaction. Under the optimized extraction conditions, the wide linear range of 1-100 µg L^{-1} with coefficients of determination better than 0.998 and low detection limits of 0.3µg L^{-1} with satisfactory precision (RSD < 4%) were obtained. Compared to other methods, MWCNT/ZrO_2 hollow fiber solid phase microextraction demonstrated a good capability for determination of PAHs in complex coffee and tea samples.

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Paper code: 686

Electrochemical determination of diuron using platinum nanoparticle and molecularly imprinted technology

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Diuron is a herbicide belonging to the urea family which is widely used to eliminate weeds at uncultivated levels and in products such as citrus, rice, cotton, soy, sugarcane, potato, wheat, coffee [1] and, moreover, in runways, railways and pipelines. Because of its stability and shelf-life in water and soil, diuron lead to environmental impacts on plants and mammals. In plants, it is absorbed through the root, then stems and breaks, and eventually prevents photosynthesis. In addition, in humans, it can be led to formation of Methemoglobin in the blood, liver, and spleen abnormalities and disturbs the processes of the natural release and transfer of hormones in the body [2]. Molecular imprinting is a process where a layer is synthesized in the presence of a molecular template, a process that generates cavities within network that are complementary to the template molecule in size, shape, and position of functional groups [3]. In this work, a sensitive electrochemical sensor based on imprinted technology was applied to determine diuron. Cyclic voltammetry and differential pulse voltammetry were applied to investigate the electrochemical response of the diuron on the electrode surface. To prepare the modified pencil graphite electrode (PGE), initially, a mixture of chitosan and carbon nanotubes is placed on the PGE surfac. Then, the electrode was applied as the working electrode in the electrochemical cell containing 60 mM KNO_3, 2.4 mM 3-methyl-4-nitrophenol, 0.5 mM diuron, 0.26 mM Pt(IV), and 2.7 M H_2SO_4 and a layer was formed on the electrode surface. After that, the modified PGE was placed into the methanol (60% v/v) solution to remove diuron and form imprinted layer. Finally, the imprinted PGE was placed into the diuron solutions with different concentrations and the peak current at 0.6 V was measured. Diuron was determined in water samples using constructed sensor.

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Paper code: 696

ZnTe/Quinhydrone nanocomposite-modified glassy carbon electrode as a promising ethanol electro-oxidation catalyst in acid media for fuel cell applications

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The ZnTe semiconductor nanorods were synthesized by a novel chemical route. The ZnTe nanorods were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), FT-IR spectroscopy, photoluminescence spectroscopy, UV–vis and cyclic voltammetry techniques. Then, this product and quinhydrone were used for the electrocatalytic oxidation of ethanol in acid medium. The ZnTe/QH/GCE fabricated by drop casting 5 µl of their suspension with weight ratio of 1:1 (ZnTe: Quinhydrone, 5mg/ml prepared in Milli-Q water) on a cleaned glassy carbon electrode surface showed a higher electrocatalytic activity toward ethanol oxidation. Furthermore, the ZnTe/QH/GCE displayed a higher stability with 93% retention of the initial current density after 5000 s in long term current-time curve. This newly prepared ZnTe/QH nanohybrid could be a promising anodic catalyst for the direct ethanol fuel cells (DEFCs) application.

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Paper code: 713

Electrocatalytic *Activities* of the Pt/CNP Nanocomposite on Carbon Ceramic Electrode for Ethanol Oxidation

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Direct ethanol fuel cells (DEFCs) have high mass energy density and can be handled, transferred and stored easily [1, 2]. Compared with other fuels, ethanol is less permeable through polymeric membranes, less toxic, cheaper, and easier to store. So that, the study of electrooxidation of ethanol and the construction of a DEFC has increasing interest in the current decays [3]. It is well known that platinum (Pt) is an effective electrocatalyst for ethanol oxidation. However, problems such as CO poisoning on the Pt catalyst becomes an important issue by decreasing the number of active reaction site available and the breaking the carbon-carbon bond in larger alcohol molecules need to high energy. Therefore, it is necessary to use new type of electrocatalysts to improve the velocities of ethanol oxidation and new supports for electrocatalysts to reduce the amount and the cost. Carbon nanomaterials with several form and structure such as carbon nanotubes (MWCNT and SWCNT) [4], nanostructured carbon black [5] and etc. have been used as support for metal nanoparticles electrocatalysts and can improve their electrocatalytic performance.

In this work, the Pt nanoparticles (PtNPs) and Pt nanoparticles doped on/in the carbon nanoparticles **(**PtNPs/CNPs) on carbon-ceramic electrode as a homemade substrate were used as electrocatalysts for the oxidation of the ethanol .The morphology, structure, composition and electrochemical behavior of the PtNPs and PtNPs/CNPs modified carbon-ceramic electrodes were characterized by scanning electron microscopy, energy dispersive X-ray spectroscopy, X-ray diffraction and cyclic voltammetric methods. It was found that PtNPs/CNPs modified carbon-ceramic electrode was electrocatalytically more active than Pt-alone nanoparticles modified carbon-ceramic electrode and had satisfactory stability.

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Paper code: 719

Visible light photoelectrochemical sensor for determination of progesterone based on polydopamine/quantum dots nanocomposites

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In photoelectrochemical (PEC) detection process, light is used as the excitation source and photocurrent is obtained as the detection signal. Therefore, it can exhibits charge-transfer upon photoexcitation and achieves the detection purpose via the intensity of the photocurrent. In this study, polydopamine/CdS quantum dots (QDs) nanocomposite was deposited on Ti sheet as semiconductor to make a PEC sensor. The CdS QDs were electro-synthesized on Ti sheet which followed by chemically deposition of polydopamine (PDA). The as-prepared PDA/CdS QDs/Ti displayed much higher photocatalytic activity than the CdS QDs/Ti and PDA/Ti, which was attributed to the synergic effect between CdS QDs and PDA, which included the optical property, the better dispersion and the small size. Thus, it was applied as a PEC sensor under the visible light for determination of progesterone. Results show that the best response is obtained in acetate buffer solution (pH=5) as a supporting electrolyte at applied potential of 2 V *vs.* Ag/AgCl reference electrode. Also, the photocurrent intensity increased with increasing concentration of progesterone ranging from 2 nM to 2x10^4 nM. The detection limit was obtained 1.54 nM and the RSD was 3.77 %.

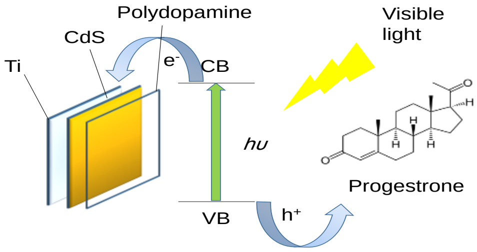

Fig. 1. The mechanism of PEC detection.

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Paper code: 745

Alignment Independent 3D-QSAR Study of BACE1 Inhibitors as Anti-Alzheimer Drugs

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β-secretase (beta-amyloid converting enzyme 1[BACE1]) is involved in the first and rate-limiting step of β-amyloid (Aβ) peptides production, which leads to the pathogenesis of Alzheimer`s disease(AD).Therefore, is an appropriate target for developing novel anti-Alzheimer drugs. In order to understand the structural characteristics correlated with the potency of BACE1 inhibitors, a Molecular Interaction Fields (MIF) based alignment independent three-dimensional quantitative structure-activity relationship (3D-QSAR) study was conducted. The predicted values of pIC50 are in good agreement with the experimental results of biological activity, indicating that the 3D-QSAR model can be select for further studies. The resulted model PLS analysis indicated that the compound activities were in good agreement with experimentally observed values (R^2=0.73, Q^2_{LOO}=0.57 and R^2_{Pred}=0.842).

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Paper code: 747

Studies on removal of tetracyclines by Fe_3O_4@Cu@folic acid-LDH magnetic core-shell nanocomposite

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Recently, magnetic based sorbents have been applied in many areas to remove, isolate and/or concentrate the desired components from aqueous solutions. Magnetic iron oxide nano-particles have been studied extensively as a new adsorbent with large surface area and small diffusion resistance [1].

In this study, Fe_3O_4@Cu@folic acid-LDH magnetic core-shell nanocomposite was synthesized by co-presipitation method. The resulting material was characterized by several methods such as, XRD, SEM, FT-IR and TEM. Result showed that Fe_3O_4@Cu@folic acid-LDH core-shell nanocomposite was combined with Fe_3O_4 and folic acid-LDH. Also, the obtained nanoparticles were spherical with the diameters of about 50 nm.

The Fe_3O_4@Cu@folic acid-LDH was used to remove tetracyclines from aqueous solutions in batch method. To investigate the tetracyclines adsorption at high concentrations, 10 mg of absorbent were added to 20 mL of tetracyclines solution (the concentration of trtracyclines varying from 30 to 200 mg L^{-1}) and stirred for 20 min at a constant temperature of 25°C. Then the sorbent was settled by applying a strong magnetic field and the analyte concentrations in the supernatant solutions were determined using high performance liquid chromatography (HPLC). The adsorption mechanism is probably the non-electrostatic π-π dispersion interaction and hydrophobic interaction between TCs and folic acid intercalated LDH. A systematic study of adsorption process was performed by varying ionic strength, sorption time, temperature, sorption amount and pH. From tetracycline adsorption kinetics study, it was found that the equilibrium was reached within 100 min following the pseudo-second-order model with rate constant (k_2) of 0.0015 g mg^{-1} min^{-1}. For oxytetracycline the same kinetic model was obtained, but the equilibrium time was 80 min with rate constant (k_2) of 0.0035 g mg^{-1} min^{-1}. The sorption data for both of analytes can be well interpreted by the Langmuir model with the maximum adsorption capacity of 256.4 mg g^{-1} for tetracycline and 222.2 mg g^{-1} for oxytetracycline. The results were shown that the adsorbent can be used to remove tetracyclines from water and sewage samples.

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Paper code: 754

Imidazolium-based bifunctional periodic mesoporous organosilicas as a novel sorbent for microextraction by packed sorbent

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Microextraction by packed sorbent (MEPS) was adopted as a simple, fast, and on-line sample preparation technique after its introduction in 2004 by Abdel-Rehim [1]. MEPS is a miniaturization of the conventional SPE and very promising technique for sample preparation. Sorbent type is a core aspect of MEPS. MEPS selectivity depends on sorbent type because the analytes are retained by the sorptive materials via different reversible interactions (hydrophobic, polar, and ionic) [2].

The present work focuses on the development of imidazolium-based bifunctional periodic mesoporous organosilicas (BFPMO) nanostructure as novel sorbent for MEPS. Here, it is believed the integrating of PMO and IL providing new organic–inorganic hybrid materials that can open novel branch toward to MEPS technique. For this purpose, chlorophenoxy acid (CPA) herbicides were tested as model compounds in aqueous matrices at a trace level. The factors that influenced on the extraction efficiency of CPAs including the number of draw/eject cycles of the sample, draw/eject flow rate, the washing volume of water, the nature of the eluting solvent and ionic strength were investigated and optimized. Finally, the proposed method was successfully applied to the analysis of trace CPAs in environmental samples.

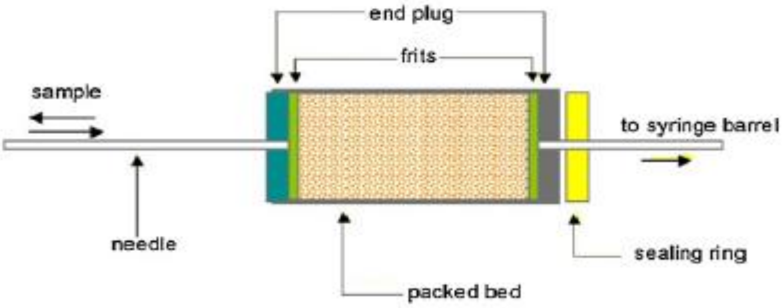

Fig. 1 Schematic diagram of MEPS and sorbent in BIN.

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Paper code: 757

Photoelectrooxidation of ethanol on a *lanthanum cobalt oxide*/platinum modified FTO electrode

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In recent years, direct ethanol fuel cells (DEFCs) have gradually attracted more interest as an alternative power source [1]. Ethanol is a promising fuel because it can be produced easily from abundant biomass, and it has lower toxicity than methanol [2]. In addition, the high theoretical mass-energy density of ethanol (~8.0 Wh g^{-1}) is appropriate for the rising demand for future energy [3]. Platinum is most commonly used as an anode material in DEFCs. Although ethanol electrooxidation on Pt electrodes has been widely investigated, some critical problems still exist when only pure Pt electrodes are used [4]. In the present study, a new photoelectrocatalyst composed of *lanthanum cobalt oxide* ($LaCoO_3$) was prepared for electrooxidation of ethanol. The photoelectrocatalyst was characterized by X-ray diffraction (XRD) and transmission electron microscopy (TEM). The surface of the fluorine doped tin oxide (FTO) electrode was modified with $LaCoO_3$ photoelectrocatalyst using drop casting method and then Pt nanoparticles through electrochemical deposition. Cyclic voltammetry, chronoamperometry, scanning electron microscopy (SEM) and energy dispersion spectroscopy (EDS) were used to investigate the surface of the modified electrode. The effect of several parameters such as ethanol concentration, amount of the Pt nanoparticles and $LaCoO_3$ photoelectrocatalyst controlling the electrooxidation of ethanol were examined and optimized. The results obtained in this study, indicate that the proposed electrode possess a high electrocatalytic activity for ethanol electrooxidation.

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Paper code: 767

Investigation of expander formulation in the negative active material on key performance characteristics of lead-acid batteries

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Lead-acid battery has been widely used for automotive yet, due to low cost, high power and 100% recyclable. the battery forms from sponge lead ($Pb/PbSO_4$) as negative electrode, with a lead dioxide ($PbO_2/PbSO_4$) as positive electrode in sulfuric acid solution. several additives introduced to modify negative active materials (NAM) to improve the batteries performance. Modern expander formulations are usually a blend of barium sulfate($BaSO_4$), lignosulfonate (LS) and carbon black(C). The function of $BaSO_4$ is to act as a site for the precipitation of lead sulfate as the battery is discharged. C is added to the expander to increase the NAM electrochemical surface area. .[1] The most pronounced effect of LS on battery performance is the improvement in low-temperature performance at high rates of discharge.[2]

The purpose of the present work was to examine various expander formulation on cold cranking test, dynamic charge acceptance, capacity as key performance characteristics of lead-acid batteries. It was made three series of expander: the first one containing 33% LS, 20% C, and 47% $BaSO_4$.; the second one had 28% LS, 17% C, 55% $BaSO_4$.; and the last one w 22% LS, 13% C, 65% $BaSO_4$.

Using 1% of the expanders, three pastes and subsequent three king of negative plate were produces.

The plates were studied by scanning electron microscope (SEM) in two states: before charging the plates and after a charge-discharge cycle. SEM images indicated different morphology and particle size for plates with different expander. electrochemical impedance spectroscopy was used to investigate the discharge plates. The results have been shown that R_{ct} in the first formulation is ten time more than the second one. but it was not considerable difference between R_{ct} of the second plate and the last one. Using the different negative plates, three 74Ah batteries were made and standard testes were done over them. The results show that plates that prepared with second expander have best dynamic charge acceptance, capacity. Whereas the first plates that its expander with 33%LS, has best cold cranking result.

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Paper code: 769

Voltammetric determination of sulfasalazine by using glassy carbon electrode modified with 2,4-dinitrophenyl hydrazine

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Sulfasalazine (salazosulfapyridine,2-hydroxy-5-[(E)-2-{4-[(pyridin-2-yl) sulfamoyl] phenyl} diazen-1-yl]benzoic acid), is a sulfa drug, a derivative of mesalazine (5-ASA), has been made special attention for its therapeutic importance. It used to treat a certain type of bowel disease called ulcerative colitis and Crohn's disease [1].

In this work, a new method was introduced to modified glassy carbon electrode (GCE) with 2,4-dinitrophenylhydrazine (DNPH) and then, sensitive, inexpensive, rapid and selective voltammetric determination of sulfasalazine (SSZ) performed. Electrode modification, conditions, optimization and electrochemical detection of this molecule was studied by cyclic voltammetry (CV), differential pulse voltammetry(DPV) and chrono-amperometry. The modified electrode presented good linear correlation to SSZ concentration in the range of 1 to 10 μM with low detection limit of 0.35 μM. The proposed method was used for the voltammetric determination of SSZ in human plasma samples.

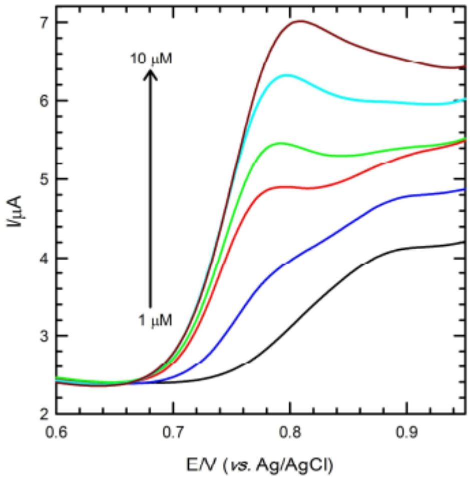

Fig. 1 Differential pulse voltammograms of GCE/DNPH in PBS (0.1 M, pH 7.0) containing different concentrations 1, 2, 4, 6, 8, 10 μM SSZ

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Paper code: 770

Multi-walled carbon nanotube/ polypyrrol nanocomposite modified glassy carbon electrode as a new sensor for determination of Buprenorphine

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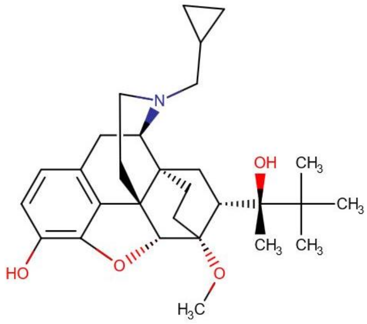
Buprenorphine (BN, Scheme 1) is a strong semi-synthetic opiate painkiller with as sovereignty of 20–40 times higher than that of morphine [1,2]. Several methods have been reported for the determination of BN. Among these methods, electrochemical methods show some advantages such as extreme simplicity, high sensitivity, easy and low-cost [3]. The present work reports preparation and characterization of a new potentiometric sensor for determination of BN based on doped polypyrrole films. A glassy carbon electrode was coated with a thin layer of multi-walled carbon nanotubes (MWCNTs) and subsequently electro-polymerized with polypyrrole. The prepared electrode was used for the voltammetric determination of buprenorphine. Surface morphology and electrochemical properties of the fabricated composite electrode were examined by atomic force microscopy and cyclic voltammetry (CV). The effect of several experimental variables, such as pH of the supporting electrolyte, drop size of the cast MWCNTs suspension and number of electropolymerization cycles were optimized by monitoring the CV responses of the modified electrode toward BN. The modified electrode is applicable to determine BN in the linear range of 0.06-40 µM with a detection limit 28 nM. The sensor was used for recovery of analytes in urine samples.



Scheme 1. Buprenorphine molecular structure

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Paper code: 774

Sensing platform for adefovir based on *molecularly imprinted* polymer-coated carbon nanocomposite

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In this paper, a novel electrochemical sensor with sensitive and selective binding sites for adefovir detection is reported, which is based on a carbon nanocomposite glassy carbon electrode (C/GCE) modified with molecularly imprinted of poly(*o*-phenylenediamine) templated with adefovir. The surface feature of electrode was characterized by cyclic voltammetry (CV), differential pulse voltammetry (DPV), electrochemical impedance spectroscopy (EIS) and field emission scanning electron microscopy (FESEM). Several important parameters controlling the performance of electrode were investigated and optimized using response surface methodology (RSM) [1,2]. Under optimal conditions, the changes in DPV peak currents of the redox probe, hexacyanoferrate, were linear to adefovir concentrations in the range from 0.1 to 15 μmol L^{-1}, with the detection limit of 0.05 μmol L^{-1} (S/N = 3). The biological applicability of the developed sensor has been delineated by the determination of adefovir in human plasma and urine samples using the standard addition method. The proposed sensor exhibited high degree of selectivity for adefovir in comparison to other structurally similar biomolecules present in biological samples, along with long term stability, good reproducibility and excellent capacity of regeneration of molecular recognition sites.

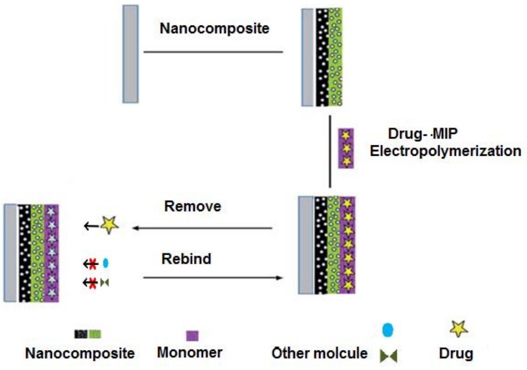

Fig. 1 Fabrication procedure for the MIP/nanocomposite and rebinding mechanism in MIPs

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Paper code: 776

Sensitive nonenzymatic electrochemiluminescence hydrogen peroxide sensor using polypyrrole/ ployluminole / titanium dioxide nanoparticles

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A thin layer of a poly (pyrrole-luminol) composite was synthesized, through electrodeposition of luminol and pyrrole in acidic medium on a graphite electrode modified by casting of titanium dioxide (TiO_2) nanoparticles with 30 - 35 nm in diameter. The properties of the nanocomposite were studied by FE-SEM and EDX techniques. In alkaline media, luminol undergoes a two-step oxidation process at around 0.48V and form excited luminol (3-aminophthalic acid dianion, the ring-opened intermediate form), which in turn emit light at 425 nm [1, 2]. Features of merit include broad linearity from 1pM to 4µM (R^2= 0.996) with a limit of detection as low as 0.40 pM (S/N=3), good reproducibility (RSD of 4%) for the analysis of a 4.0 µM hydrogen peroxide solution (n=4) and long-term stability. The presence of ascorbic acid at concentrations as high as 100 nM did not produce any electrochemiluminescence signals, which was held as proof of the selective behavior of the electrode modified with Ppy/Plu/TiO_2 towards H_2O_2 using method. The ECL process consumes luminol since this ring opened and the process is not reversible. The sensor was also used in the analysis of H_2O_2 concentration in mouthwash formulations.

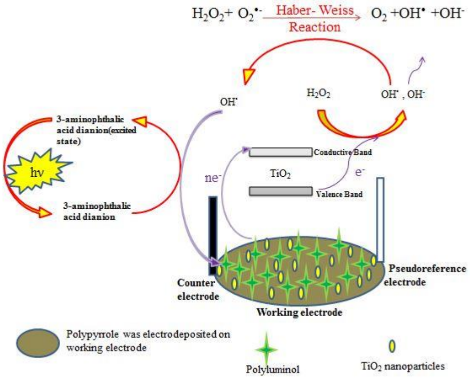

Fig. 1 The electrochemiluminescence mechanism of nanocomposite

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Paper code: 783

A nanocomposite consisting of poly(pyrrole)-poly(aniline) copolymer, graphene oxide and Fe_3O_4 nanoparticles as novel sorbent for the extraction and preconcentration of polycyclic aromatic hydrocarbons from aqueous samples

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Recently, magnetic solid-phase extraction (MSPE), a new mode of SPE method, based on the use of magnetic nanoparticles (MNPs) has been developed [1,2]. In this work, magnetic graphene oxide was functionalized by polyaniline and polypyrrole copolymer and used as an efficient sorbent for the extraction of polycyclic aromatic hydrocarbons (PAHs) followed by GC–FID. The sorbent was characterized by vibrating sample magnetometry (VSM), Fourier transform infrared spectroscopy (FT-IR) and transition electron microscopy (TEM, Fig. 1). The optimal extraction conditions include: sorbent amount, 35 mg; sorption time, 10 min; salt concentration, 30% *w/w*; type and volume of the eluent, toluene, 1 mL; elution time; 5 min. Under the optimal extraction conditions, limits of detection (LODs) and the linear dynamic ranges were achieved in the range of 0.003–0.01 ng mL^{-1} and 0.01–200 ng mL^{-1}, respectively. The absolute extraction recovery (ER%) and relative standard deviations (RSD%) were in the range of 50.4–78.3% and 5.2–8.5%, respectively. Finally, the applicability of the method was successfully confirmed by the extraction and determination of PAHs in the real water samples.

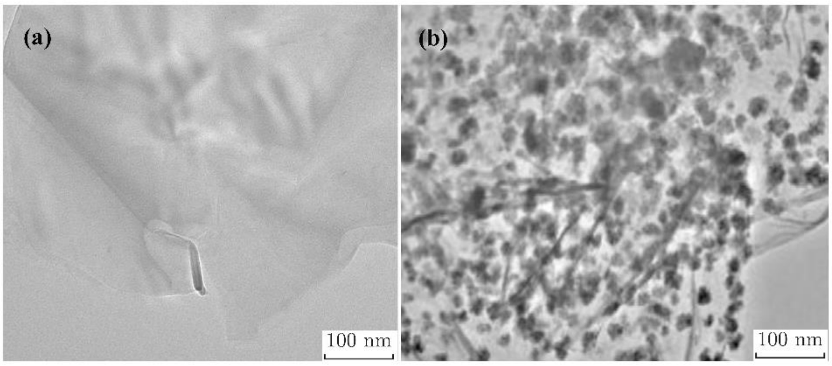

Fig. 1 TEM images of (a) graphene, and (b) nanocomposite.

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Paper code: 785

Host-guest complex of curcumin with beta-cyclodextrin and its antioxidant activity

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This study was to synthesize and characterization the host-guest complex of curcumin with β-cyclodextrin (β-CD) which has antioxidanting activity property. The host-guest interaction of curcumin with β-CD in order to complexation drug in β-CD were investigated at 25°C. The interactions host-guest complex was characterized by fourier transform infrared (FTIR) and ultraviolet-visible (UV-vis) spectroscopies. The solution of curcumin is prepared in 0.06 mM concentration with methanol. Curcumin is the phytochemical that gives yellow color to turmeric [1]. UV-vis spectra were analysised of curcumin/β-CD complex at maximum wavelength 418 nm of curcumin. The formation constant was calculated by using a modified Benesi-Hildebrand equation to big number of 1.8×10^5 M^{-1}. The stoichiometry of host-guest complex was found by using of Job`s plot to be 1:1 for β-CD with curcumin.

Curcumin is reported to have a number of pharmacological activities including antioxidant, HIV antiproteases activity, anti-inflammatory, analgesic, anticancer, etc [2]. The aim of research has the antioxidant activity of curcumin and its host-guest complex were determined by the scavenging of stable radical 2,2´-diphenyl-1-picrylhydrazyl (DPPH) [3]. Kinetic studies for remove $DPPH^{\cdot}$ in presence curcumin and curcumin/β-CD complex were done at amount of 95%. The results obtained indicated that the curcumin/β-CD host-guest complex was the most reactive than its free form into antioxidant activity. Therefore, most common pharmaceutical application of β-CD is to enhance curcumin solubility in aqueous solutions.

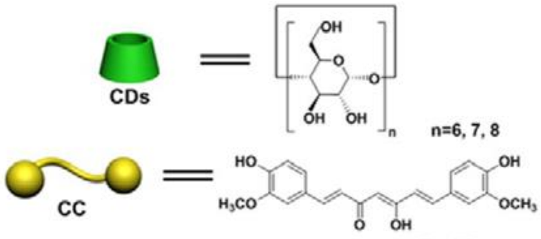

Fig. 1 The chemical structure of β-cyclodextrin and curcumin.

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Paper code: 787

Investigation of Zeolitic Imidazolate Frameworks Ability as Sorbent in Stir Bar Sorptive Extraction Method

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In this work, the zeolite imidazole framework-8 (ZIF-8) was initially synthesized by the solvothermal method. After confirmation of its structure, it was used to provide a new composite of acrylate-based polymer (PA) and ZIF-8 as a coating on a stir bar with suitable mechanical and chemical stability. Different manipulation methods was used for this purpose. This monolithic coated (PA/ZIF-8) devise was used in a stir bar sorptive extraction (SBSE) method. During the preparation of PA/ZIF-8 coating, the solvent type, the monomer to the solvent ratio, the monomer to cross linker ratio and the amount of ZIF-8 powder were optimized. In the optimization process, carvedilol (CAR) was used as a target compound and the extraction efficiency of this drug using proposed SBSE method was investigated by high performance liquid chromatography (HPLC) with photo diode array detector (PDA). In all steps, PA coated stir bar was also prepared for comparison of its extraction efficiency with PA/ZIF-8 coated stir bar.). Repeatability in the production of ZIF-8/PA sorption coating on the stir bar was determined by calculating the relative standard deviation (RSD) of the extracted carvedilol field surface with three stir bar in a batch and in three different batch 6.6% and 6.96%, respectively. In order to investigate ability of optimized PA/ZIF-8 and PA coatings, haloperidol (HLP), losartan (LOS), loratadine (LOR), diazepam (DZ), nordiazepam (NDZ) and chlorpromazine (CPZ) were also tested as target compounds and their extraction efficiency were obtained. The results showed that HLP, LOS, LOR, DZ and NDZ are extracted on PA/ZIF-8 and PA coated stir bars at similar extraction and desorption conditions. But in the case of CAR and HLP, the use of PA/ZIF-8 stir bar showed an improvement of 100% in the concentration factor obtained from PA stir bar.

Finally, effective parameters on extraction efficiency of CAR and HLP such as pH and volume of sample, extraction and desorption time and type of desorption solvent were optimized. Then the proposed method (monolithic PA/ZIF-8 coated-SBSE-HPLC-PDA) was validated and used for determination of CAR and HLP in human plasma samples.

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Paper code: 789

The application and formation of inclusion complex of γ-cyclodextrin with turmeric

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Gama-cyclodextrin (γ-CD) is one of cyclic oligomers of glucose that can form water-soluble inclusion complexes with small molecules or fragments of large compounds. γ-CD is also used for increasing stability and bioavailability of drugs, and other additional applications [1]. This research is to synthesize and characterization the inclusion complex of gama-cyclodextrin (γ-CD) with turmeric which has antioxidanting activity property. The interaction inclusion complex was characterized by fourier transform infrared (FTIR) and ultraviolet-visible (UV-vis) spectroscopies at 25°C. UV-vis spectra were analysised of turmeric/γ-CD complex at maximum wavelength 418 nm of turmeric in 0.06 mM concentration with methanol. The formation constant was calculated by using a modified Benesi-Hildebrand equation to number of 5.9×10^{5} M^{-1}. The stoichiometry of inclusion complex was found by using of Job`s plot to be 1:1 for γ-CD with turmeric.

Turmeric, is a yellow pigment extracted from the ground rhizome of curcuma commonly used as a spice and food colorant [2]. The aim of research has the antioxidant activity of turmeric and its inclusion complex were determined by the scavenging of stable radical 2,2´-diphenyl-1-picrylhydrazyl (DPPH$^{\cdot}$) [3]. Kinetic studies were done to remove DPPH$^{\cdot}$ in presence turmeric and turmeric/γ-CD complex at amount more of 100%. The spectra shown interaction between the OH group of γ-CD and the phenolic hydroxyl group of turmeric. The results were indicated that the turmeric/γ-CD inclusion complex most reactive than its free form into antioxidant activity. Therefore γ-CD can used to enhance turmeric solubility in aqueous solutions for pharmaceutical applications.

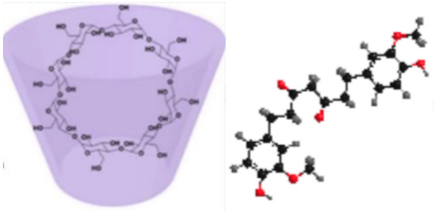

Fig. 1 The chemical structure of γ-cyclodextrin and turmeric.

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Paper code: 808

Decolorization of Industrial Wastewater Using Some Coagulants by Electrochemical Method and UV/VIS spectroscopy

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Existence of color in water increases the potential for the formation of tri-halomethanes, and the generative compounds in it may be deposited in the distribution network and re-suspended. Industrial waste from the textile industry and dyeing operations, pulp and paper production, food industry, chemical production and ore mining may be produce color in the water due to the association with natural streams and river makes the purification process indispensable. Colorant wastewater containing orange, carbazite beryllite bloween, malachite green, purple and electrolyte solution of sodium chloride salt, was purified in a designed glass cell with dimensions of 15 cm × 10 cm, metal electrodes with dimensions 14 cm × 9cm × 2mm. The UV/VIS spectroscopy was used to indicate its removal from absorption. The whole process of testing, taking into account the main factors, was determined by the effect of pH, contact time effect, color concentration effect and temperature effect, and each time in ten steps to obtain optimal conditions was conducted. The best results were obtained in 14 g/l electrolytes, 8 volt applied voltage, pH = 5, iron electrode type and 2 cm distance, temperature 25 °C in 10 minutes. Using this method, we were able to dye 99.9% of simulated wastewater.

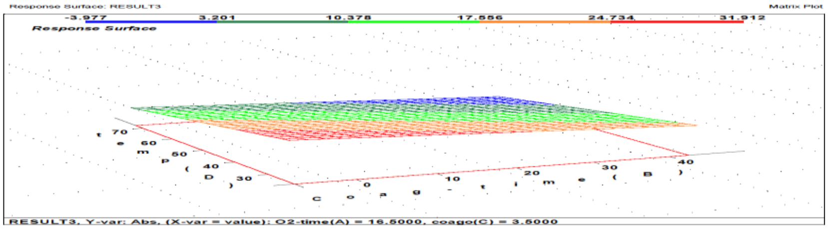

Figure1. Effect of time and coagulant temperature on reducing color removal

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Paper code: 817

Electrochemical detection of phenol using semiconductor based modified electrode

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In present work, the fast, simple and cost-effective electrodeposition method in order to fabricate ZnO thin layer as a well-known semiconductor, on conductive fluorinated-tin oxide (FTO) layer is described. The omissible polymer, Polyvinyl Alcohol (PVA), was used as an effective additive for controlling and improvement of ZnO nanoparticles growth on the FTO surface while electrodeposition process occurred, then its elimination via annealing process resulted in a highly porous nanostructure ZnO semiconductor on FTO surface (nano-ZnO/FTO). Characterization of the surface morphology of fabricated ZnO thin film by field emission-scanning electron microscopy (FE-SEM) exhibits highly porous uniform surface that can effectively increase sensing surface and sensitivity of the fabricated sensor as a result. Step by step monitoring of nano-ZnO/FTO sensor was performed using electrochemical techniques such as cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS) [1,2]. Fabricated nano-ZnO/FTO electrode was used for phenol detection in aqueous solutions using impedimetric assessment. The impedimetric results showed low detection limit and broad linear range.

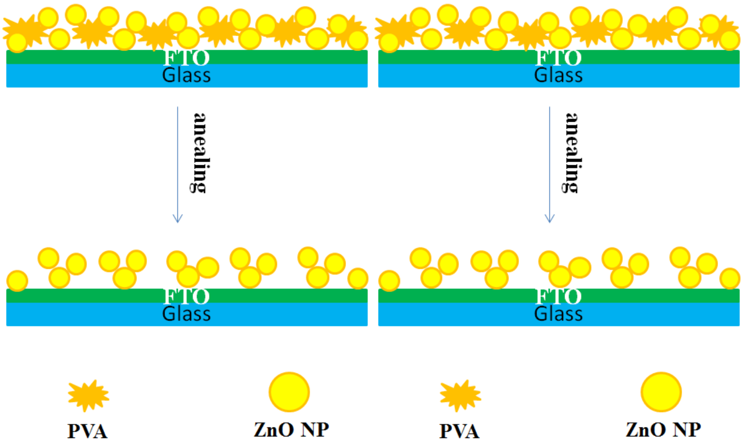

Fig. 1 schematic representation of nano-ZnO/FTO electrode fabrication process

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Paper code: 818

A novel microfluidic paper – based device with colorimetric assay for determination of catechol using poly(*N*-vinylpyrrolidone) -capped silver nanoparticles

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Due to the harmfulness of catechol to the environment and human health, various analytical methods have been developed for its determination, including electrochemiluminescence, spectrophotometry, gas chromato-graphy, electrochemistry, capillary electrophoresis and high performance liquid chromatography(HPLC)[1]. However, these methods suffer from sophisticated operations and expensive instrumentations. In this work, a paper-based device [2] was fabricated that can rapidly detect very low concentration of catechol using modified silver nanoparticles that were synthesized by facile PVP-stabilized method [3]. AgNPs paper-based sensor changed from light yellow to dark grey color after the addition of catechol due to nanoparticle growth and clusters formation. Two-dimensional optical scanners have been used as a low-cost detection system. Under optimized measurement conditions, the color intensities were altered as a function of catechol concentration. The color intensity change was linear with catechol concentration over the range of 50 μM–0.9 mM with a correlation coefficient of 0.993. This colorimetry method can detect as low as 5μM of analyte within <30 minutes on a white filter paper which was comparable to analytical laboratory-based methodologies. The proposed method was successfully applied for the determination of catechol in real samples, including tap water, perfume and cigarette smoke and satisfactory results was obtained.

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Paper code: 835

Extraction of Caffeine from coffee by Homogeneous Liquid-Liquid Micro-extraction (HLLME) method and determination with Spectrophotometer UV-Vis

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Caffeine, which stimulates the central nervous system of the human body, is the most popular stimulant all over the world and it is added manually in some products, such as energy drinks. Caffeine is an alkaloid which naturally exists in tea, coffee, cola and cocoa.

The extraction of caffeine in coffee has always been a concern for researchers and industry owners. In the homogeneous liquid-liquid micro-extraction, the homogeneous solution contains the sample and the extraction phase. The solution is converted to a two-phase by changing the conditions and its extraction phase precipitates. Recently, the use of mathematical models in the chemical and food industry has been considered to improve performance and increase efficiency. The Response Surface Method (RSM), with the lowest data, can determine the optimal value of several variables simultaneously [1].

In this study, homogeneous liquid-liquid micro-extraction (HLLME) and UV spectroscopy method were applied to extract caffeine in coffee and the obtained data was analyzed using RSM. The optimized parameters including extraction pH (3.9), extraction temperature (40 °C) and concentration of extraction phase of triton x-114 (1%) were calculated. The relative standard deviation of 5.0%, the coefficient of correlation of 0.996 and the linear range of 0.1-2 μg.mL^{-1} of the method were determined. This method has been used to measure caffeine value in coffee.

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Paper code: 849

Extraction of dopamine by DC potentially-reinforced bulk-liquid membrane transport (PR-BLMT) combined with UV- Vis spectrophotometer method

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The transfer method was investigated using direct potential-reinforced bulk-liquid membrane transport (PE-BLMT) for extraction of dopamine. The purpose of this study was to evaluate the ability of the mentioned method to isolate and transfer dopamine. The RE-BLMT method is a simple method based on a combination of two known EME extraction approaches and a BLMT transmission [1]. Variables such as pH, phase and receiver, ion strength, BLM type and volume, extraction time, applied voltage and electrode type were studied. Using this method linearity ranged from 0.2 to 4 μg mL-1 with the coefficient of correlation of 0.99. The relative standard deviation (RSD) for the seven replications was 4.8% and the transfer efficiency was 90%. The RE-BLMT method was used to transfer and determine the concentration of dopamine in drug samples.

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Paper code: 851

Spectrophotometric determination of furazolidone in real samples after its microextraction using hollow fiber reinforced with MIP@MWCNT

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Furazolidone (FZD) is one of the nitrofuran antibiotics that was utilized as a feed additive for growth promotion and bacterial infection curing agent in animals and birds especially in hen and rooster [1]. But, due to its carcinogenicity and mutagenicity effects, its usage has been banned by European Union (Commission Regulation 1442/95) [2]. However, because of its low price and high effectiveness, it is still used illegally in some countries including Iran. Thus, developing a fast, simple, sensitive and reliable analytical method for monitoring the furazolidone residues in food, and biological matrixes is of great importance. Several analytical instrumental techniques such as chemiluminescence, spectrophotometry and high-performance liquid chromatography (HPLC) have been reported for the determination of furazolidone [3]. However, its determination at low levels in complicated biological samples with high concentration of interfering matrix requires a sample preparation step for its separation and enrichment prior to its spectrophotometric measurement.

Herein, hollow fiber reinforced with molecularly imprinted polymer supported on multiwalled carbon nanotube has been fabricated and used as the sorbent for microextraction and preconcentration of furazolidone from real samples. The fabricated sorbent has the advantages of rigidity, stability, high selectivity, low manufacturing cost as well as excellent mechanical properties. The sorbed furazolidone was eluted with 500 μL of the mixture of hydrochloric acid and methanol (1:5 v/v) and quantified by fiber optic linear array spectrophotometry. The effect of some experimental parameters on the extraction of the analyte were studied and optimized. Under the optimized conditions, the calibration graph was linear (R^2 = 0.9996) over the range of 10.0–100.0 μg L^{-1} with the detection limit of 2.6 μg L^{-1} for the preconcentration of 50 mL of the sample. The relative standard deviation (RSD %) at the 30.0 μg L^{-1} level of FZD (n = 6) was 3.7%. The developed method showed high selectivity toward the furazolidone and was successfully applied for the determination of trace amount of furazolidone in poultry tissues and water samples.

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Paper code: 861

Simultaneous determination of N-acetylcysteine and acetaminophen at the modified electrode assisted by chemometeric approaches

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N-acetylcysteine (N-AC) is widely used as a medicine in the treatment of diseases such as amyotrophic lateral sclerosis, chronic obstructive pulmonary disease, alzheimer's disease and eye infection [1]. Acetaminophen (AC) commonly known as paracetamol which is one of the most commonly used oral analgesics and antipyretics [2]. It has an excellent safety profile when administered in proper therapeutic doses, but hepatotoxicity can occur after its overdose [3]. Untreated overdose of AC can cause liver failure and death within days. In this case, intravenous N-AC is used for the treatment of AC overdose. Due to this fatal effect, simultaneous determination of these compounds (N-AC and AC) is very important. So that, in this work, a sensitive voltammetric sensor based on a carbon paste electrode modified with silica nano particles (BF_3@MCM-41) with a combination of 4,4′-Dihydroxybiphenyl (DHB) (BF_3@MCM-41/DHB/CPE) was designed for simultaneous determination of N-AC and AC. The modified electrode demonstrated good sensitivity, selectivity, and stability. To simultaneous determination of N-AC and AC in blood serum samples containing unexpected electroactive interference with a very high degree of overlapping, three-dimensional voltammetry data were generated by changing the pulse height as an instrumental parameter. The obtained data subsequently analyzed by parallel factor analysis (PARAFAC). The results show that PARAFAC could be applied with great success for electroanalytical determination of highly overlapped electroactive species in real samples. Finally, the performance of the proposed method for determining both compounds in real samples was confirmed using standard method such as HPLC.

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Paper code: 865

Spectrophotometric determination of brilliant green in aqueous samples after supramolecular solvent extraction

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Brilliant green (BG) is one of the triphenylmethane dyes that has been widely used to color silk and wool in textile industry [1]. BG has also been used in fish farming industry because of its high efficiency in the prevention and treatment of certain fish disease and its low cost [2]. BG dye is toxic and has mutagenic and carcinogenic effects that affect aquatic biota and humans. Due to its carcinogenic properties, the use of BG as veterinary treatment is banned by the USA, European and many other countries [3]. So, there is a serious need to develop a fast, sensitive, inexpensive, and simple method for determining the BG from real samples.

In the present study, a simple supramolecular solvent based dispersive liquid-liquid microextraction method was developed for the separation and preconcentration of brilliant green prior to its determination by spectrophotometry. The method is based on the extraction of brilliant green with coacervates made up of decanoic reverse micelles in tetrahydrofuran-water mixture. Sodium dodecyl sulfate was used for the ion-pair formation with brilliant green. The influence of the effective parameters such as pH, type and volume of the extraction solvent, volume of disperser solvent, and sample volume on the extraction of brilliant green was investigated and optimized. Under the optimized conditions, the calibration graph was linear in the range of 1.0-17.5 µg L^{-1} of BG. The limit of detection (LOD) and limit of quantification (LOQ) were 0.28 µg L^{-1} and 0.94 µg L^{-1}, respectively. The repeatability expressed as the relative standard deviation for six replicate measurements at 5.0 ng L^{-1} brilliant green was 3.6%. The method was successfully applied to the extraction and determination of brilliant green in different water and fish farming water samples.

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Paper code: 870

Spectrophotometric Study of the Interaction between Pyridoxinewith Some Transition Metal Ions in Non-aqueous Media

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Vitamin B_6, also called pyridoxine, is one of 8 B vitamins. All B vitamins help the body convert food (carbohydrates) into fuel (glucose), which is used to produce energy. These B vitamins, often referred to as B-complex vitamins, also help the body metabolize fats and protein. B-complex vitamins are needed for healthy skin, hair, eyes and liver. They also help the nervous system function properly [1].

Electronic spectral behavior and complex formation reaction for pyridoxine in various non-aqueous media for understanding of these media function has been investigated. In this research, the complex formation reaction of $C_8H_{12}ClNO_3$ pyridoxine ligand with nitrate salts of cadmium, nickel, zinc, mercury, cobalt and copper in binary solvents of acetonitrile and dimethyl sulfoxide has been investigated [2]. According to the experiments conducted in this study, the best non-aqueous solvent was dimethyl sulfoxide, because the pyridoxine is dissolved in the presence of this solvent and reacted to the complex formation reaction.

The trmodynamic of complex formation reaction was studied spectrophotometrically and the formation of both 1:1 and 1:2 complexes with Pyridoxine and cations was stablished. The complex formation constants K_f were determined by computer fitting of the absorbance – mole ratio data. The presence of isobestic points confirmed the formation of simple complex formation. By decreasing the proportions of the dimethyl sulfoxide, the formation of the complexes increases, which correlates with the solvent receptor.

Pyridoxine

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Paper code: 885

A high-capacitance flexible solid-state super capacitor based on polyvinyl chloride, carbon nanotubes and polyaniline

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Flexible super capacitors are desirable as potential energy storage systems for wearable technologies [1,2]. Herein, we synthesize PVC-MWCNT-PANI nanocomposite films via sonicating of a mixture containing poly vinyl chloric, multi walled carbon nanotubes and polyaniline in NMP solvent and then drying in 100 °C. The surface morphology of the fabricated films was characterized using scanning electron microscopy (SEM) while their electrochemical activity was investigated using cyclic voltammetry (CV), galvanostatic charge/discharge and electrochemical impedance spectroscopy (EIS) procedures. The electrochemical measurements of the samples confirmed that PANI-PVC film does not show suitable capacitive behavior where the introduction of MWCNTs in the composite can significantly improve the capacitive behavior characteristic of PANI-PVC film. The modified electrode exhibited much higher specific capacitance (20 mF cm^{-2}) compared to the PVC-MWCNT (3 mF cm^{-2}) at a current density of 0.5 mA cm^{-2}, indicating its great potential for flexible super capacitor applications.

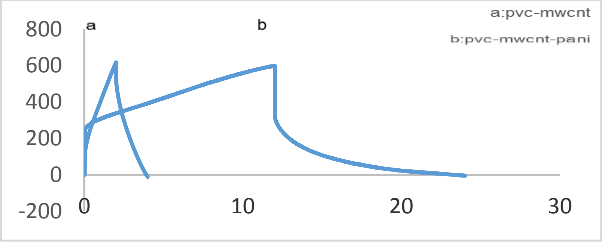

Fig. 1 Galvanostatic charge–discharge curves.

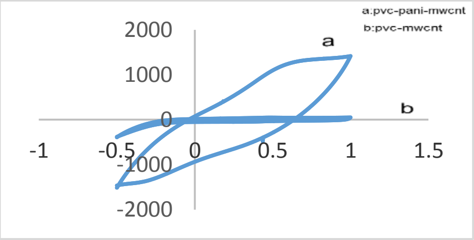

Fig. 2 Cyclic voltammograms plots.

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Paper code: 905

Determination of pK_a of Cinnamic acid using Net analyte signal as a chemometric method on the spectrophotometric data

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The acidity constants of organic compounds have an important role in some analytical methods such as acid-base titration, solvent extraction, ion transfer and complex formation [1-3].In the present paper, Net analyte signal analysis (NAS) has been used to the spectrophotometric investigations of the pKa of Cinnamic acid in water at 25 ˚C. NAS is an efficient chemometrics algorithm for analysis of acid–base equilibrium systems by spectrophotometric method.The contribution of species which have spectral overlapping with other have been obtained from the absorbance data matrix by NAS. This process made the determination of successive acidity constant of Cinnamic acid feasible. There was a very close the resulted values by NAS (pK_a=4.46) and the declared values (pK_a=4.44).

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Paper code: 906

Spectrophotometric determination of acidity constant of Cinnamic acid using rank annihilation factor analysis (RAFA)

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A significant parameter for understanding and quantifying chemical phenomena reaction rates, biological activity, biological uptake, biological transport and environmental fate [1] can be dissociation constants. In order to the determination of dissociation constants, several procedures such as potentiometric titration, spectrophotometric determination and conductometry, have been reported [2,3]. Rank annihilation factor analysis (RAFA) was a means employed in order to determine spectrophotometrically the acidity constant of Cinnamic Acid in water at 25 ˚C and an ionic strength of 0.1 M. A general method in rank annihilation factor analysis (RAFA) is annihilation of the contribution of one chemical component from the original data matrix. The contributions HA were annihilated from the absorbance data After recording the electronic absorbance spectra of the acid at different pH, making possible the determination of successive acidity constant. It was obtained that there was a very close and exact agreement between the resulted values by RAFA (pK_a=4.44) and the declared values(pK_a=4.44).

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Paper code: 914

Designing paper biosensors to the colorimetric measurement of bisphenol A by using gold nanoparticles modified with aptamer

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Different methods for measuring bisphenol A have been reported, which are often expensive and require professional knowledge. The first approach is to provide a low-cost method for measuring bisphenol A by available devices [1]. aptamer and gold nanoparticles are interconnected. A specific concentration of NaCl being added to the obtained red solution [2]. Then the red solution is dropped on the hydrophobic paper and the image is recorded by the scanner. In the next step, the bisphenol A solution is added to it and the color changes from red to blue. scaning is being done again and color analysis is performed by adobe Photoshop software. The color intensity will be proportional to the concentration of bisphenol A. The limit of visual detection (LOD) was found to 0.23 ng/L by photoshop software analysis. This is a new method for measuring bisphenol A in which Wattman paper is used as a reaction bed. And the available software such as adobe Photoshop and computer is used to quantitatively and quantitatively measure bisphenol by colorimetry. This method is able to measure bisphenol A at 1ppt level quantitatively and shows it's sensitive. This is an efficient method for measuring bisphenol A in water samples.

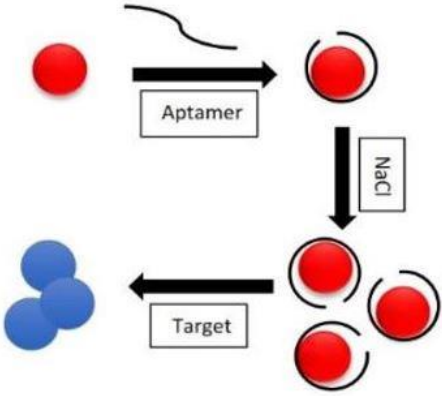

Fig. 1 Color change process

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Paper code: 915

Simultaneous determination and pharmacokinetic study of antidiabetic drugs by HPLC-UV using novel MSPE method

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Herein, silica-coated iron oxide magnetic nanoparticle modified with imidazolium-based polymeric ionic liquid (Fe_3O_4@SiO_2@PIL) was used as a sustainable sorbent for reliable magnetic solid-phase extraction (MSPE) and simultaneous preconcentration and determination of trace three antidiabetic drugs involving empagliflozin, canagliflozin and metformin in human plasma by HPLC-UV. The predominant factors affecting the extraction efficiency of the analytes were investigated in detail and optimized with one at a time approach. The limit of detections (LODs, S/N = 3) for empagliflozin, metformin and canagliflozin were 1.3, 6.0 and 0.8 ng mL^{-1}, respectively. Reasonable linearity ($0.997 \geq r^2 \geq 0.993$) and broad linear concentration ranges of 5.0–1200.0, 20.0-1800.0 and 5.0–1000.0 ng mL^{-1} were obtained for empagliflozin, metformin and canagliflozin, respectively [1]. Satisfactory intra-assay (3.8-7.5%, $n = 9$) and inter-assay (3.2-8.5%, $n = 12$) precisions as well as remarkable accuracies (≤ 9.1%) displayed good efficiency of the method [2]. Ultimately, the method was applied for the quantitation of low dose administration of invokamet in 4 healthy fed participants after oral administration and main pharmacokinetic data such as; T_{max}: 3.2 ± 0.3 and 4.1 ± 0.5, C_{max}: 390.4 ± 50.2 and 859.7 ± 91.2 for CANA and MET were achieved respectively.

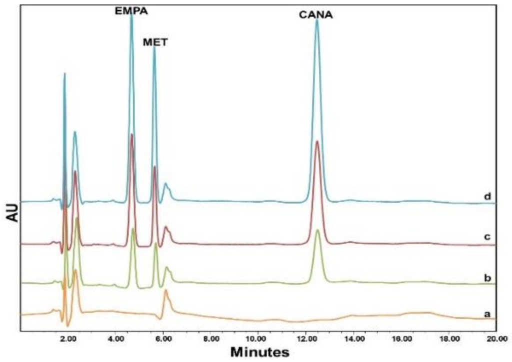

Fig. 1 The chromatograms of EMPA, MET and CANA in human plasma; (a) blank; spiked plasma at (b) 100.0 ng mL^{-1}, (c) 250.0 ng mL^{-1} and (d) 400.0 ng mL^{-1} concentration levels of each drug

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Paper code: 919

Cobalt-Nickel Loaded on Hydroxyapatite Wrapped Multiwalled Carbon Nanotubes as a New Catalyst for Oxygen Evolution Reaction

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A new catalyst based on MWCNTs coated with Hydroxyapatite (HA) was used for oxygen evolution reaction (OER) in alkaline media by immobilizing Ni and Co in the HA/MWCNTs structure. The solid state approach was used for synthesis of HA/MWCNTs and simple impregnation method was applied for loading Ni and Co on the HA/MWCNTs [1]. The mono and bimetallic catalysts were casted on a glassy carbon electrode which was finally coated with a Nafion layer. Different conditions such as the percentage of HA, amount of Ni and Co in the impregnation solution and the loading of Nafion were optimized. Under the optimized conditions, the best activity for OER was obtained for the bimetallic catalyst containing Ni and Co (Fig. 1). In fact, the best OER result was achieved via loading of Ni and Co ions on 40% HA /MWCNTs composite from an equimolar (50mM) impregnation solution of Ni^{2+} and Co^{2+}. The onset potential of 1.50 V (vs. RHE) and high stability during 10000s were achieved using this ideal catalyst.

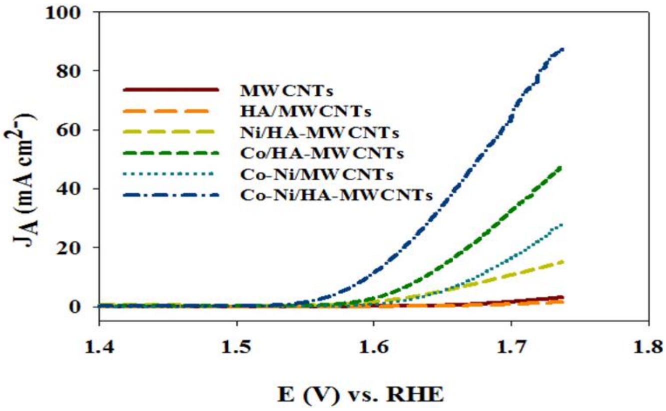

Fig. 1 linear sweep voltammetry (LSVs) of OER activity of different electrodes

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Paper code: 920

Designing and fabrication of novel electrochemical sensor for simultaneous determination of hydroxylamine and phenol

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Hydroxylamine, NH_2OH, and phenol have received growing attention due to thier extensive application in manufacturing of semiconductors, pharmacologica industry, agriculture, military and industrial fields [1]. Despite these benefits, they are toxic and harmful to humans, animals, and even plants. These substances may cause harmful effects on the central nervous system, heart, liver and kidneys in addition to inhibit a number of cellular enzymes. Also, they are irritant of skin, eyes and mucous membranes [2]. Thus, using of a sensitive analytical method for the simultaneous determination of hydroxylamine and phenol at low concentration is of great importance in biological processing, industrial and environmental fields and pharmacologica industry. So that, in this work, a sensitive voltammetric sensor based on a carbon paste electrode modified with MgO nanoparticle and organic compound as a modifier was designed for determination of hydroxylamine. The modified electrode demonstrated wide linear range from 5.0 to 650.0 µM and low detection limit of 1.65 µM for hydroxylamine. Also, the designed electrode was used to simultaneous determination of hydroxylamin and phenol.

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Paper code: 930

Fabrication of an optical pH sol-gel sensor based on Thionine dye

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In the present work, an optical chemical sensor was constructed by incorporating the thionine (TN) dye molecules (Figure 1) into a sol-gel silica matrix and it was used for determination the pH of the aqueous solutions. Entrapment of TN dye molecules into the silica matrix, was made via an acid-catalyzed sol-gel reaction of tetraethyl orthosilicate (TEOS) and the thionine molecules [1]. The thionine molecules in the immobilized form, showed a different spectral behavior than its solution form. After optimization the experimental conditions, the fabricated optical sensor showed a fast response to pH changes in the range of 11-13 with a response time about one minute. The experimental results, showed that the proposed pH sensor, has a good reproducibility and stability and also a low leaching and a long lifetime of over 7 months. The fabricated optical sensor can be used for pH measurement in real samples.

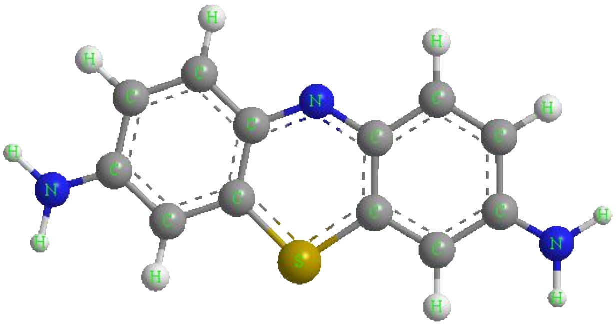

Fig. 1 The chemical structure of Thionine acetate.

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Paper code: 936

Zn^{2+}-mediated fluorescent ZnS quantum dots as indirect sensor for selective and sensitive detection of glutathione

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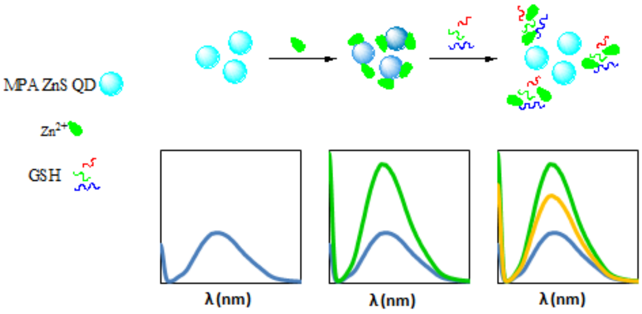
The QDs-based fluorescence chemosensing could be performed by different strategies. In many analytical sensing procedures, handling the surface chemistry of quantum dots (QDs) has been utilized to achieving the goal, according to the interaction between the mediator and QDs surface as well as the analyte and mediator [1,2]. In this study, an indirect turn-off fluorescence sensing strategy was proposed for the determination of reduced glutathione (GSH), utilizing the zinc sulfide quantum dots. The quantum dots were prepared by precipitation method using mercaptopropionic acid as stabilizer (MPA-ZnS QDs). The fluorescence of the water soluble ZnS QDs, changed very slightly with the direct addition of GSH. Interestingly, the emission of ZnS QDs can be strongly ameliorated in the presence of Zn^{2+} and subsequently, this fluorescence intensity was efficiently quenched by different concentrations of GSH. The fluorescent Zn^{2+}-MPA-ZnS QDs hybrid system was developed for the detection of GSH with a LOD of 0.920 µM and a linear range of 2.0-104.0 µM. The RSD for five replicate measurements of 65 µM GSH was 1.9%. To examine the selectivity of Zn^{2+}-MPA-ZnS QDs set for GSH, the effect of some substances, including amino acids, dopamine, urea, uric acid, ascorbic acid, glucose, sucrose and fructose was studied. The quenching effect of GSH on this hybrid system was significantly higher than all of the investigated species. The fluorescence spectra were recorded by a Perkin-Elmer luminescence spectrometer (model LS-50B, 3.5 cm × 1.0 cm × 1.0 cm quartz cell, excitation and emission wavelength were 305 and 425 nm, respectively)



The general approach for GSH detection by using the surface passivated QDs.

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Paper code: 944

Modified Graphite Paste Electrode with Strontium Phen-Dione Complex for Simultaneous Determination of a Ternary Mixture of 4-aminophenol, Uric Acid and Tryptophan

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For the first time, the $[Sr(OH_2)_4(phen\text{-}dione)_2](Cl)_2$ complex (Sr-Phen) was synthesized and characterized by different spectroscopy techniques such as ^{1}H-NMR, UV-Vis, FT-IR as well as elemental analysis. The prepared complex was used for modification of graphite paste electrode for simultaneous determination of 4-aminophenol (AP), uric acid (UA), and tryptophan (Trp). Detailed investigations by electrochemistry methods were used in order to elucidate the properties of the modified graphite paste electrode with Sr-Phen. The proposed modified electrode displays intense and indelible electrooxidation responses for simultaneous determination of AP, UA, and Trp to three well-separated peaks in potential range from 0.4 to 1.1V using cyclic and differential pulse voltammetry methods in pH 2.0. Based on the experimental results the detection limits of 3.40, 1.06 and 1.32 µM were obtained for AP, UA and Trp, respectively. Finally, the proposed modified electrode was used for simultaneous determination of AP, UA and Trp in real samples.

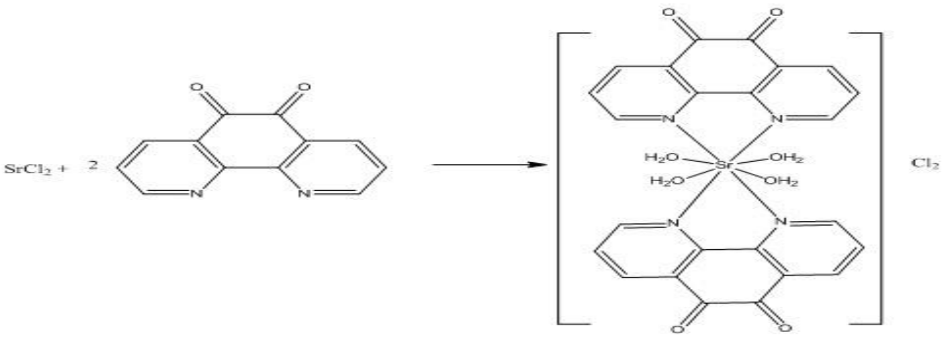

Fig 1. The proposed structure of $[Sr(phen\text{-}dione)_2(OH2)_4](Cl)_2$ complex.

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Paper code: 945

Modified Graphite Paste Electrode with Strontium Phen-Dione Complex for Simultaneous Determination of a Ternary Mixture of Dopamine, Acetaminophen and Xanthine

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In this study, modified graphite paste electrode with $[Sr(OH_2)_4(phen\text{-}dione)_2](Cl)_2$ complex (Sr-Phen) was used for simultaneous electrochemical determination of dopamine (DA), acetaminophen (AC), and xanthine (XN). The proposed modified electrode was shown a sensitive and selective response for simultaneous determination of DA, AC and XN to three well-separated peaks in the potential range from 0.4 to 1.1V using CV and DPV methods in a phosphate buffer solution with pH 3.0. Some kinetic and thermodynamic parameters for the electrochemical oxidation of DA, AC, and XN were also determined. Under the optimum conditions the calibration curves were linear up to 220, 150 and 60 µM with a theoretical detection limits (S/N=3) of 800, 90 and 60 nM for DA, AC, and XN, respectively. Moreover, GPE/Sr-Phen were successfully used to determine DA, AC, and XN in human urine and blood serum samples.

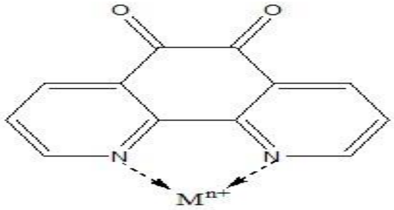

Fig 1. Chemical structure of phendione ligand coordinated to metal ion (M^{n+})

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Paper code: 965

Preconcentration and determination of phenylalanine in some pharmaceutical and food samples by cloud point extraction coupling with UV-Visible spectrophotometry

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Phenylalanine (Phe) is an essential amino acid, which is necessary for infants' growth and nitrogen equilibrium in adults. However, phenylalanine's accumulation could cause neurological damages which are the results of deficiency in phenylalanine hydroxylase enzyme, considered as the major enzyme for its metabolism. (1)This enzyme typically begins the procedure of parsing of phenylalanine amino acid molecules which is essential for protein synthesis in the body mutations in the phenylalanine hydroxylase gene will cause a disease called phenylketonuria (PKU).

In this work,(2) cloud point extraction in combination with UV-visible spectrophotometry, was used for the extraction of Phenylalanine from some pharmaceuticals and dietary drinks. Lauryl alcohol, 7 ethylene oxide (LAE 7) was used as surfactant for separation and preconcentration of Phenylalanine from sample solutions. Some important parameters such as surfactant concentration, extraction time, temperature and pH were investigated and optimized in order to maximize the extraction efficiency. It was observed that the maximum efficiency of phenylalanine extraction was obtained with 20% (V / V) surfactant LAE 7, 30 minutes at 60 ° C and pH 8.under optimized conditions, the calibration range for L-Ph 10-1000 mg / L^{-1} with a detection limit of 0.1 mg / L and precision as a standard deviation in the range of 0.4-0.9% .This method has been successfully used to determine phenylalanine in real samples, including colchicine1, ciprofloxacin 500 and Co-Trimoxazole 400/80 tablets and dietary drinks.

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Paper code: 967

Trace determination of nitrotoluenes in water by hollow fiber protected stir bar liquid phase microextraction based on magnetic ionic liquids

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In this work, a novel hybrid approach called hollow fiber protected stir bar liquid phase microextraction (HF-SBLPME) that combines the advantages of stir bar sorptive extraction (SBSE) [1] and hollow fiber protected liquid phase microextraction (HF-LPME) [2] has been employed for the accurate and sensitive determination of ten nitrotoluenes (NTs) in complex water samples. The extraction is carried out using a 2cm hollow fiber which was also filled with a magnetic ionic liquid (MIL) as extraction phase, in such a way that the MIL inside the hollow fiber is stirred in the solution at high stirring rates. Five magnetic ionic liquids ($[\text{aliquat}^+]_2[\text{MnCl}_4^{2-}]$, $[\text{P}_{6,6,6,14}^+]_2[\text{MnCl}_4^{2-}]$, $[\text{P}_{6,6,6,14}^+][\text{Ni(II)(hfacac)}_3^-]$, $[\text{P}_{6,6,6,14}^+][\text{Dy(hfacac)}_4^-]$ and $[\text{P}_{6,6,6,14}^+][\text{Mn(hfacac)}_3^-]$) were evaluated as extraction solvents. Once the stirring is ceased, the hollow fiber was magnetically stirred into the sample solution, and subsequently the MIL along with concentrated analytes were subjected to a gas chromatography-mass spectrometry (GC-MS) system. The main parameters that affecting the extraction efficiency (i.e., MIL amount or hollow fiber size, pH of solution, extraction time and ionic strength) were evaluated by Response Surface Methodology (RSM) and a multivariate optimization was done using Box-Behnken Design (BBD) [3]. Under the optimized conditions, the method was successfully validated showing good linearity ($R^2 \approx 0.986$), dynamic linear range (30 ng.L^{-1}-0.05 mg.L^{-1}), limits of detection and quantification in the low ng.L^{-1} levels (less than 10 ng.L^{-1}), good intra- and inter-day repeatability and reproducibility (RSD<7%) and good enrichment factors (1950-2785). This sensitive analytical method was applied to the determination of trace amounts of NTs in two natural water samples (industrial and rainwater) with satisfactory relative recovery values (91–106%), highlighting that the matrices under consideration do not affect the extraction process.

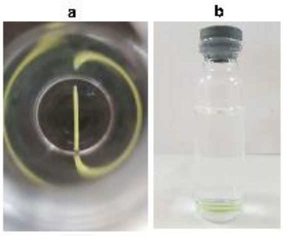

Fig. 1. Schematic image of HF-SBLLME fiber. (a) Top view (b) HF-SBLLME fiber in sample solution.

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Paper code: 968

Potentiometric Determination of HPO4$_2^-$ with Chitosan- Cu by Carbon Paste Electrode

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In the present work, using modified copper chitosan, HPO_4^{2-} anion is measured by potentiometric method. A room temperature ionic liquid, 3-methyl-imidazolium tetrafluoroborate and paraffin for compare of conductive effect are used. Response time, pH range, electrode selectivity, electrode life have been investigated. Carbon nanotubes (WCNTs) were used in the composition of the carbon paste to improve conductivity and transduction of chemical signal to electrical signal. Also, the effect of different carbon nanotubes (single-wall carbon nanotubes, multi-wall carbon nanotubes and COOH functionalized single-wall carbon nanotubes, COOH functionalized multi-wall carbon nanotubes and NH_2 functionalized single-wall carbon nanotubes and NH_2 functionalized multi-wall carbon nanotubes) on the electrode's response has been investigated. The electrode has a short response time (~5 s) and can be used for at least 50 days without any considerable divergence in potentials, and the working pH range was 6.9–8.3. fabricated sensor for determining of HPO_4^{2-} demonstrated a maximum Nernstian slope equal to 29.2 mVdecade^{-1} along a linear range from 1×10^{-6} to 1×10^{-2} mol.L^{-1} and detection limit of 4.35×10^{-7} mol.L^{-1}. Finally, the proposed electrode was successfully used as an indicator for potentiometric determination of HPO_4^{2-} in Hydroponic farm wastewater samples.

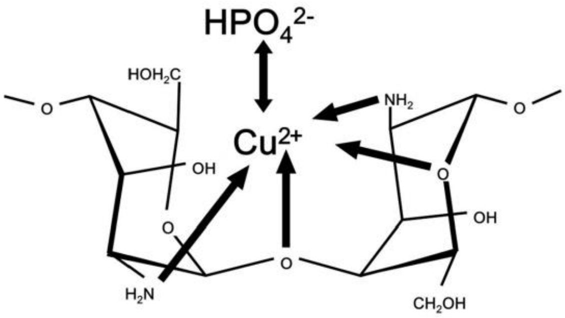

Fig. 1 The The proposed mechanism of crosslinking on a chitosan bead using Cu(II).

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Paper code: 980

Analysis of antidepressant drugs by using HS-SPME based on nano-structured conductive polymer fiber couple to ion mobility spectrometry

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This work describes the development of a simple, rapid, and selective method based on headspace solid-phase microextraction combined with ion mobility spectrometry (IMS-HS-SPME) equipped with corona discharge ionization for determination of antidepressant drugs such as sertraline, imipramine and alprazolam. The fiber was coated using electrochemical deposition technique. The effect of type of anion dopants on the extraction characteristics of the fiber was investigated. The sulfonated reduced graphene oxide (SRGO) and dodecyl benzenesulfonate were used as anion dopant. The extraction properties of these two fibers toward antidepressant drugs were studied using a HS-SPME devise. The results showed that PPy-DS possesses a better efficiency toward the sertraline than PPy doped with PPy-SRGO. The HS-SPME system was equipped with a cooling device on the upper part of the sample vial and a circulating water bath for adjusting the sample temperature [1]. The HS-SPME conditions such as solution pH, extraction time, extraction temperature, salt effect, desorption time, and desorption temperature were investigated and optimized [2]. The calibration graph was linear in the range from 100 ppb to 3 ppm, and the detection limit was 100 ppb. Finally, the proposed IMS-HS-SPME method was applied for analysis of antidepressant drugs in real samples.

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Paper code: 987

Pesticides determination in crops by solvent assisted stir bar dispersive solid phase microextraction based on magnetic nano-composites

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In this study, a novel method combining the principles and benefits of solvent assisted dispersive solid phase microextraction (SA-DSPME) [1] and stir bar sorptive extraction (SBSE) is presented. This new approach, termed solvent assisted stir bar dispersive solid phase microextraction (SA-SBDSPME), involves the addition of a magnetic nano composite (MNC) and a neodymium-wire (1.5 cm) magnetic stir bar into the sample solution. The proposed method was based on the dispersion of the synthesized MNC (Nio@TiO2@GO-CTAB) into the aqueous sample to maximize the interaction surface. In this way, the dispersion of the sorbent at a very low milligram level was received by injecting a solution of the MNC and disperser solvent into the aqueous sample. The cloudy solution created from the dispersion of the MNC in the sample solution. In the high stirring rates, the rotational forces surpass the magnetic field and the MNC disperses into the sample solution in a similar manner to DSPME. But, As long as the stirring rate is maintained at low speed, the MNC resists rotational (centrifugal) forces and remains on the stir bar surface in a manner closely resembling SBSE. After extraction, the stirring is stopped and the MNC returns to the neodymium-wire without the requirement of an additional external magnetic field. The MNC-coated stir bar containing the preconcentrated analytes is thermally desorbed directly into a gas chromatographic system coupled to a mass spectrometric detector (TD-GC-MS) using a SPME syringe. Several parameters affecting the extraction efficiency were studied by Fractional Factorial Screening (FFS) and a multivariate optimization was done using Central Composite Design (CCD) [2]. To prove the utility of the proposed method, the extraction of nine organophosphorus pesticides from typical agricultural crops was done as model analytical application and excellent analytical features were achieved in terms of linearity ($R^2 \approx 0.991$), enrichment factors (1925–2644), limits of detection (lower than 20 $ng.L^{-1}$), intra- and inter-day repeatability and reproducibility (RSD<6%) and relative recoveries (94-102%, 91-103% and 92-105% for rice, tomato and onion samples, respectively).

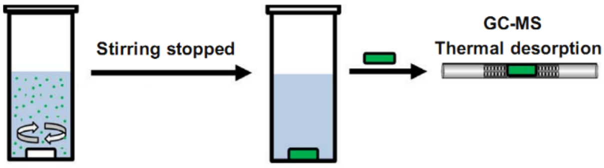

Fig. 1. Schematic diagram of SA-SBDSPME.

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Paper code: 996

Voltammetric determination of hydrazine at the surface of a modified carbon paste electrode with TiO_2 nanoparticles

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Hydrazine (N_2H_4) is a small and reactive molecule with powerful reducing capabilities. As known, hydrazine and its derivatives have different usages such as using in pesticides, chemical blowing agents, pharmaceutical intermediates and photography chemicals [1]. Despite these benefits applications for hydrazine, it is volatile and toxic and is absorbed by oral, dermal, or inhalation routes of exposure [2]. Critical exposure is able to damage the liver, kidneys, and central nervous system in humans. Thus, a sensitive analytical method for determination of hydrazine at low concentration is great importance in biological processing, industrial, environmental fields and pharmacological industry. The fabrication of electrodes modified with nanoparticles has been the focus of recent attention owing to enhancement of the response signal, increased sensitivity and better reproducibility. So that, in this work, a sensitive voltammetric sensor based on a carbon paste electrode modified with TiO_2 nanoparticle and organic compound as a modifier was designed for determination of hydrazine. The modified electrode demonstrated wide linear range from 20.0 to 620.0 µM and low detection limit of 6.67 µM for hydrazine. Also, this sensor was used for determination of hydrazine in real samples.

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Paper code: 998

Combining magnetic solid-phase extraction and dispersive liquid-liquid microextraction methods for preconcentration environmental pollutants

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In this study, the combination of two methods of magnetic solid-phase extraction (MSPE) and dispersive liquid-liquid microextraction (DLLME) was used to preconcentration of polycyclic aromatic hydrocarbons (PAHs) in aqueous samples. To perform of MSPE procedure, a magnetic graphene modified with polyaniline (Fe_3O_4@GO/PANI) was synthesized and characterized by scanning electron microscopy, Fourier-transform infrared spectroscopy and vibrating sample magnetometer. The PAH compounds were initially extracted by MSPE and the desorption solvent was used as a dispersing solvent in the DLLME method. Finally, the extraction solvent was injected into the gas chromatography for the determination of polycyclic aromatic hydrocarbons. The factors affecting the efficiency of both extraction methods include adsorbent amount, desorption conditions, extraction time, salt concentration, sample pH, extraction solvent and volume, which were investigated and optimized [1,2]. The method showed good linearity in the range 0.03–100 ng mL^{-1} for all analytes, with correlation coefficients ranging from 0.9920 to 0.9948. The method detection limits (S/N=3) were in the range of 0.01–0.05 ng mL^{-1} and the limits of quantification (S/N=10) between 0.03–0.1 ng mL^{-1}. Repeatability of the method was assessed through five consecutive extractions of independently prepared solutions at concentrations of 0.1, 10 and 100 ng mL^{-1} of the compounds. The repeatability was obtained in the range of 3.1–8.2%. The proposed method was successfully applied in the analysis of PAHs in environmental samples (tap, well and wastewater samples). The recoveries of the method ranged between 89.6–98.1%. The procedure proved to be efficient, environmentally friendly and fast.

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Paper code: 1003

Modification of carbon nanotubes with a Keplerate polyoxomolybdate as efficient sorbent for the extraction (HF-μ-SPE) of naproxen in hair samples

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In continuation of our ongoing research on the development of novel catalytic methods for oxidation of organic compounds in green media [1-3], we describe the modification of CNT with polyoxomolybdates. In this work, we described a synthesis method of the polyoxomolybdate (POMo) and the modification of carbon nanotube (CNTs) through a chemical modified approach. POMo was prepared by a one-step reaction at room temperature and characterized by FT-IR, XRD, Uv-Vis and TEM [4]. These uniform nano-polyoxomolybdate has an average size of 5–25 nm. In this research, the Keplerate carbon nanotubes/silica composite was used in the pores and lumen of a hollow fiber as the hollow-fiber micro-solid-phase extraction device. Based on chemical adsorption between POMo and carboxylic acid groups in CNT, which were introduced to the CNTs by adding dilute nitric acid, POMo was successfully located on the CNTs as the modifier. The hollow-fiber was used for the microextraction of the analyte from hair sample under the optimized conditions as sensitive technique to determinate naproxen. After optimizing the reaction conditions (pH, salt, volume of donor and desorption phase, extraction and desorption time), extraction of naproxen in the presence of hollow-fiber combined with fluorescence spectrophotometry was performed.

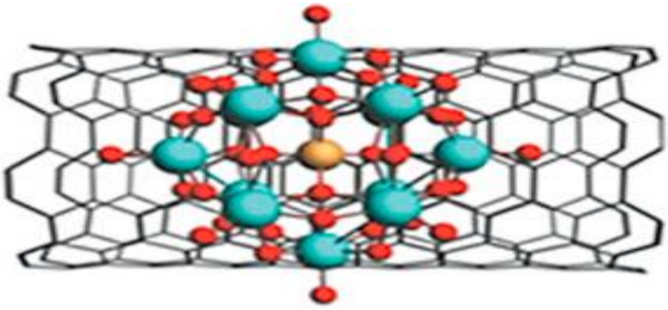

Fig. 1 Representation of models under study

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Paper code: 1014

A new, facile and efficient agarose gel based electromembrane extraction for preconcentration, clean up and determination of propranolol in blood serum

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In obtaining more reliable results regarding the procedure type, a suitable sample preparation technique is required for preconcentration and cleanup of the real samples [1-2]. Herein, for the first time a new, rapid and efficient method was developed to determine a drug named propranolol in blood serum, using agarose gel based electromembrane extraction technique (AG-EME). In order to facilitate the migration of propranolol from sample solution through agarose gel membrane, an electrical driving force was used. The variables influencing the extraction efficiency were electrical field voltage (V), amount of agarose in membrane (w/v%), amount of acetic acid in membrane (w/v%), pH of donor (pH_d) and acceptor (pH_a) phase, and extraction time (min). The first three variables were investigated based on one variable at a time. The other variables were modeled and optimized utilizing response surface methodology (RSM). Based on the non-linear Nelder-Mead optimization, at pH_d=7.9 and pH_a=3.3 with extraction time of 37 min, the maximum predicted extraction efficiency (98.8±2.2) was in agreement with the experimentally acquired value (99.2±7.0). Limits of detection (LOD) and quantification (LOQ) were 0.09 and 0.29 $\mu g\ mL^{-1}$, respectively. The method was used to determine the propranolol drug in the blood serum sample at different concentration levels.

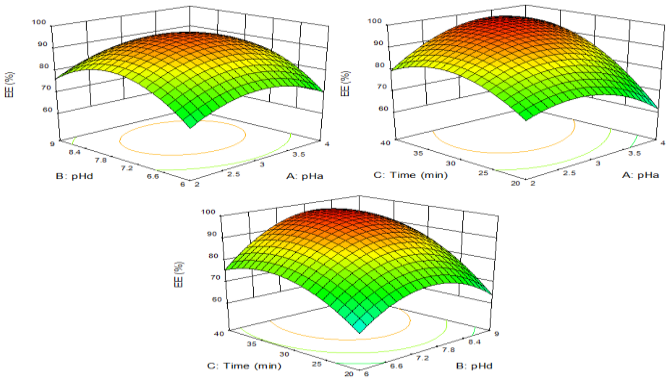

Fig. 1 The response surface plots for extraction and determination of propranolol by the proposed AG-EME procedure.

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Paper code: 1020

High-Performance Visible-Light-Driven Ag–gC_3N_4/Pt Photoelectrocatalysts for Methanol Oxidation

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The world's demand for energy has increased dramatically over the last few decades and will continue to do so. Therefore, it is urgent to find alternative energy sources and perhaps unconventional way of energy conversion with much improved energy efficiency [1]. Fuel cells have received increasing attention because of their high energy conversion efficiency and environmental affinity [2]. Among different type of fuel cells, direct alcohol fuel cells (DAFCs) were attracting increasing interest as a compact power sources for portable applications, mainly due to the relatively simple handling, storage, and transportation of the fuel [3]. Among fuel cells, the direct methanol fuel cell (DMFC) is one of the most attractive ones because of high energy conversion efficiency and low environmental intrusion and without a reformer [4-7].

Traditional electrocatalysts together with optically active semiconductors are selected as the promising catalysts for the improvement of anodic reactions. In order to fabricate the modified electrode, firstly, Pt nanoparticles were electrodeposited on the surface of FTO electrode. Then, graphite carbon nitride (gC_3N_4) decorated with silver nanoparticles (Ag NPs) was casted on the surface of Pt/FTO electrode. The Ag–gC_3N_4/Pt/FTO electrode displayed much higher catalytic properties for methanol oxidation compared to the Pt/FTO electrode. Interesting, when the modified electrode was upon visible light irradiation, both the catalytic activities and stabilities were improved greatly. The synergistic effect of Pt catalyst and photo-irradiation promotes the electrocatalytic performance and stability. Our result provides a new insight into developing highly efficient photoelectrocatalyst for application in direct methanol fuel cells in the presence of visible light illumination.

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Paper code: 1021

A novel visible light photoelectrochemical aptasensor for detection of bisphenol A

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BPA (bisphenol A) is an organic compound that is widely used to make epoxy and polycarbonate resins [1]. Epoxy resins are used extensively for many applications such as industrial flooring, adhesives, sealants, can coating and printed circuit boards [2]. Polycarbonate resins are light-weight, high performance plastics that are mainly used to make medical equipment, water bottles, digital media (e.g. CDs and DVDs) and some reusable food-contact containers [3]. The safety of BPA has been extensively studied. Numerous scientific studies and government assessment show that human exposure to BPA which is released into environment from manufacturing processes or plastic products under severe conditions (e.g. acidic, basic and other physical conditions) can affect the functions of brain, thyroid, ovary, reproductive organs and increasing the rate of cancer [4]. Therefore, it is important to determine the BPA level in food samples and environment. Photoelectrochemical (PEC) detection represents a novel and dynamically developing analytical technique which has attracted substantial research scrutiny for its satisfactory analytical performances [5]. PEC detection possesses potential merits than traditional electrochemical methods because of its total separation and different energy form of the excitatil (photocurrent). Different from electrochemical analysis, PEC detection system requires a photoactive working electrode to produce photocurrent signal under photoirradiation.

In this study, Ag-gC_3N_4 nanocomposite was used as novel photoactive materials to establish the PEC aptasensor for the detection of BPA. Here, first of all, the Ag-gC_3N_4 nanocomposite was immobilized on the surface of FTO electrode. Then the electrode was electrodeposited with gold nanoparticles (Au NPs). In the next step, SH-aptamer was adsorbed on the Ag-gC_3N_4/Au NPs nanocomposite through S-Au bond. Under optimal conditions, the proposed sensor showed a low detection limit and good selectivity for target analysis. The potential applicability of the PEC aptasensor was confirmed by detecting BPA in real samples.

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Paper code: 1028

A simple visual and highly selective colorimetric analysis of Dopamine based on gold nanoparticles decorated- Polyoxometalate using smart camera phone

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Dopamine (DA), is intensively involved in the normal functions of daily life, including movement, feeding, and neurocognition. Moreover, a number of neurological disorders such as Parkinson’s disease and schizophrenia are highly correlated to DA concentration [1-3]. Gold nanoparticle (AuNP)-based colorimetric assays are emerging as alternative approaches for detection, providing high sensitivity, specificity and ease of signal read-out. So, in this work we used various POM (polyoxometalate) - modified gold nanoparticles that synthesized in different condition. The developed approach is simple, without using complex financial instruments and adding other metal salts or ions for improving sensitivity. Dopamine induces the aggregation of POM-AuNPs, this resulting in a color change from pink (pale red) to blue or purple. The color change was in situ monitored for the quantitative determination of dopamine by using digital camera. Our results revealed that the method exhibited a dynamic range of 0.05-20 mg/L with a limit of detection of 0.01 mg/L.This method could provide quantitative information very conveniently. The purpose of this study were to develop, fast, simple and reliable apply colorimetric by digital camera method for quantification of dopamine (DA).

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Paper code: 1029

Dressed-up gold nanoparticles as the colorimetric nano-sensor for simple assay of acetaminophen in biological samples

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Acetaminophen (APAP) toxicity may be the consequence of either an acute overdose [1]. Therapeutic levels are 5-20 µg/mL (33-132 µmol/L) [2]. various chromatographic techniques, have proved to be reliable and accurate methods for quantifying APAP concentrations in biological samples [3]. However, these approaches require complex sample preparation procedures, expensive and bulky instruments, and professionally trained personnel running the tests. Therefore, they are not well suited for rapid on-site detection of APAP and may not even be available for use in developing countries. Resently, gold nanoparticle (Au NP)-based colorimetric assays are emerging as alternative approaches for detection, providing high sensitivity, specificity, and ease of signal read-out. So, in this work we used POM-(polyoxometalate) modified gold nanoparticles that synthesized by Sonochemistry method in different temperature, potential and the proportions chloroauric acid and POM. Colorimetry was performed by a digital camera and the data was obtained by the Photoshop CC 2017 software. The method was optimized for effect of pH, reaction time, volume ratio of POM-Au NP, ambient light condition and light intensity. Under optimized condition linear range and limit of detection are 5-40 mg/L, 0.5 mg/l respectively. It is important to develop a quick, simple, reliable and sensitive method, which can detect APAP. We have effectively established a novel nanosensor with high sensitivity for the visual and quantitative detection of APAP in serum from animal samples.

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Paper code: 1030

Evolution of paper based analytical devices for fire assay- fluorimetric determination of gold in geological samples using camera smart phone

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Quantitative determination of gold is often an important aspect of the discovery, development, design and operation of the precious metals mine, as well as the associated concentrator or metal production plant. The fire assay process is still the most accurate and precise method for measuring the gold content in these samples [1]. The final stage in this technique can be different: gravimetric method, that is restricted by its relatively low sensitivity and instrumental methods, which are very expensive. Paper-based analytical devices have recently attracted a great deal of interest due to a simple structure, easy fabrication and use, lightness of weight, inexpensive materials, low consumption of reagents and samples and equipment-free readouts [2]. So, in this work we coupled fire assay with paper-based method. A paper-based microspot assay was created by use of printing on filter paper. The diameter of the detection region was 4 mm, requiring ca.0.5 µL of solution to fill with uniformity, so that the amount of reagents and samples was very lower than that of conventional liquid detection methods (2mL). Briefly, the paper loaded with rhodamine B then prepared samples with fire assay method spotted in the test zones. The $Aucl_4^-$ ion reacts with the cation of the reagent to form an association complex that decrease fluorescence intensity. The signal was measured with a simple homemade box containing UV lamp as a light source and cell phone as the detector. The fluorescence intensity was determined using Adobe Photoshop CS5 in luminosity mode [3]. LOD was obtained 1ppb that 10 times was better than fire assay- flame atomic absorption. Gold ore samples were assayed by µ-PAD and the results was compared to the conventional methods. T-test analysis assumed no differences in means between the results of the two methods at 95% confidence interval.

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Paper code: 1034

Basic charge storage mechanism of cobalt sulfide electrode material for supercapacitor

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Recently, since supercapacitors have received considerable attention, a large number of studies have been developed to create efficient electrodes to respond to ever-increasing demands of supercapacitors. The boundary between the electrochemical capacitors and batteries is less pronounced. The similar material may exhibit capacitor battery-like behavior depending on the charge storage guest ions and the electrode design. In this work a system containing cobalt sulfide (CoS) electrodes and KOH (6 Molar) as electrolyte, has been studied to check its ability as supercapacitor or battery. The amount of b-value can be used to prepare guidance for the practical design of high-performance electrode materials. In this report, the calculated b-value for cobalt sulfide electrode is closer to 1 in a very wide range of sweep rate (Fig.1). Therefore, the charge storage mechanism in these studied electrodes is capacitive rather than battery-type materials.

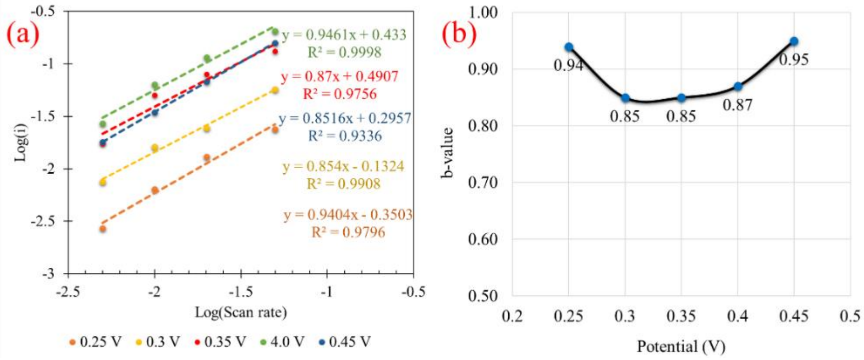

Figure 1: (a) linear plot between log i vs. log v in several potentials, (b) b-values in several potentials

Details of this procedure along with the obtained values are illustrated in Figure 1. It can be seen that the calculated *b*-value is closer to 1 in a very wide range of sweep rate (from 5 to 50 mV s^{-1}), charge storage mechanism in these studied electrodes is capacitive rather than intercalation/de-intercalation (battery-type).

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Paper code: 1035

Pt–Os–TiO_2 photoelectrocatalyst for methanol oxidation

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In recent decades, due to high energy demands, fossil fuel depletion, and environmental pollution throughout the world [1], there has been an increasing interest in the development of fuel cells, because they can directly convert chemical energy to electrical energy with higher efficiency than other sources of electrical power [2]. Among fuel cells, the direct methanol fuel cells (DMFCs) have attracted considerable interest because of a variety of merits such as low operating temperatures, ease of handling a liquid fuel, high energy density of methanol, and applications to microsized fuel cells [3–7].

Novel photoelectrocatalyst composed of Pt-Os-TiO_2/FTO was prepared electrochemically using a three-electrode system and directly electrodeposited on the surface of FTO (as working electrode). The photoelectrocatalyst with a composition of 18% TiO_2, 4% Pt and 3% Os showed the best performance for methanol oxidation. Scanning electron microscopy images showed that this composite film was even and porous. The photoelectrocatalytic oxidation behavior of methanol over the modified electrode has been studied by means of electrochemical techniques including, cyclic voltammetry and chronoamprometry methods, with or without UV illumination. Comparative experiments evince that the anodic current for methanol oxidation is increased up to 20% under UV illumination. Moreover, under UV illumination, the poisoning resistance of Pt-Os-TiO_2/FTO for methanol electrooxidation is significantly improved.

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Paper code: 1038

A liquid chromatography method for determination of p-cresol in human plasma by in situ surfactant-based solid phase extraction

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Recent researches on sample pretreatment and preparation methods have being oriented toward the development of efficient, economical, and miniaturized methods. In situ surfactant-based solid phase extraction (ISS-SPE) is a sample preparation technique in which the alkyl group of cationic surfactant interacts with the hydrophobic parts of an analyte and acts as an extraction medium. Then, the interaction between the surfactant and an ion-pairing agent forms very fine solid particles that could be dissolved in an appropriate solvent [1, 2].

A sensitive and reproducible high-performance liquid chromatography–fluorescence method was developed and validated for determination of p-cresol in plasma samples. ISS-SPE was proposed for pretreatment of plasma samples prior to HPLC analysis. The separation was carried out on a C_{18} column (250 × 4.6 mm, 5 µm) by isocratic elution with sodium acetate buffer (pH 3.8) and acetonitrile (40:60, v/v) as the mobile phase. The method was validated and found to be linear in the range of 0.5 to 8 µg mL^{-1} with the limit of quantification of 0.038 µg mL^{-1}. The variations for intra-day and inter-day precisions were both less than 8.2% and the extraction recoveries were more than 97%.

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Paper code: 1040

Application of smart camera phone for End point detection of precipitation titration technique

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Solution scanometry, a new, simple, fast and inexpensive method, was applied for the determination of the accurate detection of precipitation titration end points without using any indicator [1]. In this work we used mobile for detection of end points of the titration of sulfate by barium. The photo of cell containing precipitate was taked with a smartphone, and the image was analyzed in the CMYK and RGB color mode by a photoshop program [2]. The results revealed that among the color values, the magenta value was suitable for the accurate detection of end points. To improve the accuracy of the end point detection, second derivative titration curves were obtained. The titration errors were acceptable and were always less than 10%. The performance of our smart-phone method was also tested with water samples including city tap water, Lake and mineral water and satisfactory result was gained.

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Paper code: 1045

Application of ligandless liquid-phase microextraction based on a deep-eutectic solvent for determination of trace amounts of lead in edible oils by flame atomic absorption spectrometry

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In this work, a simple, sensitive, and efficient ligandless liquid-phase microextraction method based on a deep eutectic solvent for preconcentration of trace amounts of lead in edible oils is proposed. Flame atomic absorption spectrometry (FAAS) is used for the final analysis of lead. The green solvent of a deep eutectic type is formed by mixing choline chloride and tetra-n-butyl ammonium hydroxide (TBA) [1]. A 1:1 mixture of a deep eutectic solvent and 2% ethanol (200 µL) is added to an oil sample. The mixture is vortexed and transferred to a water bath and stirred for 5 minutes. After completion of the extraction, the phases are separated by centrifugation, and the enriched analytes in the deep eutectic solvent phase are determined by FAAS. In order to obtain the maximum extraction efficiency, the effects of some parameters such as the molar ratio of choline chloride/TBA (composition of the solvent), volume of ethanol as the diluent solvent, amount of sample, extraction time, and extraction temperature [2] are investigated. Under the optimized conditions, a linear range of 0.04-1.20 µg.mL^{-1}, a limit of detection of 0.015 µg.mL^{-1} and a preconcentration factor of 24.7 were obtained. Also, the relative standard deviations for six replicate determinations of lead were obtained to be 3.85%, 1.20% and 1.10% in 0.08, 0.5 and 1.0 µg mL^{-1}, respectively. The developed method was also successfully applied for the determination of lead in different edible oils.

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Paper code: 1063

Simultaneous Evaluation of Factors Affecting the Size of Gold Nanoparticles by Response Surface methodology

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Gold nanoparticles are of great interest for researchers in many fields [1]. The size distribution of the particles is an important physical characteristic that influences particle behavior [2]. Thus, the development of techniques for the controlled synthesis of gold nanoparticles of well-defined size is a big challenge [3].

In this work, Au NPs were synthesized using sodium borohydride as reducing agent. The effect of five parameters including the concentration of gold salt ($HAuCl_4$) and reducing agent ($NaBH_4$), the molar ratio of gold (in form of gold chloride) to reducing agent, the rate of addition of the reducing agent with aid of syringe pump and pH was studied on the size of generated gold nanoparticles calculated by using theory and UV-Vis spectrum of gold nanoparticles. Using the central composite design and response surface methodology (RSM), the quantitative relationship between the variables and their impacts on the response was investigated. Regression analysis based on $R^2{}_{(adj)}$ values for evaluating the optimum models was used. The best fitted empirical models achieved with $R^2 = 0.97$. Our results imply moderate correlation between experimental and predicted responses. Furthermore, the analysis of the results has shown that all parameters have important effects on the size of nanoparticles. A decrease in size was obtainable with decreasing of the rate of addition of the reducing agent, the molar ratio of gold to reducing agent and increasing of pH, concentration of gold salt and reducing agent.

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Paper code: 1065

Dispersive solid phase extraction and preconcentration of Reactive blue194 using magnetic carbon nanotube and utilization of smart Mobile Phone for colorimetric analysis

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In this work the applicability of carbon *magnetic* nanotubes as a magnetic solid phase sorbent for the extraction/preconcentration of Reactive Reactive Blue 194 (RB194) were studied. Carbon *magnetic* nanotubes were synthesized by the solvothermal method in polyol media [1]. The method utilizes the unique properties of carbon *magnetic* nanotubes including high surface area and superparamagnetism causing rapid separation. To optimize of important factors such as the adsorption time, NaOH concentration, adsorption pH, desorption time, amount of adsorbent and volume of eluent, central composite design method was used [2]. After *extraction of RB194,* the concentration of dye was determined colorimetrically with the aid of smart mobile phone. The calibration curve had two linear range of 20-200 µg L^{-1} and 1-10 mg L^{-1} of RB194. Limit of detection was 4 µg L^{-1}. The relative standard deviations of six replicate measurements were 2.2% and 3.0% for 0.1 and 3 mg L^{-1} of RB194, respectively. The proposed method was used for analysis of RB194 in environmental waters and satisfactory results were obtained. The recoveries were in the range of 95–108 %.

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Paper code: 1066

A validated HPLC–FL method for estimation of metoprolol in exhaled breath condensate

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Exhaled breath condensate (EBC) is one of the most accessible biological samples because it contains water vapor and hundreds of different compounds of exo- and endogenous origins in trace concentrations. In addition, EBC analysis is a non-invasive biological sample which is potentially useful for assessing the response to pharmacological therapy. Therefore, it could be as an alternative blood and urine tests [1, 2].

In the present study, a simple and sensitive HPLC–Fluorescence method was developed for determination of metoprolol in EBC samples. The separation was carried out on a C_{18} column (250 × 4.6 mm, 5 μm) by isocratic elution with sodium phosphate buffer (pH 3.8) and acetonitrile (40:60, v/v) containing 0.2% SDS as the mobile phase. Under optimized conditions, the proposed method was successfully applied to determine metoprolol in EBC samples of patients.

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Paper code: 1095

The application of new method based on EM-DLLME for analysis of five poly aromatic hydrocarbons by gas chromatography–mass spectrometry

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Electro membrane extraction (EME) is a method based on analyte migration from an aqueous sample into an acceptor solution under an applied electrical potential[1]. In this work, A highly efficient and simple two-step method, electro membrane extraction followed by dispersive liquid-liquid microextraction (EM-DLLME) and analysis by gas chromatography–mass spectrometry (GC–MS), was developed for the determination of trace level of five poly aromatic hydrocarbons in environmental water samples. This method was applied for determination of tricyclic antidepressants, previously[2]. At this work, for electroactivating of analytes was used initial derivatization the same of that was used in voltammetric technique [3]. In the first step, the analytes were extracted, under electrical potential, from the sample solution into the acceptor solution (acidic aqueous solution), which was held in a polypropylene membrane tube with toluene as the supported liquid membrane. The acceptor solution from the first step was then employed as the sample solution for the second step of (EM-DLLME). In this step, the target analytes were extracted into a solvent with lower density than water (1-octanol) that was dispersed in the sample solution with the assistance of vortex. The extract was separated from the sample solution by centrifugation and collected as the upper layer. Finally, the extract was injected into a GC–MS system for analysis. Five poly aromatic hydrocarbons, naphthalene, acenaphtylene, acenapthene, fluorene and phenanthrene were selected here as model compounds for developing and evaluating the method. The amount of extraction increases when the potential is applied, compared to when the potential is not applied. At the beginning of the research, the response was different in two modes, without potential and with potential. This is relevant to the applied potential area and in a particular potential region, the poly aromatic compounds are partially charged and ionized. Several factors influencing the extraction were investigated using Taguchi design. With the EM-DLLME procedure, high enrichment factors of up to 2710 were achieved. Under the most favorable conditions, good limits of detection (lower than 0.03 μg/L), linearity ($R^2 \cong 0.988$) (from 0.07–15 to 0.1–20 μg/L, depending on the analytes), and repeatability of extraction (RSDs below 7.5%, n=5) were obtained. The proposed method was applied to determine poly aromatic hydrocarbons in rain-water samples and good relative recoveries (89-106%) obtained under the optimized conditions.

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Paper code: 1108

Simultaneous chiral separation of tramadol and methadone in tablets, human urine, and plasma by capillary electrophoresis using maltodextrin as the chiral selector

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The chiral separation has gained importance in pharmaceutical industry since more than half of the drugs currently in use are chiral and about 90% of the last ones are marketed as racemates consisting of an equimolar mixture of two enantiomers [1]. Various analytical techniques have been successfully employed for the enantioseparation such as capillary electrophoresis using various chiral selectors [2]. This paper focuses on the simultaneous stereoselective separation of tramadol and methadone enantiomers using Maltodextrin as the chiral selector in a CE-based analysis. The best separation for the both enantiomers were achieved on an uncoated fused-silica capillary at 25 °C using 100 mM phosphate buffer (pH 8.0) containing 20% (w/v) maltodextrin with dextrose equivalent of 4–7 and an applied voltage of 16 kV (Fig. 1). The relative standard deviations (n = 3) of 20 µg mL^{-1} TRA and MET were 2.28 and 3.77 %, respectively. The detection limits were found to be 2 µg mL^{-1} for TRA and 1.5 µg mL^{-1} for MET. The developed method was successfully applied to the measurement of drugs concentration in their tablets, urine and plasma samples.

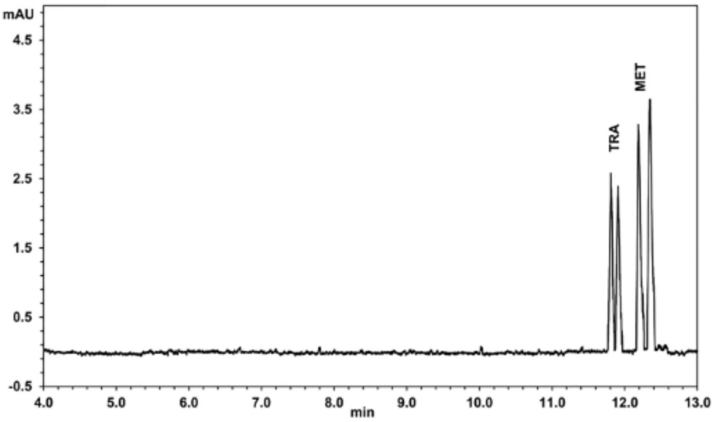

Fig. 1 A typical electropherogram of chiral separation of a mixture of standard solution of TRA and MET (20 µg mL^{-1}).

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Paper code: 1124

Abstract Extraction of Dopamine by Homogeneous Liquid –Liquid Extraction method (HLLE) and determination with UV-Vis Spectroscopy

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Dopamine (DA), 3,4 dihydroxyphenylethylamine, is an organic chemical substance in the catecholamines and phenylethyleamines group, which plays a number of important physiological roles in the brain and body [1,2]. In this study one of the homogenous liquid-liquid extraction methods, which is cloud point extraction, was used in order to preconcentrate and extract dopamine and amount of dopamine was determined by UV-Vis spectroscopy method. Triton x-114 was chosen as a surfactant due to low water content. The significant parameters to extraction were optimized. Experimental result show that high extraction efficiency can be obtained at the optimized parameters: pH=4 of sample solution; 1.5% v/v Triton surfactant; time of equilibration 15 min; equilibration of 40 ºC; time and rate of centrifuge 10 min and 5000 rpm respectively. At the optimum conditions the calibration plot of dopamine was drawn with good linearity ($R^2 \geq 0.999$) and using this plot, figures of merit of the proposed method were investigated. The given method presents suitable working linear ranges (0.05 - 1 $\mu g.L^{-1}$), good limit of detection (0.02 $\mu g.L^{-1}$), relative standard deviation (%RSD ≤ 4.7) and good recycle percentage (recovery > 88%). Finally, the proposed method was used for two types of real samples.

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Inorganic Chemistry

Paper code: 24

Mononuclear copper(II) complexes containing chelating ligand of 2-methyl-N-(pyridine-2-yl-methyl)propane-2-amine as chromotropic probes

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Chromotropism is the change in color of a substance due to the physical and chemical properties of its ambient surrounding medium, such as temperature (thermochromism), solvent (solvatochromism), electrons (electrochromism), pressure (piezochromism), light (photochromism), pH (halochromism) and ion (ionochromism). Chromotropism properties of inorganic compounds have been studied during the past four decades. This phenomenon has many applications in thermo-sensitive, imaging, photo switching, sensor materials, pollutant sensor and as Lewis acid-base indicators [1]. Among the metal complexes whose color changes are due to the d–d transitions, the copper(II) ion can be an excellent candidate due to its diverse coordination numbers, various geometrical structures and the presence of a strong Jahn–Teller effect. A combination of the copper(II) ion with appropriate ligands has been reported to afford metal-ion responsive chromotropic molecules. Multidentate ligands stabilize the resultant complexes due to chelate effect. The metal binding is also more strengthened when a 5- or 6- membered chelate ring is formed [2,3]. Herein, the synthesis of two mononuclear copper(II) complexes of formula $[L_2CuX]X$ where L is a bidentate ligand of *N*-(pyridin-2-ylmethyl)propane-2-amine and X =Cl and Br (Fig. 1), is reported. The complexes are fully characterized by physic chemical techniques. The chromotropic behaviors of the complex, including thermochromism, solvatochromism, and halochromism, is investigated.

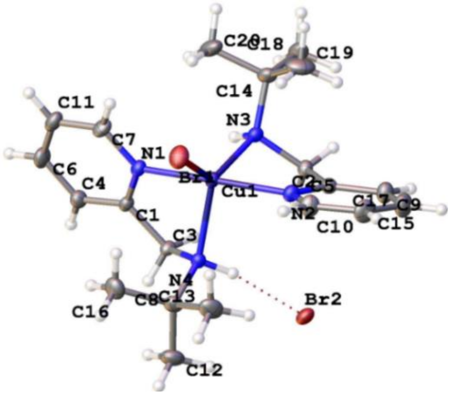

Fig. 1 Thermal ellipsoid plot of the cation in $[L_2CuBr]Br$.

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Paper code: 29

Synthesis, X-ray structural properties of hexacoordinate nickel(II) complex incorporating 4-methylpyrazole and azide ligands

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Mixed ligand complexes plays an important role in numerous chemical and biological systems. Nickel(II) complexes of mixed ligands accompanied by heterocyclic nitrogen donors as pyrazole base ligands and thiocyanate, azide, halides etc. have been used extensively in organometallic and inorganic chemistry [1-3].

In this research work a novel mixed-ligand nickel(II) complex, *trans*-$[Ni^{II} (N_3)_2 (Pz^{me})_4]$, ($N_3$ = azide and Pz^{me} = 4-methylpyrazole) has been synthesized and characterized by X-ray crystallography. The X-ray diffraction reveals that the nickel(II) ion in the title complex is in a distorted octahedral arrangement of two trans N-donor atoms of azide ligands and four another N-donor atoms of pyrazole derived ligands. The complex crystallizes in the monoclinic crystal system, space group *C2/C* with *a*= 12.901 (2)Å, *b*= 10.5003 (8)Å, *c*= 14.118 (1) Å, α= 90.00º, β= 116.398 (2)º, γ= 90.00º lattice specification.

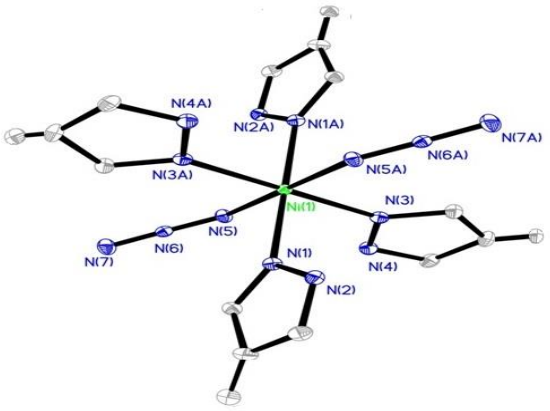

Fig. 1 The ORTEP plot of *trans*-$[Ni^{II} (N_3)_2 (Pz^{me})_4]$ showing 40% probability displacement ellipsoids and the atomic numbering scheme.

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Paper code: 53

Formation and Photocatalytic Activity of $BaTiO_3$ Nanoceramics via Sol-gel Process

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Barium titanate ($BaTiO_3$) is a versatile elctroceramics that finds widespread application and So many studies have been focused on various chemical methods for the synthesis of $BaTiO_3$ powders, for example sol-gel, co-precipitation, hydrothermal and spray pyrolysis [1]. The sol-gel process has been intensively studied because it facilitates the preparation of powders with high purity, small grain size, and good uniformity. oxide photocatalyst has drawn much attention for degrading organic chemicals from wastewater through the advanced oxidation process (AOP), generally with the assistance of UV irradiation. Among these oxides, perovskite-type materials have unique potential which displays photostability and preeminent photocatalytic activity [2]. $BaTiO_3$ is a typical perovskite photocatalyst with unique physical and chemical properties, which highly depend on its morphology and particle size; thus, high purity and nanoscale structure are highly desired [3].

We reported a facile sol-gel approach to synthesize $BaTiO_3$ nanoceramic for degradation of Methylene Blue (MB) and Eosin Y (EY). $BaTiO_3$ powder was prepared at low temperatures, starting with two different precursors; Barium hydroxide and titanium tetraisopropoxide. It was found that, phase $BaTiO_3$ was formed after calcination at 400°C for 2h. Ceramic was characterized by Energy dispersive X-ray analysis (EDX), FT-IR, SEM, UV-vis spectroscopy and X-ray diffraction (XRD). XRD analysis and SEM reveal pure perovskite phase structure and uniform grain size. The degradation efficiency for photocatalytic reaction was calculated as

$$\text{Efficiency (\%)} = C_0\text{-}C_e/C_0 * 100$$

Where C_0 and C_e correspond to the initial and final concentration of dye before and after photo-irradiation. In this equation E% shows the dye photocatalyst degradation percent. Percentage of destruction with MB and EY were obtained respectively 53% and 48%. Parameters such as concentration of substrate, amount of photocatalyst, pH of the solution, temperature of reaction medium and time of irradiation of light for photocatalysis degradation were investigated. Ceramic show the maximum adsorption at low pH for MB and minimum adsorption at low pH for EY.

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Paper code: 54

Synthesis, Properties, and Photocatalytic Activity of Perovskite-Phase $Ba_{0.75}Sr_{0.25}TiO_3$ Nanoceramics

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Photocatalysis has long been studied for clean energy and environmental applications. Over the past two decades, the number of applications based on photocatalysis has increased sharply, while a wide range of materials systems have been developed [1–2]. TiO_2-based materials are the most studied for photocatalytic applications, ternary and other complex oxide systems have been increasingly explored as photocatalysts. Among the various classes of materials studied, perovskites-based photocatalysts have unique photophysical properties and offer distinct advantages [3].

An aqueous solution of barium and titanium was obtained by mixing 14.66 g $Ba(NO_3)_2$ in 40 ml deionized water and 2ml titanium tetraisopropoxide (TIP) in 4 ml glacial acetic acid. 14.66 g of $Sr(NO_3)_2$ solved in deionized water added to the above solution. Then powder calcination at 400°C for 2h. Ceramic was characterized by Energy dispersive X-ray analysis (EDX), FT-IR, SEM, UV-vis spectroscopy and X-ray diffraction (XRD). XRD analysis and SEM reveal pure perovskite phase structure and uniform grain size.

Parameters such as concentration of substrate, amount of photocatalyst, pH of the solution, temperature of reaction medium and time of irradiation of light for photocatalysis degradation of methylene blue (MB) were investigated. Ceramic show the maximum adsorption at high pH hence the photodegradation also found maximum at high pH.

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Paper code: 68

In situ oxidation of 2,9-dimethyl-1,10-phenanthroline for synthesis of nickel(II) complexes containing highly preorganized acidic ligand

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Preorganized ligands have proven to be important in inorganic chemistry, biomedical, environmental, and industrial fields.[1] Ligand preorganization means that the free ligand has the same conformation as is required to complex the target metal ion. These ligands have a rigid phen backbone, with only limited movement possible for the donor groups at the 2 and 9 positions of the phen, leads to high levels of preorganization. 1,10-Phenanthroline-2,9-dicarboxylic acid (H_2PDA) with flat and rigid skeleton is one of the most prominent preorganized ligands which is used to prepare coordination compounds with selectivity metal ion, luminescence and magnetic properties.[2] As continuation of our efforts to develop systems containing dicarboxylic acids,[3] we employed H_2PDA to synthesis Ni(II) coordination complexes formulated as $[Ni(PDA)(H_2O)_2]$ (**1**) and $[Ni(PDA)(phen)].5H_2O$ (**2**) (Fig. 1). These compounds have been characterized by melting point, elemental analysis, infrared spectroscopy (IR), and thermogravimetric (TGA) analysis.

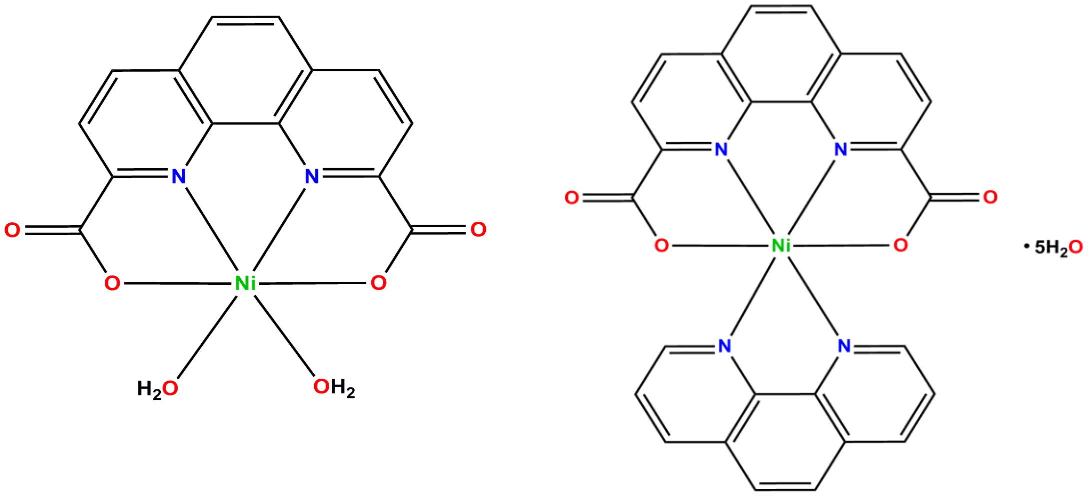

Fig.1 The molecular structures of **1** and **2**.

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Paper code: 69

Mixed ligand coordination complex of Mn(II) containing oxidized pyridine-2,6-dicarboxylic acid and 1,10-phenanthroline: Synthesis and characterization

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For the last two decades, the synthesis of mixed ligand coordination compounds with transition metals and their applications have become an attractive field because of the excellent properties such as catalysis, ion exchange, microelectronics, nonlinear optics, porous materials, etc. The use of acid–base mixed ligands is a very suitable method for the preparation of these compounds. Naturally, acid and base ligands are perfect partners that can compensate charge balance, coordination deficiency, repulsive vacuum, and weakly interaction all at once.[1] For this purpose, polycarboxylic acids and N-heterocycle bases are very excellent candidates.[2] As an aromatic polycarboxylate ligand derived from pyridinedicarboxylic acid, pyridine-2,6-dicarboxylic acid *N*-oxide (H_2pydco), has limited steric hindrance and weak stacking interactions and can form various coordination structures through carboxylate and *N*-oxide bridges.[3] In this work, H_2pydco as a primary ligand and 1,10-phenanthroline (phen) as secondary ligands were employed to synthesis mixed ligand coordination complex of Mn(II). This compound has been characterized by melting point, elemental analysis, infrared spectroscopy (IR), and thermogravimetric (TGA) analysis. The purpose molecular formula [Mn(pydco)(phen)(H_2O)] (**1**) is confirmed by results (Fig. 1).

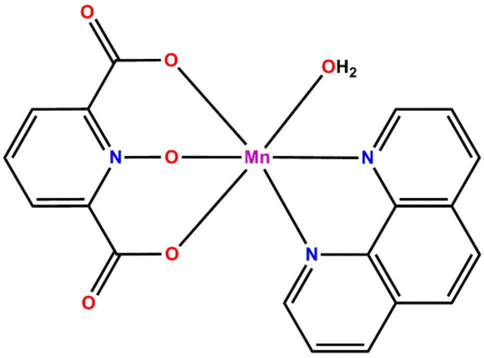

Fig.1 The molecular structure of **1**.

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Paper code: 71

Construction of two zinc and copper(II) coordination complexes containing pyridine-2,6-dicarboxylic acid *N*-oxide based on mixed-ligand synthetic strategy

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The design and construction of coordination compounds with unique structural motifs and desirable properties has attracted extensive interest in supramolecular and materials chemistry. A major part of the research and its success are due to the vital role of the concept of mixed organic ligands in the design. Pyridinedicarboxylic acid derivatives and neutral multidentate N–donor ligands are excellent candidates for the formation of novel mixed-ligand architectures with beneficial properties.[1] As continuation of our efforts to develop systems containing pyridinedicarboxylic acids,[2] we decided to oxygenate nitrogen of pyridine ring of pyridine-2,6-dicarboxylic acid as *N*–oxide to investigate synthesis, coordination modes, and structure types of these compounds in view of crystal engineering concepts. In this work, we have prepared two Zn and Cu coordination compounds by employing pyridine-2,6-dicarboxylic acid *N*-oxide (pydco) and 1,10-phenanthroline (phen) ligands, ($[Cu(pydco)(phen)(H_2O)].2H_2O$) (**1**) and $[Zn(pydco)(phen)(H_2O)_2]$ (**2**) (see Figure 1). These compounds have been characterized by melting point, elemental analysis, infrared spectroscopy (IR), and thermogravimetric (TGA) analysis.

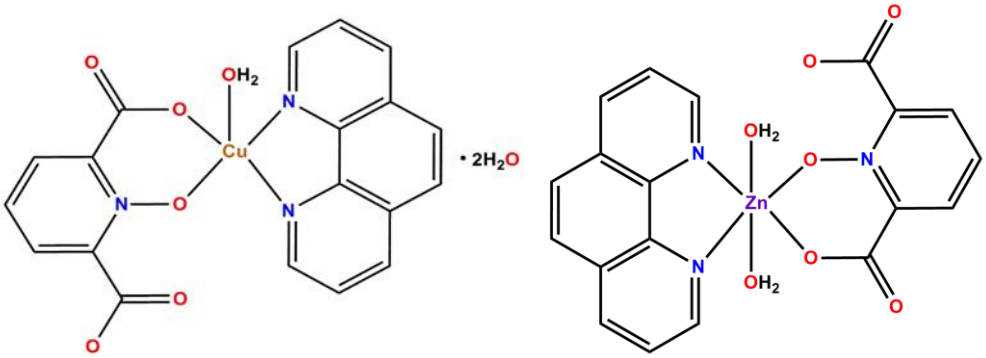

Fig.1The molecular structures of **1** and **2**.

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Paper code: 103

Interaction of Ethylenediamine 2-pyridinecarboxcylatopalladium(II) nitrate with CT-DNA/BSA and its anti-tumor activity

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Cis-Diamminedicholoroplatinum (II) (*cis*platin), first identified as antitumor drug in late 1960. Thousand's analog of this compound has been synthesized, characterized and tested for their antitumor activities. It has been reported that many active complexes could react with DNA and inhabit its synthesis[1]. The long-term application of Pt complexes is thwarted by issues, leading scientists to examine other metals such as palladium, which could exhibit complementary modes of action (given emphasis wherever known). Several research groups have focused on the application of an eclectic array of palladium complexes as potential anti-cancer agents[2].

In this study, a new palladium (II) complex of formula [Pd (en)(2-pyc)]NO_3 (where en is 1,2-diaminoethane and 2-pyc is 2-pyridinecarboxylate anion) has been designed, synthesized and characterized. We selected 2-pyc as ligand because of its planar π aromatic moiety which assisted the interaction of the complex with bio macromolecules specially DNA[3]. The synthesized complex has been characterized by elemental analysis, conductivity measurements, and UV-Vis, FT-IR and ^{1}H NMR spectroscopic techniques. The interaction of this complex with calf thymus DNA (CT-DNA) and bovine serum albumin (BSA) has been investigated using UV-Vis spectroscopy in 30 mmol/L Tris-HCl buffer of pH = 7.00 at two different temperatures of 300 and 310 K. In these studies, K_{app}, apparent association constant was found to be 1.3×10^4 M^{-1} and 1.9×10^5 M^{-1} for DNA and 1.5×10^4 M^{-1} and 1.1×10^5 M^{-1} for BSA at 300 and 310 K, respectively. These results indicate that the titled complex can interact with DNA as well as BSA with moderately binding affinity. Furthermore, the concentration of the Pd(II) complex in the midpoint of transition from native to denatured DNA or BSA, $[L]_{1/2}$, was calculated which increased from 0.034 mM to 0.038 mM for DNA and from 0.023 mM to 0.036 mM for BSA by increasing the temperature from 300 to 310 K. Moreover, the thermodynamic parameters ($\Delta G°$, $\Delta S°$ and $\Delta H°$) for the interaction of the complex with DNA and BSA have been calculated using the K_{app} values and van't Hoff equation. The *in-vitro* antitumor properties of the Pd (II) complex against human tumor cell line K_{562} were examined using MTT assay. The 50% cytotoxic concentration (Cc_{50}) of the complex was determined 32 µM, indicating its potential anticancer activity, possibly targeting DNA.

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Paper code: 105

Pt–Au Complexes Built on a Diphosphine Scaffold: Cytotoxic Properties

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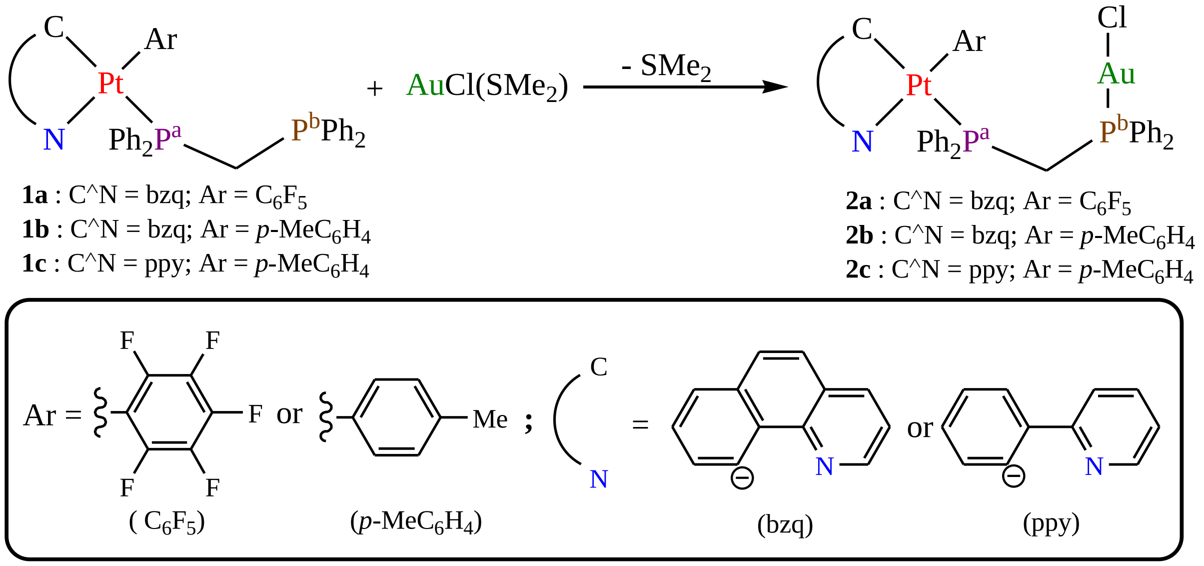
Platinum complexes are well-established drugs in modern anticancer chemotherapy. However, their effectiveness is still hindered by clinical problems, including acquired or intrinsic resistance, a limited spectrum of activity, and high toxicity leading to side effects [1]. A recent strategy in the field of metal based anticancer drugs consists in the design of bimetallic or even multimetallic agents bearing diverse metal centers with distinct biological and pharmacological features. This strategy is aimed at exploiting the possible synergism existing among the individual metal centers, which may contribute to overcome resistance [2].

We report here on the preparation, characterization and stability of some bimetallic Pt(II)–Au(I) complexes. The new compounds are depicted in Fig 1. They contain a cycloplatinated(II) moiety and a gold(I) chloride fragment linked through a bifunctional diphosphane ligand 1,1-bis(diphenylphosphino)methane (dppm).



1a : C^N = bzq; Ar = C_6F_5
1b : C^N = bzq; Ar = p-MeC_6H_4
1c : C^N = ppy; Ar = p-MeC_6H_4

2a : C^N = bzq; Ar = C_6F_5
2b : C^N = bzq; Ar = p-MeC_6H_4
2c : C^N = ppy; Ar = p-MeC_6H_4

Fig. 1 Synthetic route for the formation of Pt(II)-Au(I) complexes.

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Paper code: 109

Activation of C-I Bond by Cycloplatinated(II) Complexes Comprising Tricyclohexylphosphine ligand: Kinetics and Mechanism Investigations

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The cycloplatinated(II) complexes incorporating monophosphine ligands, with general formula of [Pt(C^N)(Me)(L)] (L = monophosphine ligand), are normally good choices in order to study of the mechanism of oxidative addition reaction with alkyl halides. [1]. Phosphine ligands are important in the sense that their electronic and steric effects, induced by their substituents, have a considerable impact on the rate constants and activation parameters of such reactions. Electron-withdrawing or electron-donating properties of the substituents and their Tolman cone angle values control the electronic and steric properties of the phosphine ligands, respectively [2].

Herein, we have investigated the kinetic and mechanism of the oxidation reaction of cycloplatinated(II) complexes incorporating tricyclohexylphosphine ligand (PCy_3) by MeI (Fig. 1). The new Pt(IV) complexes have been identified by NMR spectroscopy and single crystal X-ray crystallography. The kinetic measurements, supported by the DFT calculations, have been performed using the UV-vis spectroscopy by monitoring the change in the absorbance spectra of Pt(II) complexes.

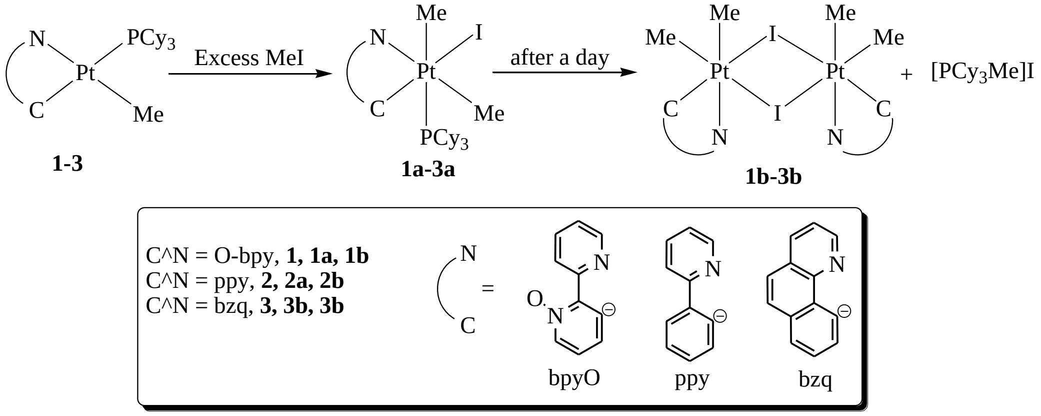

Fig. 1 Synthetic route for the formation of Pt(IV) complexes.

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Paper code: 134

Synthesis and structural determination of novel the Cu(II) nano coordination system

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Metal-organic coordination systems are one of the most important classes of inorganic materials which have been advanced in recent years [1]. Metal-organic coordination systems are a class of organic–inorganic materials consists of metal ions linked together through multi-dentate organic ligands, to form a polymeric chain. These materials have found various applications such as in catalysis, sensing, luminescence, separation and storage used [2].

In this work we investigate the coordination behaviors of Cu(II) with pyridin-2-isonicotinohydrazide (L) Schiff-base ligand $[[Cu_2(L)_2Cl_2].(H_2O)]_n$. The compound was characterized by scanning electron microscopy (SEM), elemental analysis, IR spectroscopy, X-ray powder diffraction (XPRD), and single crystal X-ray analysis. The X-ray structure revealed that the Cu(II) atom is coordinated by one oxygen and three nitrogen atoms from two “L” ligands and one chloride anion with a CuN_3OCl donor set with square pyramid geometry. We describe a simple sonochemical synthesis method for a nano structure of this coordination system and its use in the preparation of CuO nano-particles. CuO nanoparticles were obtained by thermolysis of coordination polymer at 180 °C with oleic acid as a surfactant. The average diameter of the nanoparticles was estimated by XPRD to be 38 nm.

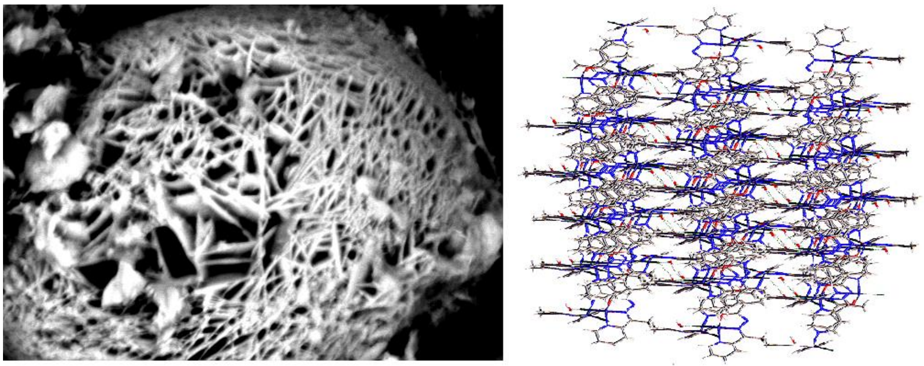

Fig. 1 Right: packing of the structure on a molecular level, Left: morphology of the nano-card house.

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Paper code: 136

Sonochemical and the structural characterization of novel the Cd(II) nano metal-organic polymer

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In two past decades new classes of molecular materials, known as coordination compounds or metal-organic hybrid materials have attracted remarkable attention due to their interesting properties. The research activities in this area have spread widely and rapidly and their fundamental properties are studied more than before [1]. Such compounds in most cases result from self-assembly. The self-assembly process is led by the interactions between primary structural units and their growth in several dimensions [2].

In the present work, we investigate the coordination behaviors of Cd(II) with pyridin-2-isonicotinohydrazide (L) Schiff-base ligand. The compound was characterized by scanning electron microscopy (SEM), elemental analysis, IR spectroscopy, X-ray powder diffraction (XPRD), and single crystal X-ray analysis. The X-ray structure analysis revealed that the Cd(II) atom is coordinated by one oxygen and three nitrogen atoms from two “L” ligands and two oxygen atoms of single nitrite anion with a CdN_3O_3 donor set with distorted octahedral geometry. We describe a facile sonochemical method for synthesis of a nanostructures of this coordination polymer and its use in the preparation of cadmium(II) oxide nanoparticles. CdO nanoparticles were prepared by thermolysis of compound **1** at 180 °C with oleic acid as a surfactant. The average diameter of the nanoparticles was estimated by XPRD to be 23 nm. The morphology and size of the prepared CdO nanoparticles were further studied using SEM.

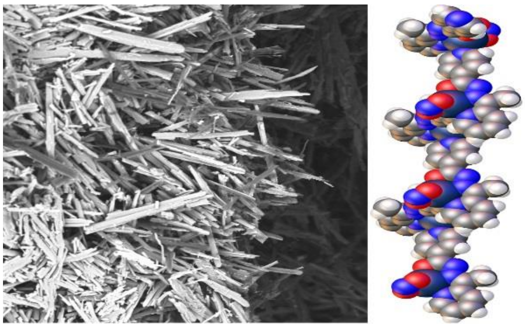

Fig. 1 Right: 1D structure on a molecular level, Left: morphology of the nano-rods.

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Paper code: 235

Synthesis and characterization of new binuclear complexes mercury(II) of pyridinium ylide

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Pyridinium ylides are important reagents in organic chemistry, especially in the synthesis of naturally occurring products with biological and pharmacological activities [1]. These compounds have been used as reducing agents in coordination chemistry. They can behave as ambidentate ligands, because the carbanion located at the Cα of the ylide or the enolate oxygen is able to donate electron density to a transition metal [2]. Herein, we report the synthesis and characterization of new binuclear and polymeric complexes of Hg(II) derived from pyridinium ylide. Pyridine and 2,3- dibromo acetophenone in 1:1 ratio react in acetone as solvent to produce the related pyridinium salt. For synthesis of ylide a solution of potassium carbonate was added to a solution of pyridinium salt in water. The mixture was stirred for 20 min and then extracted with dichloromethane. Reaction of pyridinium ylides $C_5H_5NCHC(O)C_6H_5$ (m-Br) (ylide) with HgX_2 (X = Cl, Br and I) in 1:1 ratios leads to binuclear products of the type $[HgX_2(ylide)]_2$. Characterization of the complexes by IR, 1H and 13C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom (Fig. 1).

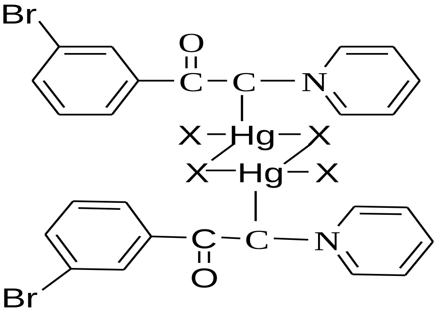

Fig.1. $C_5H_5NCHC(O)C_6H_5$ (m-Br) with HgX_2 (X = Cl, Br and I)

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Paper code: 238

Synthesis and characterization of silver(I) and mercury(II) complexes with pyridinium ylide and study on their antibacterial properties

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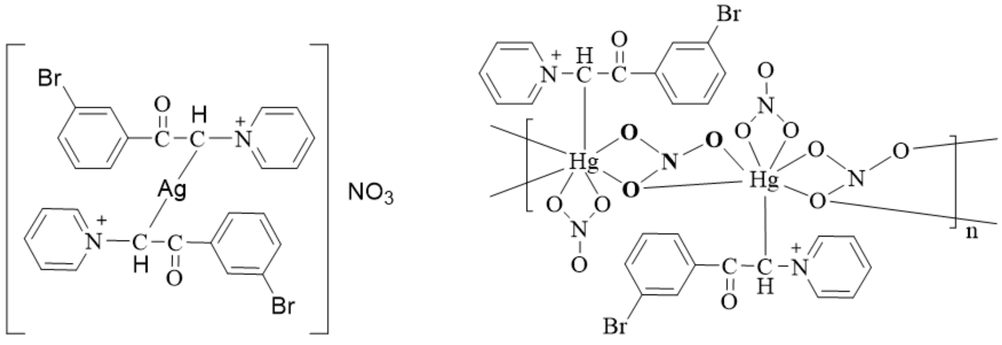
Pyridinium ylides are able to form stable complexes and could be characterizat with spectroscopic techniques. The present study describes the synthesis and characterization of mononuclear Ag(I) and polymeric Hg(II) complexes of pyridinium ylides The synthesis of complexes derived from ylides and Ag(I) began in 1975 by Yamamoto et al [1]. Herein, synthesis and characterization of α-ketostabilized pyridinium ylide of the type $C_5H_5N{=}CHC(O)R$ with $AgNO_3$ and $Hg(NO_3)_2.H_2O$, using methanol as a solvent and study on their antibacterial properties are reported. All reactions were performed in air. Reaction of pyridinium ylides $C_5H_5NCHC(O)C_6H_5$ (*m*-Br) with $Hg(NO_3)_2.H_2O$ in 1:1 and with $AgNO_3$ in 2:1 ratios leads to products of the type $[Ag(ylide)_2](NO_3)$ and $[Hg(NO_3)_2(ylide)]_n$ complexes. Characterization of the obtained compounds was performed by elemental analysis, IR, ^1H and ^{13}C NMR. The spectroscopy analyzes and literature [2] were shown that the nitrate ion exists in the Polymer chain of Hg complex but in Ag complex, the nitrate ion shows a bonding interaction with the silver ion (Fig. 1). Also, the results show that both complexes represent antibacterial activities.



(a) (b)

Fig.1. complexes(a): $[C_5H_5NCHC(O)C_6H_5(m\text{-}Br)Ag(NO_3)_2]_n$ and complexes(b): $[C_5H_5NCHC(O)C_6H_5(m\text{-}Br)Hg(NO_3)_2]_n$

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Paper code: 279

Anticancer activity of three novel Pt complexes with Amine and glycine ligand

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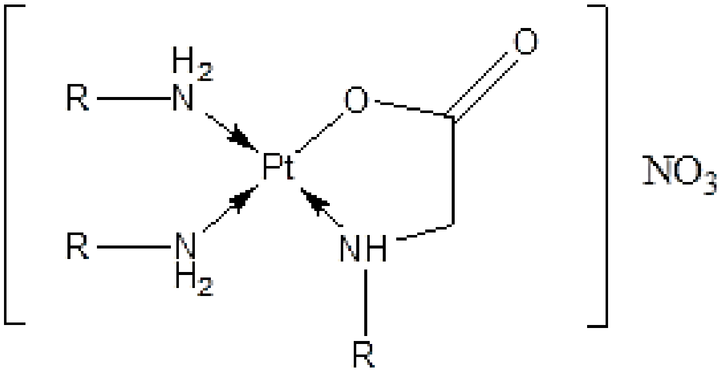
Using bidentate ligand such as amino acid derivatives is the strategy in designing new drugs. Due to presence of lipophilic functional group, toxicity of drug is reduced and influence of the drug into the cancer cell is improved [1]. Recently, three anticancer complexes were synthesized with formula of cis-[Pt(Butylamine)$_2$(Butylglycine)]NO_3, cis-[Pt(Iso-pentylamine)$_2$(Iso-pentylglycine)]NO_3 and cis-[Pt(Tert-pentylamine)$_2$(Tert-pentylglycine)]NO_3. These compounds (Fig. 1) have been characterized using analytical and spectroscopic methods such as elemental analysis, conductivity, FT-IR, UV-Vis and ^{1}H-NMR techniques. These water soluble complexes show 50% cytotoxic concentration (Cc_{50}) values against cell line, at micro molar concentration higher than cisplatin activity [2].



R : Propyl, iso-pentyl, tert-pentyl glycine

Fig. 1: Proposed structure of Pt complexes as anticancer drug

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Paper code: 281

Synthesis, characterization and cytotoxicity of three novel amino acid Platinum (II) complexes against colon cancer cell line

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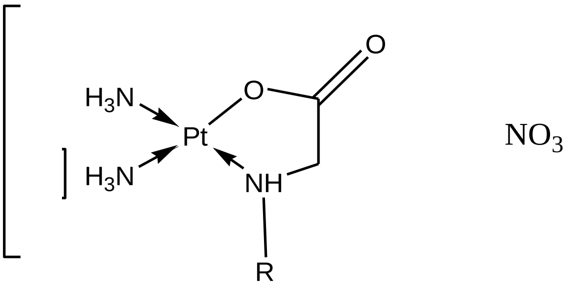
Investigation of side effects and solubility of anticancer drugs is a major challenge in chemotherapy science. Thus, design and synthesis of cisplatin analogs with higher lipophilicity as novel water-soluble anticancer drugs is valuable. In this work, three new Pt(II) complexes were synthesized with formula of cis-$[Pt(NH_3)_2(R\text{-}gly)]NO_3$, where R-gly is butylglycine, iso-pentylglycine and tert-pentylglycine see (Fig. 1). These compounds were extensively characterized by using analytical techniques; spectroscopic methods and conductivity measurement [1]. Also anticancer activity was investigated against colon cancer cell line HCT116 using MTT assay and results showed excellent anticancer activity with Cc50 values at micro molar concentration and 24-h incubation time, which are lower than that for cisplatin [2].



R : Butylglycine, iso-pentylglycine and tert-pentylglycine

Fig. 1: Proposed structure of anticancer Pt complexes.

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Paper code: 288

Two Pillared Metal–organic Frameworks Comprising a Long Pillar Ligand used as fluorescent sensor for nitrobenzene and heterogeneous catalyst for Knoevenagel condensation reaction

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Two new pillared zinc and cadmium-organic frameworks were synthesized by incorporating two different organic linkers, namely 2-aminoterephthalic acid as an oxygen-donor linker and $N_4,N_{4'}$-bis(pyridin-4-ylmethylene)-biphenyl-4,4'-diamine as a long pillaring strut. The structure of these two frameworks was analyzed using X-ray crystallography, FT-IR spectroscopy, thermogravimetric and elemental analyses. Their structural features as well as their stability were studied. These two MOFs having the same organic compositions and the same network topology but different inorganic nodes differ in their chemical stability. Also, these two frameworks respond differently to nitrobenzene when they are used as a fluorescent sensor. Furthermore, the catalytic behavior of one of these frameworks toward Knoevenagel condensation reaction was investigated.

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Paper code: 296

New Hydrazide Palladium Complexes, Synthesis, Characterization and biological studies

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Four new complexes of palladium with general formula *trans*-$[Pd(L)_2(OAc)_2]$ (E,F) and $[Pd(L)(\mu\text{-}OAc)]_2(OAc)_2$ (G,H) (L= Benzhydrazide and 2-Furic hydrazide) have been synthesized and characterized with several methods including FT-IR, ^{1}HNMR, elemental analysis, UV-Vis spectroscopy, then the fluorescence quenching reactions of complexes with bovine serum albumin (BSA) in pH 7.20 Tris–HCl buffer solution were studied and the interaction of them with calf thymus deoxyribonucleic acid (DNA) have been studied by electronic absorption titration, fluorescence and viscosity measurement. Also in order to determination of protein binding site of mentioned complexes, site-competitive replacement experiments with specific site markers including Eosin-Y, Ibuprofen and Digoxin have been done. By the analysis of fluorescence spectrum and fluorescence intensity, it was showed that these complexes have an ability to quench the intrinsic fluorescence of BSA. Further our complexes showed the ability of interaction with binding site I of BSA. In addition, fluorescence resonance energy transfer (FRET) have been calculated. Spectroscopic measurements data showed the groove binding of them to DNA. Also DNA cleavage and cytotoxicity studies of synthesized complexes have been done

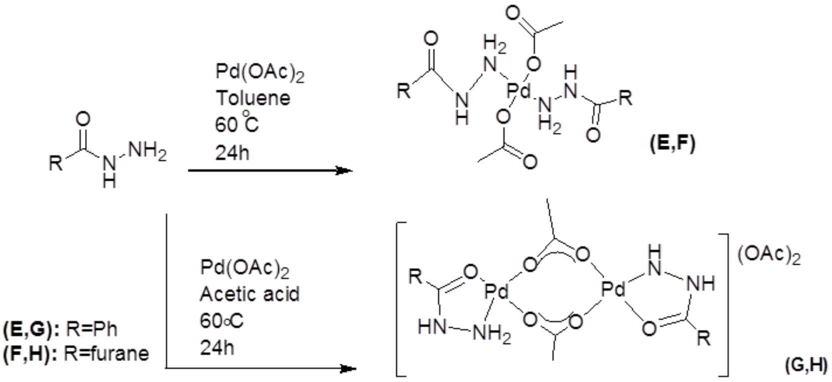

Fig. 1 General procedure for synthesis of Hydrazide complexes

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Paper code: 304

Studies of cadmium (II) macrocyclic Schiff-base complexes containing piperazine moiety

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The new Cd(II) macrocyclic Schiff-base complexes were prepared via the metal templated [1+1] cyclocondensation of 2,2'-(piperazine-1,4-diylbis(methylene))dianiline (A) and 2,6-pyridinedicarbaldehyde or 2,6-diacetylpyridine. The products were characterized by elemental analysis, mass spectrometry and spectroscopic methods such as: FT-IR, ^{1}H and ^{13}C-NMR, the crystal structure of $[CdL^1(ClO_4)_2](CH_3CN)$ (1) complex was also obtained by single-crystal X-ray crystallography. The complexes were tested for *in vitro* antibacterial properties against some bacteria. The complexes had antibacterial properties and in some cases were active even more than standards. The geometries of the $[CdL^n(ClO_4)_2]$, (n=1,2) complexes have been optimized at the BP86/def2-SVP level of theory. Also the nature of $Cd{\rightarrow}L^n$ (n=1, 2) bonds in $[CdL^n(ClO_4)_2]$, (n=1,2) complexes are studied with the help of NBO and Energy decomposition analysis (EDA). Results showed that the nature of metal-ligand bond in the complexes is slightly more electrostatic with a contribution of about 52% in total interaction energy.

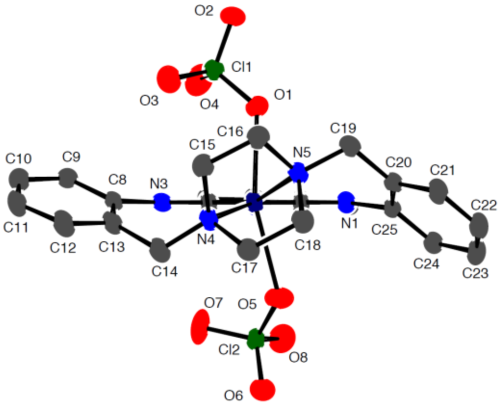

Fig.1. ORTEP representations of $[CdL^1(ClO_4)_2](CH_3CN)$

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Paper code: 308

Synthesis and characterization of macrocyclic complexes containing piperazine moieties with Mn(II), Cd(II) and Zn(II)

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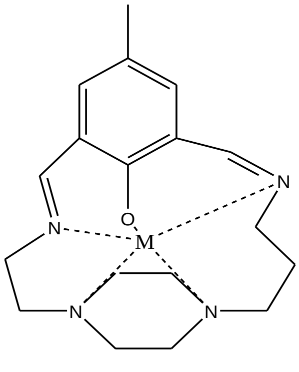
Macrocyclic chemistry has developed into one of the most active and promising research areas of chemical science located at the interface between chemistry, physics and biology. Schiff-base complexes are considered to be among the most important stereo chemical models in main group and transition metal coordination chemistry due to their preparative accessibility and structural variety.

In this work, we report the synthesis and characterization of new Mn(II), Cd(II) and Zn(II) macrocyclic Schiff base complexes have been prepared via the Mn(II), Cd(II) and Zn(II) of 2-Hydroxy-5-methyl-benzene-1,3-dicarbaldehyde with an asymmetrical linear amine, N,N'(2-aminoethyl) (4aminobutyl) piperazine. The complexes have been characterized by elemental analysis, IR and HNMR.



M= Cd(ii),Zn(ii),Mn(ii)

Fig. 1 Mn(II), Cd(II) and Zn(II) macrocyclic Schiff base complexes

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Paper code: 319

Synthesis, characterization, structure determination and theoretical studies of some new dimethylglyoxime cobalt(III) complexes

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Cobaloximes are octahedral Co$^{(III)}$ complexes with a chemical composition of Co(dmgH)$_2$LX in which the equatorial dmgH ligands are monoanions of dimethylglyoxime (dmgH$_2$), the axial base (L) is a nitrogen-coordinated molecule such as pyridine and X is an organoligand [1]. Over the past four decades cobaloximes have been extensively studied as structural and functional models for the coenzyme vitamin B$_{12}$. In the recent years the interest in these complexes has been increased due to their ability to catalyze the hydrogen evolution from acidic non-aqueous solutions at moderate potentials [2]. In this work, several [Co(DMG)$_2$(L)Cl] complexes were prepared and characterized by different spectroscopic methods such as FT-IR, UV-Vis and ^{1}H-NMR and their solid state structures were determined by single crystal X-Ray diffraction. Theoretical calculations using Gaussian09 were used to optimize the structures and calculate the molecular orbitals in gas phase and solution. The charge decomposition analysis (CDA) using molecular orbitals were used to calculate electron-donation and accepting properties of the nitrogen-coordinated molecule in the complexes and predict the ability of the complexes for H$_2$ evolution. The theoretical calculations were compared to the previously reported experimental work and proved with very good agreement.

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Paper code: 325

Synthesis, characterization and photoluminescence studies of a new Schiff base ligand and its nickel(II) complex

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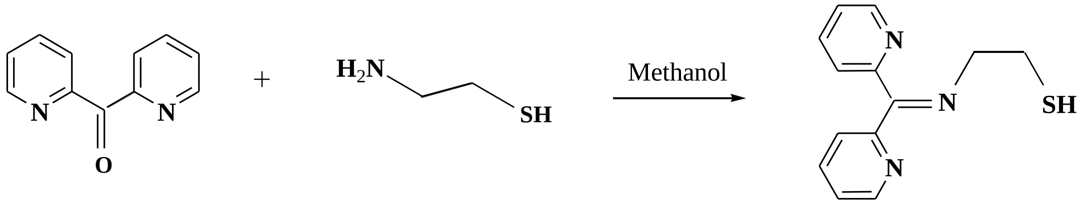
Schiff base ligands are considered "privileged ligands" because they are easily prepared by the condensation between active carbonyl groups and primary amines. Schiff base ligands are able to coordinate with many different metals, and form stabilizes complexes in various oxidation states [1]. These compounds also show a wide range of biological properties such as anticancer, antitumor, antifungal, antibacterial, antimalarial, antifilarial, antiviral and anti-HIV activities, Moreover, the biological activities of their complexes could be due to metal ion coordination. Metal complexes have been widely applied in clinics for centuries, although their molecular mechanism has not yet been entirely understood. Among different Schiff base complexes, nickel(II) imine complex has been shown to possess catalytic activity for the polymerization or copolymerization of olefins and vinylic monomers [2]. In this work, a new Schiff base ligand was synthesized from the 1:1 molar condensation of a novel ketone containing chelating ligand with cysteamine. Furthermore, the metal-to-ligand ratio was 1:1, and molar conductance data revealed that the nickel complex was nonelectrolyte. The free Schiff base ligand and its complex showed photoluminescence in methanol at room temperature. In the complex of this ligand, the sulfur group is used as a coordination site since oxidation of the SH group and formation of the disulfide bond were prevented by use of an inert atmosphere. The Schiff base ligand was coordinated to metal ion as a ligand through nitrogen and sulfur donor atoms. The Schiff base ligand and its nickel complex have been characterized by the elemental analysis and spectroscopic studies such as FT–IR, UV–Vis and ^{1}H NMR.



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Paper code: 329

Synthesis, characterization and structural studies of some new homoleptic and heteroleptic diiminic and diphosphine copper(I) complexes

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Cu(I) complexes are considered as a promising alternative with interesting photophysical properties to traditional noble-metal complexes that are mainly based on Ru(II) and Ir(III). Therefore, in recent years heteroleptic Cu(I) complexes of the type $[Cu(N^\wedge N)(P^\wedge P)]^+$, $[Cu(N^\wedge N)_2]^+$ have been developed exhibiting impressive performance, e.g., long-lived excited-states, high emission quantum yields with tunable emission spectra as well as largely adjustable redox properties [1-2].
we report synthesis and structural chemistry of some new homoleptic and heteroleptic Cu(I) complexes with new NN-diimine ligands and known heterocyclic diimines along with biphosphines. In our strategy, we tried to incorporate different substitution on the peripheral phenyl rings to pursue the stabilizing and directing effect of such group by increasing possibility of the intermolecular interaction such as C-H···π, π···π, dipolar CN···CN, $NO_2 \cdots NO_2$ and $NO_2 \cdots \pi$ of the respected Cu(I) complexes. The results showed that not only the nature of the substituents but also the rigidity and flexibility of the ligands are effective on the physicochemical properties of the related complexes.

These complexes have been characterized using ^{1}HNMR, ^{31}PNMR, and FT-IR and their solid-state structure determined by single crystal X-ray diffraction.

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Paper code: 331

Synthesis and Characterization of a new polyamine containing piperazine moiety and related potentially N_6O_2 donors ligands together with corresponding Zn(II) complexes

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Schiff base complexes have remained an important and popular area of research due to their simple synthesis, versatility and diverse range of applications [1]. Piperazine is a well-known building block for novel supramolecular structures due to the presence of two weakly held terminal amino protons [2].

We have designed and synthesized a new polyamine and related Schiff base macroacyclic ligands. These Schiff-base ligands and their complexes were characterized by elemental analysis, IR spectroscopy, ^1H and ^{13}C NMR and EI-Mass.

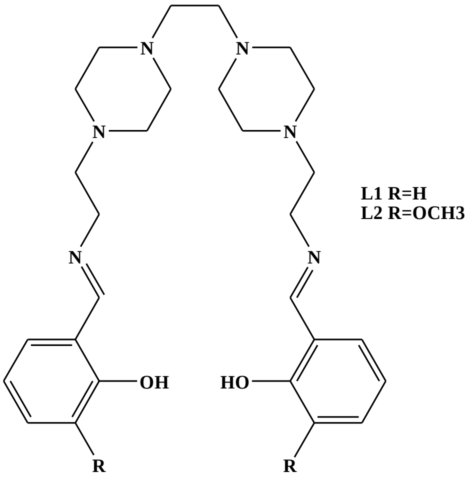

Fig. 1 The structure of L^1 and L^2

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Paper code: 332

Crystal engineering and interaction energy calculation of some new rhenium(I) tricarbonyl complexes bearing bidentate NN-donor ligand

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Crystal engineering is the understanding of intermolecular interactions in the context of crystal packing and the utilization of such understanding in the design of new solids with desired physical and chemical properties [1]. The chemistry of the last two decades of the twentieth century has been largely dominated by the endeavor to master secondary noncovalent bonding. This has determined a substantial shift of interest, from a focus on atoms and bonds between atoms to a focus on molecules and bonds between molecules, and has involved all areas of chemistry, from biochemistry to organic, organometallic, and physical chemistry, to encompass the thriving area of materials chemistry [2]. This Highlight focusses on inorganic and organometallic components, or at least metal-containing components. In this study we designed and synthesized some new rhenium(I) tricarbonyl complexes with a bidentate cyano-substituted NN-donor ligand.

Since the metal fragment has itself three carbonyl groups with facial geometry and a halogen or halogen-containing ligands either Cl, Br or –OCOCF$_3$, there might be a range of possibility of intra- and intermolecular interactions based on dipolar CO···CO, halogen bonding and classical and non-classical hydrogen bonding. On the other hand, cyano-substituents on the peripheral aromatic ring of the NN-donor ligand can also make more possibility for the intermolecular interactions in the crystal packing.

The interaction energy of different pairs of molecules in the crystal packing were calculated by G09 considering latest Grimme dispersion correction (D3) to find the most effective and directing intermolecular interaction in the crystal packing of the related complexes.

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Paper code: 334

Synthesis and theoretical studies of two new Co(III) and Cu(II) macroacyclic Schiff-base complexes containing piperazine moiety

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The new Schiff base H_2L^1, has been prepared from the condensation of 2-hydroxybenzaldehyde with 2,2'-(piperazine-1,4-diylbis (methylene))dianiline (A). In the presence of appropriate metal ions and in methanolic/ethanolic solution two Cobalt (III) and Copper (II) macroacyclic Schiff-base complexes were prepared. All resultant products were characterized by elemental analysis, mass spectrometry and spectroscopic methods such as: FT-IR, ^1H and ^{13}C NMR. the crystal structure of $[CoL^1](ClO_4)$ complex have been revealed by single-crystal X-ray crystallography. The geometries of the $[CoL^1]^+$ and $[CuL^1]$ complexes have been optimized at the BP86/def2-SVP level of theory. Also, the nature of the metal-ligand bond in the complexes is analyzed with NBO and EDA analysis. Results confirm that the nature of metal-ligand bond in the complexes is slightly more covalent with a contribution of about 53% in total interaction energies.

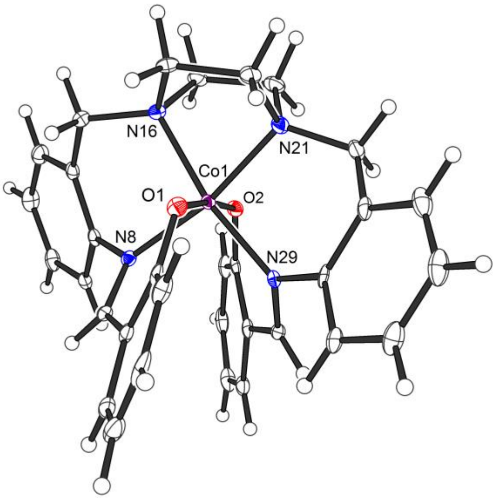

Fig. 1 ORTEP representation of $[CoL^1](ClO_4)$

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Paper code: 416

Investigation of the effect of aminodiphosphonate complexes inhibition on metals corrosion

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In this study, two of the amino diphosphonate complexes with the general structure of Cu(H3L1)2.2H2O (1), [H4L1= methyl-N(CH2PO3H2)2] and Cd2(H2L2)4(2), [H4L2= n-propyl-N(CH2PO3H2)2] were synthesized and characterized by 31P, 13C, 1H NMR and FT-IR spectral techniques. Corrosion inhibition performances of 1 and 2 were also compared with each other in order to study the effect of combinations of externally added Cd/H4L2 and Cu/H4L1 (1:1 ratio) on corrosion rates of carbon steel. It was found that at pH 3.0, Cd/H4L2 or Cu/H4L1 combinations do not have noticeable corrosion inhibition efficiency for carbon steel. In contrast, at pH 7.0, higher corrosion inhibition efficiency was achieved for Cd/H4L2. Physical characterizations such as scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDS) and Fourier transform infrared spectroscopy (FTIR) were applied to study the corrosion specimens and film material.

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Paper code: 433

Cation exchange in an anionic nanoporous MOF for study of CO_2 adsorption

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Developing new materials for CO_2 capture and separation is becoming more vital as intensive combustion of fossil fuels has increased CO_2 concentration in the atmosphere [1]. Metal Organic Frameworks (MOF) have regular accessible cages that can be used for selectivity adsorbing CO_2 increasing the MOF pore volume and surface area [2] or modifying the pore chemistry to increase CO_2 capacity [3]. In this study we focused on CO_2 adsorption capacity in an anionic MOFs of $[HDMA]_2[Zn_2(BDC)_3(DMA)_2].6DMF$ (**TMU-3)** Fig.1, BDC^{2-}: 1,4-benzenedicarboxilate, DMA: dimethylamine and DMF: N,N'-dimethylformamide) by modifying their pore volumes.

For such purpose we exchanged $[NH_2Me_2]^+$ (dimethylammonium) with series of organic cations such as tetramethylammonium, tetraethylammonium, tetrapropylammonium and tetrabutylammonium, and studied the effect of these exchanges on their BET surface area and CO_2 adsorption capacity. The exchanged materials were also characterized by IR,1H-NMR spectroscopies and by TG-DTA and XRD analyses.

The SEM images of ZnO nanostructures which were assembled by direct calcination of the exchanged MOFs were reported too.

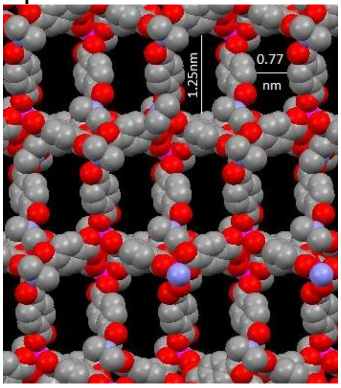

Fig. 1 Showing the existence of one-dimensional channels along the crystallographic b axis in an anionic nano-porous MOF of TMU-3, guest DMF molecules and organic HDMA+ cation are omitted for clarity.

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Paper code: 434

Interplay Between Hydrophobicity and Basicity toward the Catalytic Activity of Isoreticular Organocatalyst MOFs

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The structural diversity of metal-organic frameworks, MOFs, tailored engineering of these compounds is important for their use in catalytic processes [1]. Among the MOFs tested as heterogeneous catalysts, there have been rare reports of size selective catalysts. In the present work, we could successfully indicate that subtle substrate selectivity can be induced in the catalytic system by designing a series of isoreticular MOFs with slight structural modifications. Four MOF catalysts possess imine and/or amine basic N-donor pillars bearing phenyl or naphtyl cores owing different hydrophobic character around the basic reaction center were prepared via simple mechano-chemical synthesis. They were characterized thoroughly using TG, IR and PXRD analysis. For the first time, aldol-type condensation reaction of malononitrile with ketone-functionalized carbonyl substrates developed in the presence of the basic MOF organocatalysts (Figure 1) [2]. Moreover, it has been successfully showed that a subtle substrate selectivity can be addressed during the reaction of three slightly different α,β-unsaturated carbonyl compounds in contrast the effect of size control barriers that commonly direct heterogeneous reaction pathway.

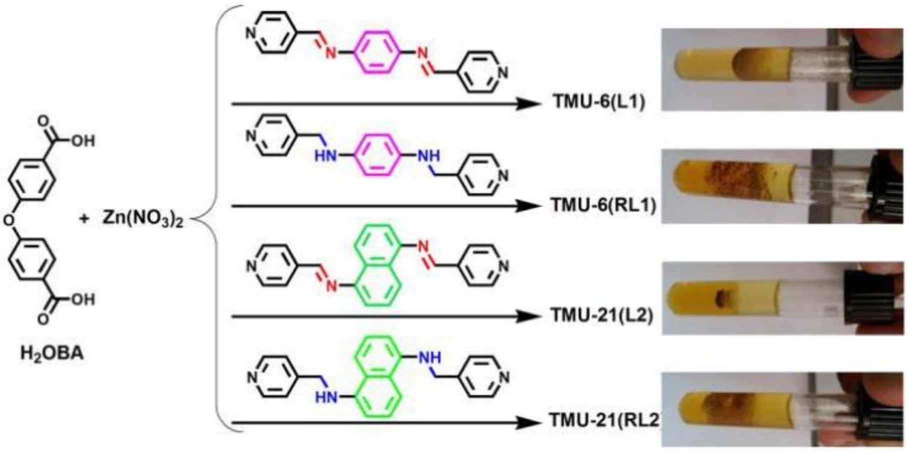

Fig. 1 Synthesis of a series of IRMOFs using four pillar ligands; according to the estimated Pka, their basicity is in the order of RL1> L1> RL2>L2. Images of the catalysts in the mixture of H_2O and PhCH3right.

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Paper code: 457

Co(II) Schiff base complexes encapsulated in the zeolite-Y as efficient and reusable nanocatalysts for epoxidation of styrene in mild conditions

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However, most of such epoxidation reactions are still using homogeneous catalysts. From the sustainable and green chemistry point of view, heterogeneous catalysts would be interesting since they offer the benefits of possible catalyst recycling, easy catalyst separation and sometimes high selectivity and activity [1]. In this respect, encapsulation of transition metal complex in zeolite-Y gained much interest in the last decade [2]. Cobalt (II) macrocyclic complexes synthesized inside the nanocavity of zeolite-Y were characterized by FT-IR, DRS, AAS, XRD, molar conductance, magnetic moment data, thermal and elemental analysis (Scheme 1).

These complexes (neat and encapsulated) were used for epoxidation of styrene with O_2 as oxidant in different solvents. Reaction parameters including temperature, catalyst amount and solvent were screened by reaction time. The supported $Co[L_2]^{2+}$-Y exhibited a moderate 62.8 % selectivity for epoxidation with 86.2 % conversion. The recycling experiment results indicated that the catalysts were highly stable and maintained activity and selectivity even after being used for five cycles.

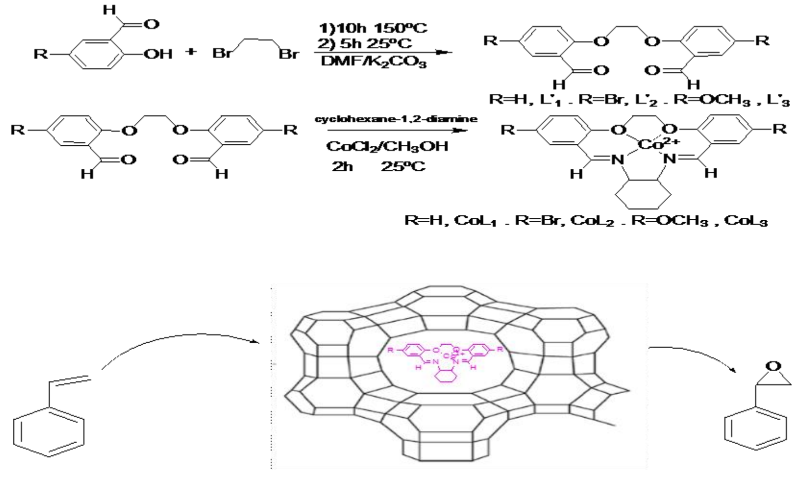

Fig. 1 preparation of neat and encapsulated Co (II) complexes and their application in epoxidation of styrene

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Paper code: 501

Synthesis and crystal structure of a novel mixed ligand copper complex

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Isothiosemicarbazone as one of the thiosemicarbazones derivatives has shown biological properties especially anticancer propreties. In these compouds an alkyl group binds to the sulfur atom, and the coordination accomplishes *via* thioamide nitrogen instead of thioamide sulfur [1]. On the other hand, interaction of nucleobases with metal ions has been a subject of several studies because of their chemical and biological importance. Among them, adenine as an N-rich nucleobase has proved to be a rather versatile metal-binding biomolecule [2]. This molecule shows wide range of binding possibilities because it exhibits at least five nitrogen donor sites, and a great variety of complexes with different metal binding patterns have been reported [2]. In this study, we synthesized a new mixed ligand copper(II) complex of isothiosemicarbazone with adenine as an auxiliary ligand and examined its structure using X-ray crystallography.

Perspective view of the centrosymmetric Cu dimer complex is presented in figure 1. Each Cu atom has a distorted square pyramidal coordination geometry in which a tridentate ONN isothiosemicarbazone ligand in addition to an adenine molecule fill the equatorial sites. The adenine molecule coordinates Cu *via* N4 in the form of neutral monodentate ligand. An oxygen atom (O1) from the other isothiosemicarbazone molecule places in the axial site and constitutes an attractive Cu1···O1^{i} (2.674 Å) (symmetry code: (*i*) -*x*,1-*y*,1-*z*) bond. Displacement of O1 is the main factor of distortion of the complex structure so that it lies 0.188 Å away from the Cu1C9N1N2N3 mean plane.

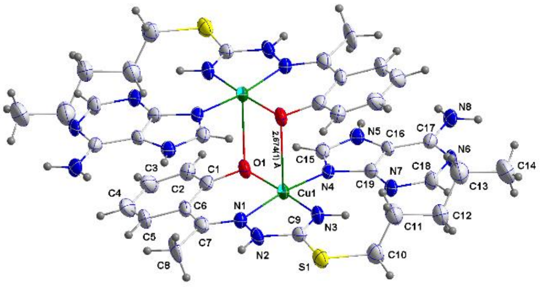

Figure 1. Crystal structure of the synthesized complex showing the atom numbering scheme.

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Paper code: 540

Synthesis, characterization and chemiluminescence study of quercetin and its metal complexes

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Quercetin is one of the most common flavonoid present in nature that has attracted the attention of many researchers because of its biological properties. It is a strong natural antioxidant and having free radical scavenging activity along with potent metal chelator [1]. As transition metal ions play a vital role in the initiation of free radical processes (via the Fenton reaction), metal chelation is widely considered as a mechanism of the antioxidant activity of flavonoids. The interaction of flavonoids with metal ions may change the antioxidant properties and some biological effects of the flavonoids [2].

In the present work we synthesized three metal(II) complexes with quercetin (M = Cu, Ni and Co). The complex formation was examined by analytical techniques including UV-Vis, IR, thermal gravimetric and elemental analyses. Reaction of luminol with hydroxyl radicals produces a chemiluminescence (CL) signal which is influenced by specific radical scavengers, so luminol chemiluminescence was used to evaluate radical scavenging of quercetin and its metal complexes. CL intensity was measured with different concentrations of ligand and complexes. This method can serve as a screening test for the antioxidant properties of substances [3].

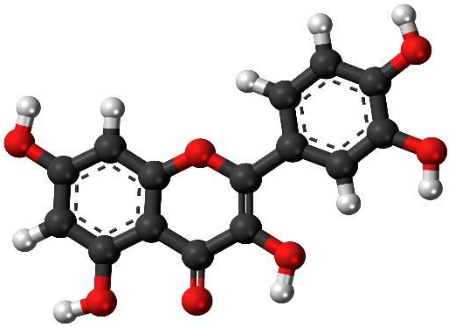

Fig. 1 Chemical structure of Quercetin.

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Paper code: 545

Synthesis, characterization and electronic absorption spectra of new mononuclear cyclopalladated benzo[h]quinolinate complexes containing phosphorus ylides

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The chemistry of Pd(II) complexes containing cyclometalated ligands has attracted great interest in recent years due to their applications in different areas [1-3]. A series of mononuclear cyclopalladated benzo[h]quinolinate complexes with bidentate phosphine ligands, namely, $[Pd(bzq)((Ph_2PCH_2PPh_2C(H)C(O)PhR)]ClO_4$ (R = Cl (**1**), Br (**2**) NO_2 (**3**) OCH_3 (**4**), were synthesized. The reactions of $[Pd(bzq)(\mu\text{-}Cl)]_2$ with bidentate phosphorus ylide (1:2 molar ratio) in presence of $NaClO_4$ led to the splitting of the chloride bridge and obtained the mononuclear complexes that benzoquinolinate and phosphours ligand are bonded to the Pd atom giving two five membered rings. These complexes were fully characterized by elemental analysis, IR, ^1H, ^{31}P, and ^{13}C NMR. The spectroscopic data revealed that the phosphorus ylide is coordinated to palladium *via* the phosphine group (PPh_2) and methene group (CH). These analyses being consistent with a 1:1:1 stoichiometry bzq/ylide/Pd(II) for compounds **1** through **4**. In addition, the UV-vis absorption spectra of complexes were recorded in dichloromethane solvent at 298 K. All of the complexes exhibit absorption bands at high energy due to the intraligand transitions ($\pi \rightarrow \pi^*$) and absorptions at lower energy which are attributed to MLCT transition ($\pi \rightarrow \pi^*$). Also the absorption spectra of complex **3** were recorded in several solvents such as acetonitrile and acetone.

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Paper code: 562

Synthesis, structural characterization and cytotoxic activity of Mn(IV) complex of dithiocarbazate

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Cellular resistance and systematic toxicity are the two major defects of platinum-based anticancer drugs. Complexation of tridentate ONS-chelating ligands of dithiocarbazates derivatives with metals such as Mn is known in chemotherapeutic properties including antitumor effects. A new Mn(IV) complex, [MnL$_2$] (Fig. 1) [L: *S*-ethyl-3-(2-hydroxyphenyl)methylenedithiocarbazate)], is synthesized and characterized using single crystal X-ray diffraction analysis, mass spectrometry and IR spectroscopic technique. This compound crystallizes in the monoclinic system with $C2_1/c$ space group. Single crystal X-ray diffraction analysis reveals that the complex has distorted octahedral structure and each of the two ligands are coordinated to the metal ion through phenol oxygen, azomethine nitrogen and thioamide sulfur donor atoms. This coordination selects *cis* configuration for the two phenolic oxygen and also thioamide sulfur atoms, and likewise the configuration of the *trans* for two azomethine nitrogen atoms compared to their counterpart in the opposite ligand. The $\pi \cdots \pi$ (4.342 Å) and C4-H4···S1^i (2.920 Å) (symm. code *i*: 1/2-x, 1/2-y,1-z) interactions lead to the formation of the dimer. These dimers interact to grow a one-dimensional ribbon along the *a* direction. Moreover, in vitro cytotoxicity of the complex against the MCF-7 (Human Breast cancer cell) and Hela (Human cervical cancer cell) cells was assayed by MMT method. Cytotoxicity study shows that the complex has significant activity against human cervical cancer cell line.

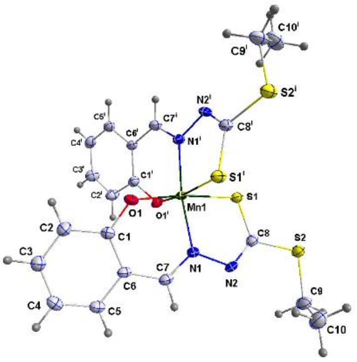

Fig. 1 ORTEP diagram of [MnL$_2$] with atom-numbering scheme.

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Paper code: 570

Synthesis of new dithiocarbazate Sn(IV) complex; investigation of the crystalline structure and cytotoxic activity

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Metal complexes of *S*-alkyldithiocarbazates comprise an important class of compounds due to the interesting physical and chemical properties and also play significant role in biological systems. A new Sn(IV) complex, [$SnCl_2L$.DMSO] (Fig. 1) [L: *S*-ethyl-3-(2-hydroxyphenyl)methylenedithiocarbazate)] (*sedtc*), is synthesized and characterized using single crystal X-ray diffraction analysis, mass spectrometry and spectroscopic techniques such as IR, ^{1}H- and ^{13}C-NMR. Compound **1** crystallizes in the triclinic system with $P\bar{1}$ space group. The X-ray diffraction data revealed a distorted octahedral structure where the *sedtc* tridentate ONS ligand is coordinated to the metal ion *via* phenolic oxygen, iminic nitrogen, and thioenolate sulfur donor atoms. In this compound the two chlorine atoms are arranged *cis* relative to each other (96.81(3)º). The H_2L ligand and one chlorine atom are located at the equatorial position and the other chlorine atom and DMSO solvent occupied the axial position. The adjacent molecules in this compound form dimers with ten-members graph set, $R_2^2(10)$, by a pairwise hydrogen bond H7-C7^i···Cl2 (2.819 Å) (Symm. Code *i*: 2-x, 1-y, 1-z). The dimer form one-dimensional chain along the *ac* plane bisector through the C10-H10C···π (3.397 Å) and H12B-C12···Cl2 (2.868 Å) interactions. Moreover, *invitro* cytotoxicity of the complex against the MCF-7 (Human Breast cancer cell) and Hela (Human cervical cancer cell) cells are assayed by MMT method. Cytotoxicity study shows that ligand coordination to the metal increases cytotoxic activity relative to the free ligand and the complex has significant activity against human cervical cancer cell line.

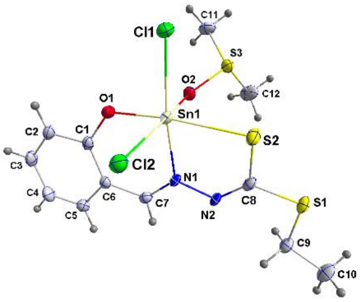

Fig. 1. ORTEP diagram of *cis*-[$SnCl_2L$.DMSO] with atom-numbering scheme.

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Paper code: 599

Synthesis and characterization of new palladium(II) complexes derived from pyridinium ylide and investigation of their catalytic activity

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The catalytic complex of palladium is one of the most powerful tools for creating a C-C bond in organic synthesis. As a result, various types of palladium complexes have been developed with different ligands [1]. Herein we used the pyridine ylide as a ligand for synthesis Pd complex. This ylide is capable of forming stable complexes that can be identified by spectroscopic and X-ray crystallographic method. Also, they can behave as ambidentate ligands, because the carbanion located at the Cα of the ylide or the enolate oxygen is able to donate electron density to a transition metal [2]. We studied on the catalytic properties of palladium(II) complex with the new pyridinium ylide in Suzuki–Miyaura cross-coupling. Results showed that ylide, with an electron-donating structure, was most efficient and enabled the coupling of various aryl halide with aryl boronic acid in good to excellent yields. The ease of preparation of the ylidic ligand, its high solubility in organic solvents, very low catalyst loading and stability toward air and moisture make it an ideal catalytic system for Suzuki cross-coupling reaction.

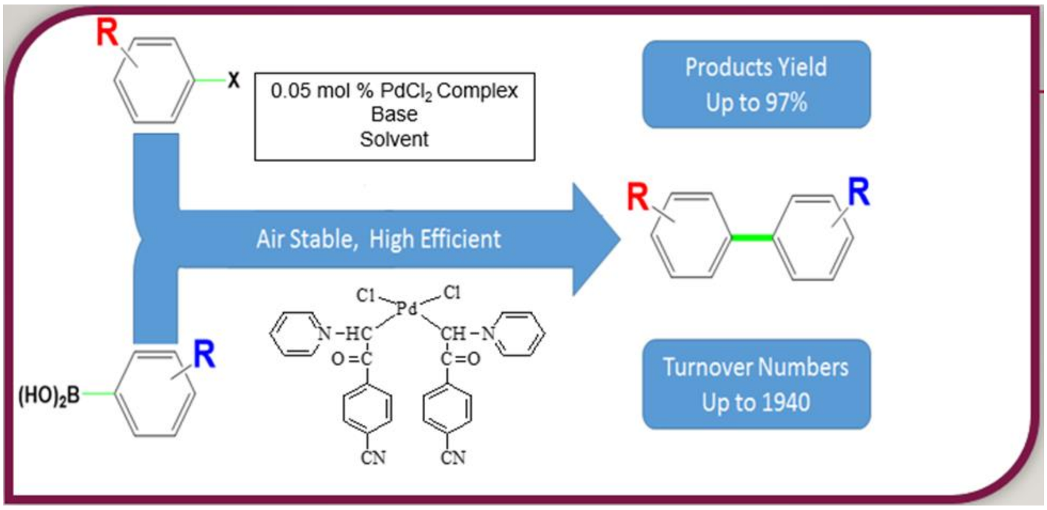

Fig.1. $C_5H_5NCHC(O)C_6H_5$(*p*-CN) with Pd(II)

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Paper code: 600

New Molecular Azo-Azomethine Receptor for Colorimetric Detection of Inorganic Anions

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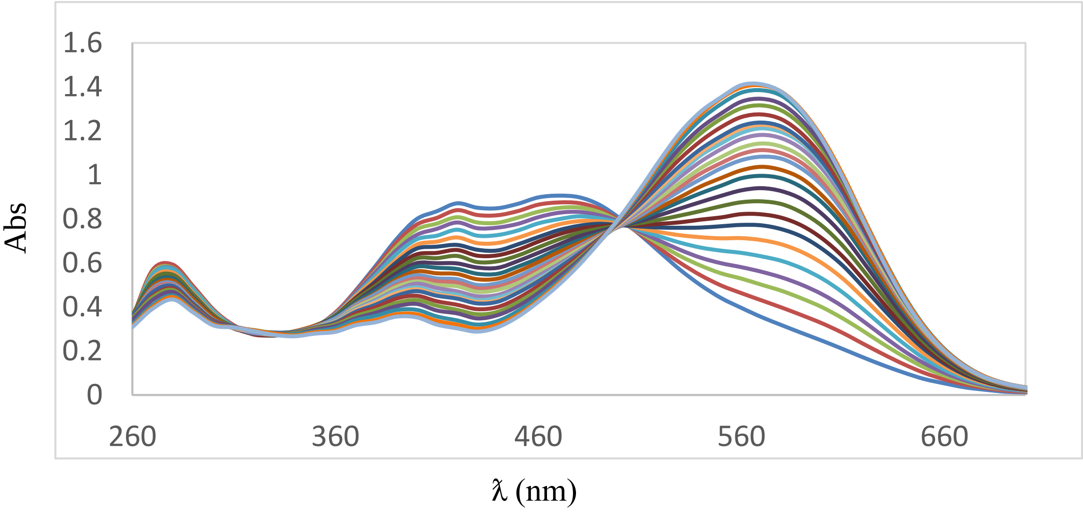
A new azommerhine receptor, HL, was synthesized by reaction of 2-(3,4-dimethoxy phenyl)ethan-1-amine and 2-hydroxy-5-((4-nitro phenyl)diazenyl)benzaldehyde in pure EtOH. The sensing ability of HL was investigated qualitatively towards various anions, such as F^-, Cl^-, Br^-, I^-, NO_3^-, AcO^-, CN^-, HSO_4^- and $H_2PO_4^-$ (as their sodium salts), by visual examination of color changes in dry DMSO. Furthermore, the anion recognition behavior of, HL, was explored using UV-Vis spectroscopy in dry DMSO and also in semi-aqueous solution (DMSO: H_2O, 7:3, v/v). The prepared receptor could instantly detect inorganic CN^-, AcO^- over other anions in semi-aqueous media, at low limit of CN^- about 7×10^{-7} M. which is lower than the World Health Organization (WHO) permissible level.

Moreover, the stoichiometry between HL with CN^-, AcO^- were determined from UV-Vis spectral changes with the help of Benesi–Hildebrand method. The results indicated that the mentioned anions interact with HL in a 1:1 stoichiometry with binding constants of CN^-: 3.1×10^4 M, AcO^- : 3.6×10^4 M .



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Paper code: 601

Synthesis and characterization of new mercury(II) complexes derived from α-keto stabilized new pyridinium ylide

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Metal carbene complexes are of much interest in synthetic chemistry [1]. One of the most abundant carbene complexes are Cα coordinated Hg(II) complexes. Pyridine ylides $R_2N=C(R')(R'')$ (R, R′, R″=alkyl or aryl groups) are very reactive species with interesting applications in organic synthesis [2]. These compounds can behave as ambidentate ligands, because the carbanion located at the Cα of the ylide or the enolate oxygen is able to donate electron density to a transition metal [3]. Considering the importance of metal carbenes, and particularly pyridinium ylide, synthetically simple and general routes for their preparation are highly desirable. Herein, we report the synthesis and characterization of new binuclear and polymeric complexes of Hg(II) derived from α-keto stabilized pyridinium ylide. Reaction of α-keto stabilized pyridinium ylides $C_6H_5NCHC(O)C_6H_4R$ (R=m-CN) with HgX_2 (X= Cl, Br, I) in 1:1 ratio leads to binuclear products of the type $[HgX_2(ylide)]_2$. Also, polymeric products of the type $[(ylide)Hg(NO_3)_2]n$ obtained by the reaction of mentioned ylide and $Hg(NO_3)_2$ in 1:1 ratio. The reaction yielded the desired Hg(II) complexes in excellent yields. Characterization of the complexes by IR, ^1H and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom (Fig. 1).

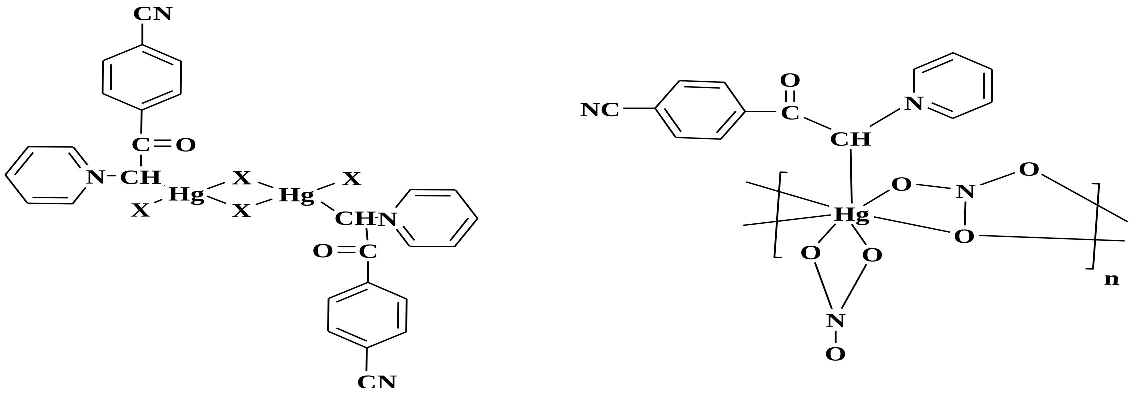

Fig.1. $C_5H_5NCHC(O)C_6H_5$ (*p*-CN) with HgX_2 (X = Cl, Br and I)

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Paper code: 620

Synthesis and characterization of new binuclear and polymeric complexes mercury(II) stabilized of pyridinium ylide

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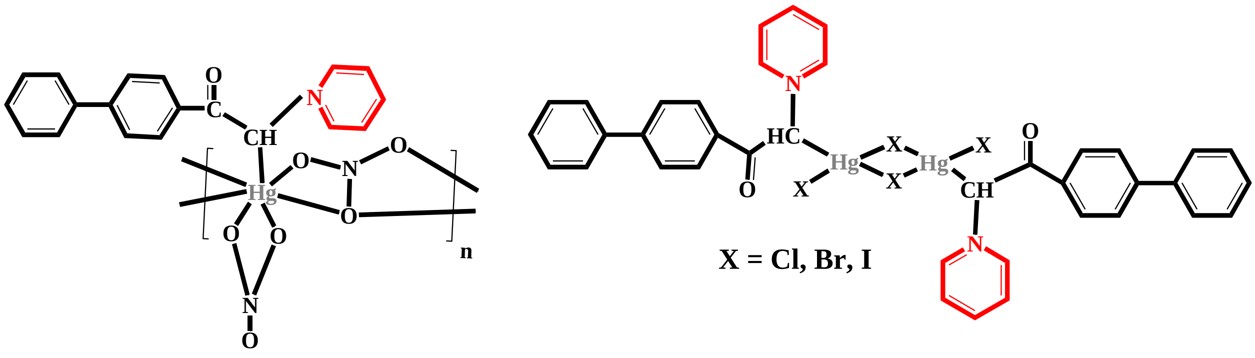
Several pyridinium ylide complexes of transition metals have been reported [1,2] and the change of the structure and reactivity of the ylide upon coordination has posed interesting compounds. In this work, Hg(II) transition metal has chosen to study the nature of pyridinium ylides and synthesized some complexes. The ylide used in this project is from a 1:1 ratio of salt and K_2CO_3 in a water solvent for 30 minutes [1]. The new pyridine ylide can act as a ligand that is used in different ways to various intermediates. Reaction of ylide $C_5H_5NCHC(O)C_6H_5R$ (R=p-Ph) with HgX_2 (X = Cl, Br and I) and $Hg(NO_3)_2$ in 1:1 ratio leads to binuclear and polymeric products of the type $[HgX_2(ylide)]_2$ and $([Hg(ylide)]NO_3)_n$ Respectively. These complexes were synthesized by using methanol as solvent and studied by IR, ^{1}H and ^{13}CNMR spectroscopy techniques [2]. The schematic representation of this complex is shown in (Fig. 1).



(a) (b)

Fig. 1: Polymeric (a) and binuclear (b) structure of Hg(II) complexes

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Paper code: 623

Synthesis and characterization of palladium(II) complexe derived from α-keto stabilized pyridine ylide and study on its catalytic properties

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New prepared ylide has been considered in this research for the preparation of palladium complexes whit catalytic applications [1]. A palladium complex combined with this kind of ylides is the most commonly used catalytic system for these type of reactions [2]. According to this report, this ylide was synthesized in a 1:1 ratio with potassium carbonate as a base in ice bath which was used to synthesize the palladium complexes (II). By doing this reaction, it is possible to develop research on the use of materials for the synthesis of palladium metal catalysts that can greatly increses the yieds of products. Characterization of the complex by IR, 1H and 13C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom (Fig. 1). Also In this work, the Suzuki–Miyaura reaction of various aryl halides using [Pd(μ-Cl$_2$){C$_6$H$_5$NC(H)C(O)PhR}]$_2$ (R=p-Ph) have been investigated. Well-defined pyridine bis-ylide Pd(II) complex were found to be an effective catalyst for the Suzuki coupling of various aryl halides including with phenyl boronic acid, giving the desired coupling products at low catalyst loading in moderate to good yields.

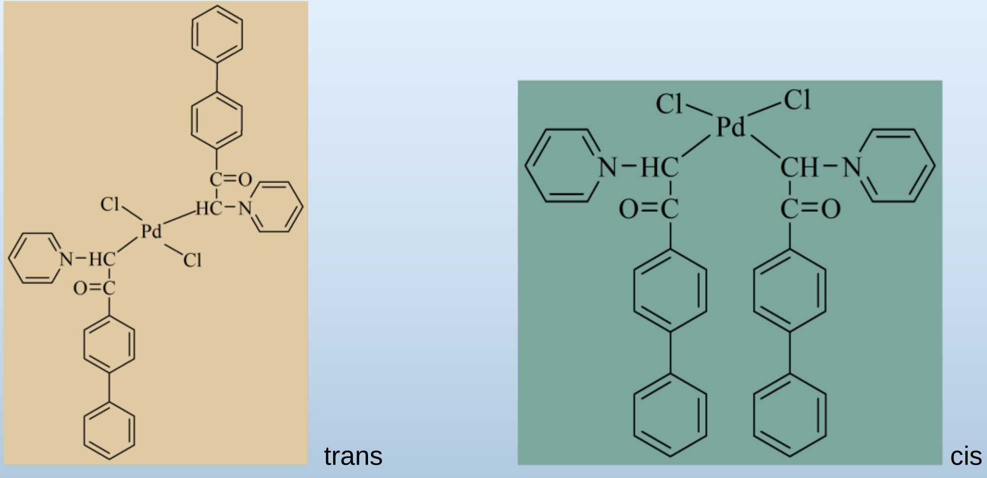

Fig.1. $C_5H_5NCHC(O)C_6H_5$ (p-Ph) with Pd(II)

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Paper code: 637

Synthesis and spectroscopic characterization of Hg(II) complexes of new unsymmetrical Phosphorus ylide

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The reaction of $Ph_2PCH_2PPh_2$ (dppm) with ethylchloroacetate in chloroform produce the new phosphonium salts $[Ph_2PCH_2PPh_2CH_2C(O)OCH_2CH_3]Cl$ (**1**). Further, by reacting the phosphonium salt with appropriate base, the bidentate phosphorus ylide, $Ph_2PCH_2PPh_2{=}C(H)C(O)OCH_2CH_3$ (**2**) was obtained. The reaction of this ligand with mercury(II) halides in dry methanol led to the formation of the mono nuclear complexes $[HgX_2(Ph_2PCH_2PPh_2C(H)C(O)OCH_2CH_3)]$ [X=Cl (**3**), Br (**4**), I (**5**)]. Characterization of the obtained compounds was performed by elemental analysis, IR, ^{1}H, ^{31}P and ^{13}C NMR. In all complexes the title ylide is coordinated through the ylidic carbon and the phosphine atom. These compounds form five membered ring under complexation.

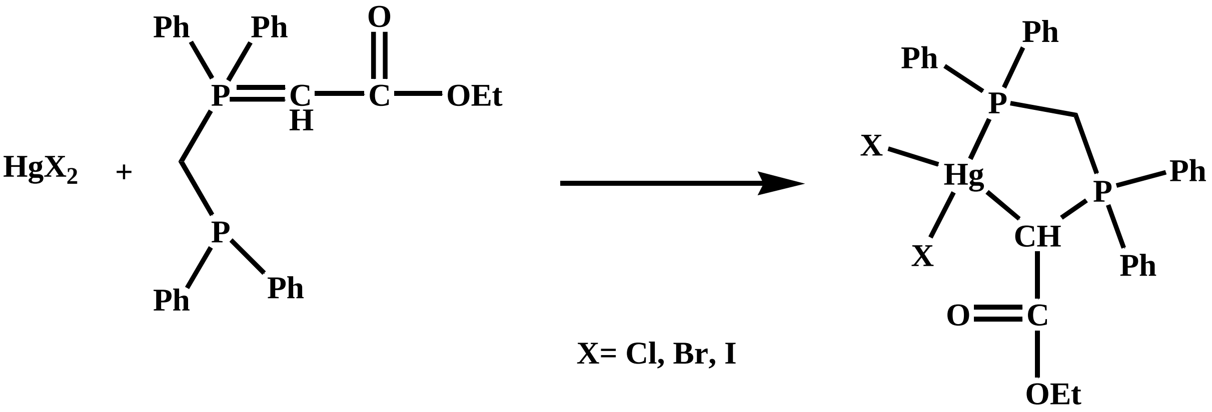

Fig. 1 Synthetic route for the preparation of compounds **3**- **5**.

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Paper code: 652

Synthesis and characterization of polymeric Schiff base ligand and its vanadium complex derived from N,N-bipyridinium

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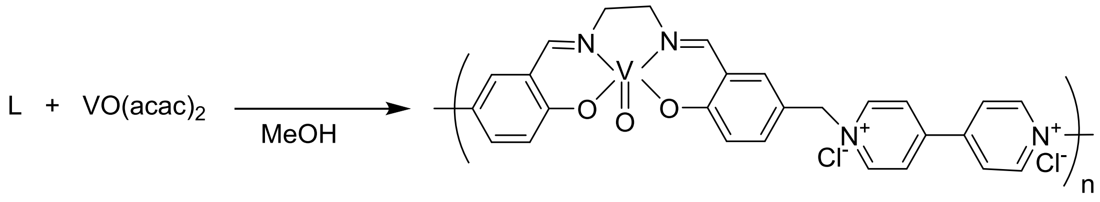
Polymeric Schiff bases are an important class of coordination polymers with multidentate donor sites, known to form polychelates with transition metal ions. Basic properties of polymeric Schiff base are due to the azomethine linkage in polymeric backbone. This report deals with the synthesis and characterization of a new polymeric Schiff base ligand and its vanadium complex. The polymeric Schiff base ligand (L) was prepared from reaction of [N,N-bipyridinium bis(methyl salicylaldehyde)] chloride and ethylendiamin. Then by reaction of $VO(acac)_2$ with L the VO- Schiff base polymer was synthesized (scheme1). L and VO- Schiff base polymers were characterized by different methods: FT- IR, UV–Vis, ^{1}H-NMR and CHN. The results of C, H and N analysis agree with the expected values. The IR spectrum provide valuable information regarding the reaction of polymeric Schiff base-ligand with metal atom. The ligand and metal–polychelate were mainly characterized using the azomethine, Ar-OH and V=O bands. The appearance of a broad strong band in the IR spectrum of the ligand in 3000–3400 cm^{-1} is assigned to Ar-OH stretching vibrations. In the metal–polychelate, this band appears as a weak band. The band at 1598 cm^{-1} in the FT-IR spectrum of L, assigned to the azomethine linkage of L. This band shifted to the higher wave number in the polychelate. In addition, a new sharp band is seen at 814 cm^{-1}, related to the V=O stretching vibrations. These observations indicating the coordination of the ligand to metal ion. The ^{1} H-NMR spectrum of the L confirmed the functional groups of L. It exhibits resonance signals at 10 ppm, 7-9 ppm and 11 ppm which is assigned to the CH=N, groups, aromatic protons and –OH groups, respectively.



Scheme 1: Elemental Analysis of L and Its vanadium complex

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Paper code: 705

Mononuclear and dinuclear complexes of stannyldimethylplatinum(IV) *via* oxidative addition reactions

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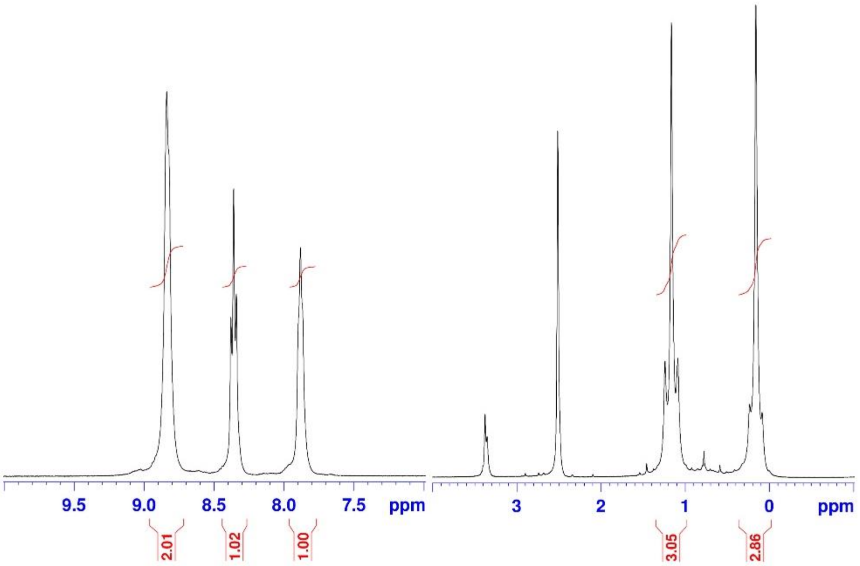
Dimethylplatinum(II) complexes of general formula [$PtMe_2$(NN)], NN is a chelating diimine ligand, have attracted a great deal of interest towards oxidative addition reactions; as it is a key step in many catalytic reactions. The oxidative addition reactions of alkyl halides to the dimethylplatinum(II) complexes containing diimine ligands have been studied extensively, although there are a few reports of organoplatinum complexes containing tin atom [1-2]. Therefore, we herein report the oxidative addition reactions of electron rich complexes [$PtMe_2$(NN)] {NN = bpy (2,2'-bipyridine), phen (1,10-phenanthroline) and bu_2bpy (4,4'-di-*tert*-butyl-2,2'-bipyridine)} with some organotin halides or pseudohalides to give the corresponding mononuclear or dinuclear dimethylplatinum(IV) complexes. The products have been fully characterized by elemental analysis, IR, multinuclear NMR (^{1}H, ^{13}C, ^{195}Pt, ^{119}Sn), HH COSY and DEPT-135 NMR spectroscopy and X-ray crystal structure determination. The results provide more information about their structural features.



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Paper code: 711

Geometrical aspects in coordination of an amino alcoholic ligand toward copper bromide

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In the Article a new ionic complex of the copper(II), [Cu(L)Br]Br, with 2-(2-(2-hydroxyethylamino)ethylamino)cyclohexanol (L) was prepared and identified by elemental analysis, FT-IR spectroscopy and single-crystal X-Ray diffraction. The spectroscopies data revealed that the ligand acts as NN'OO-donor mode toward Copper atom and in agree with the structural analysis result. In this structure, the copper atom has a CuN_2O_2Br environment and distorted square pyramidal geometry. The ligand has a one chiral carbon atom whilst two new chiral centers (nitrogen atoms of the amine groups) are formed after coordination. In the crystal network of the complex, there are intermolecular N–H···X and O–H···X (X: Br) hydrogen bonds, extending the crystal network in three directions.

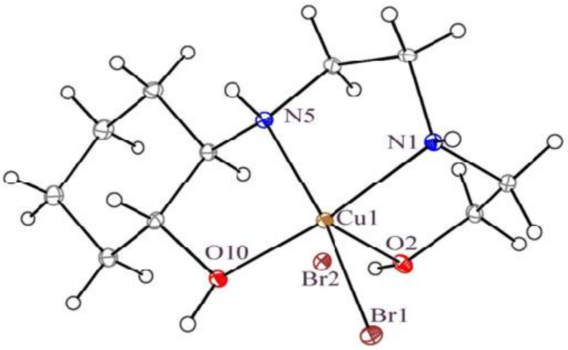

Fig. 1 The crystal structure of the complex.

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Paper code: 714

Synthesis and Spectral Study of a zinc(II) Complex with NN'O-Donor Ligand

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In this work, 2-(2-(2-hydroxyethylamino)ethylamino)cyclohexanol (L) was prepared in solvent by ring opening of epoxycyclohexane with 2-(2-aminoethylamino)ethanol and then its complex with zinc(II), $[Zn(L)Cl_2]$ were prepared and identified by elemental analysis, FT-IR, ^{1}H NMR spectroscopy and single-crystal X-Ray diffraction. The spectroscopies data revealed that the ligand acts as NN'O-donor mode toward zinc atom and in agree with the structural analysis result. The X-ray analysis showed that the zinc atom has distorted trigonal bipyramidal geometry. In the crystal network of the complex there are intermolecular N–H⋯Cl, O–H⋯Cl and O–H⋯O hydrogen bonds, extending the crystal network in three directions.

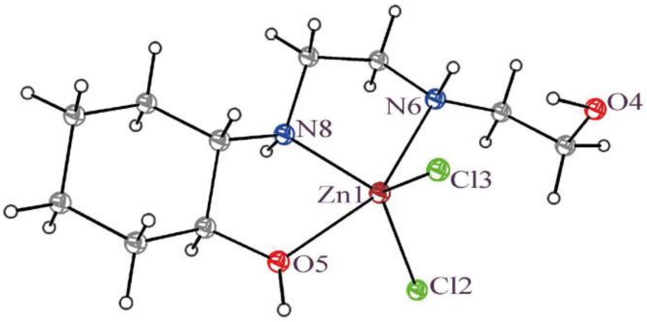

Fig. 1 The crystal structure of the complex.

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Paper code: 730

Complexation of an imidazolidin ligand toward the copper atom

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A new complex of copper, [Cu(L)$_2$], with 2-(1-(2-hydroxyethyl)-4,5-dihydro-1H-imidazol-2-yl)phenol ligand (HL) was prepared and identified by elemental analysis, FT-IR spectroscopy and single-crystal X-Ray diffraction. In this structure, the copper atom has CuN_2O_2 environment and square planar geometry. The ligand has a one chiral carbon atom. X-ray analysis of the complex revealed that the ligand is deprotonated during the complexation process and acts as anionic ligand. The complex has one center of inversion on the copper atom and C_i symmetry. In the crystal network of the complex there are intermolecular C–H···O and C–H···C hydrogen bonds, extending the crystal network in three directions.

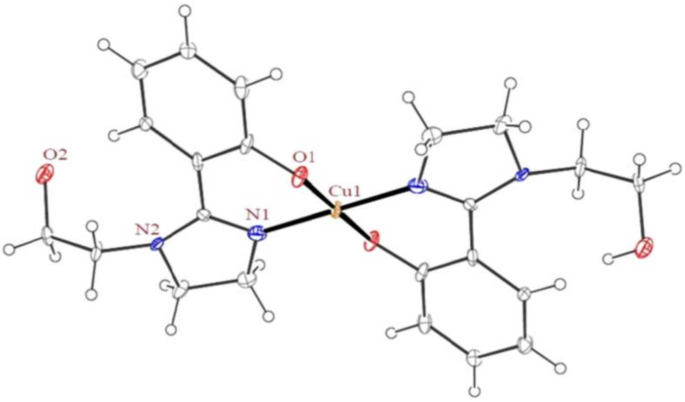

Fig. 1 The structure of the complex.

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Paper code: 755

Synthesis and characterization of cobalt complexes containing 1,10-phenanthroline-2,9-dicarboxylic acid

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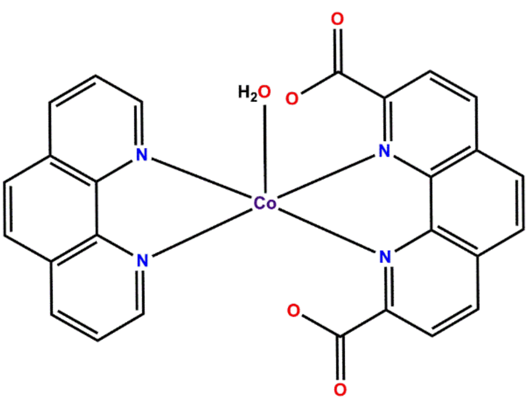
The enhanced coordination capability and rigid structure of PDA^{2-} are not only helpful to construct high-nuclearity metal cluster but also confer high thermodynamic stability on the corresponding complexes. 1,10-Phenanthroline-2,9-dicarboxylic acid (H_2PDA) has versatile chelating and bridging capabilities, which play an important role in coordination chemistry. Preorganized ligands can be good candidates for biomedical applications and sensors because of their intrinsic rigidity and selective behavior. These ligands show a promising future in the bioinorganic, nuclear and industrial fields as well as many other fields. Therefore, we synthesized Co(II) complexes with this ligand and auxiliary ligands such as 2,2'-bipyridine (bipy) and 1,10-Phenanthroline (Phen) using various methods. The chemical formulas of $[Co(PDA)(Phen)(H_2O)]\cdot H_2O\cdot CH_3CN$(**1**), $[Co(PDA)(bipy)]\cdot H_2O$(**2**) were determined by the help of elemental analysis and infrared spectroscopy (Fig. 1.).



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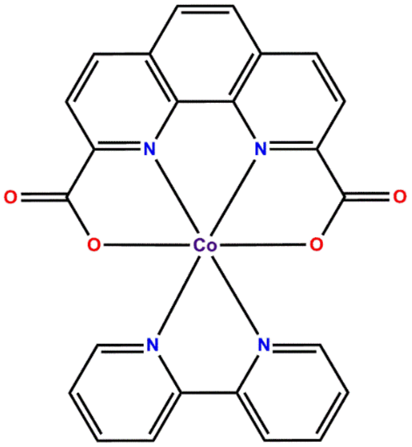

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Fig. 1. Proposed chemical formulas of 1 and 2. Water and acetonitrile molecules are omitted for clarity.

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Paper code: 760

TiO_2 conjugated with molecules of Rose red dye as a photocatalyst towards salicylic acid

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Nanoscale TiO_2 was synthesized using $TiCl_4$ as a starting material via sol-gel method. Prepared spherical TiO_2 nanoparticles were conjugated with Rose red dye and used as modified photocatalysts for degradation of salicylic acid as a model of environmental pollution. TiO_2 nanoparticles and dye-TiO_2 system were characterized with X-ray diffraction analysis (XRD), Infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), thermal analysis (TGA/DSC) and spectroscopy (UV-Vis). Based on the results of detection, the energy gap of dye-TiO_2 was calculated to be 2/9eV. Experiments showed degradation of salicylic acid by dye-TiO_2 system under visible light has better efficiency compared to bare TiO_2 nanoparticles. At the time of 120 minutes; dye-TiO_2 system could remove approximately 70% of salicylic acid, while bare TiO_2 nanoparticles had 10% efficiency. The mechanism of reaction is based on optical excitation of both of TiO_2 semiconductor and dye molecules fallowed by charge transfer. It is proposed that electron injection from the dye to ،TiO_2 is mainly responsible for the enhancement of the reaction rate of salicylic acid degradation.

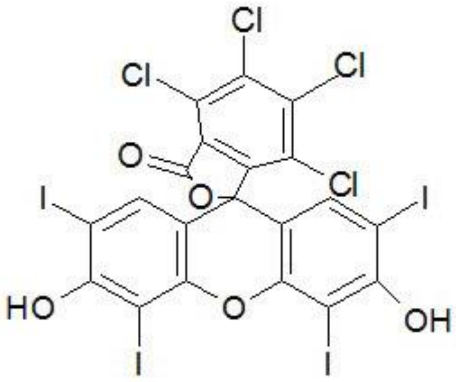

Fig. 1 molecular structure of Rose red dye.

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Paper code: 777

Synthesis and characterization of metal complexes with tridentate Schiff base ligand (NNS) derived from Pyrrole-2-carbaldehyde

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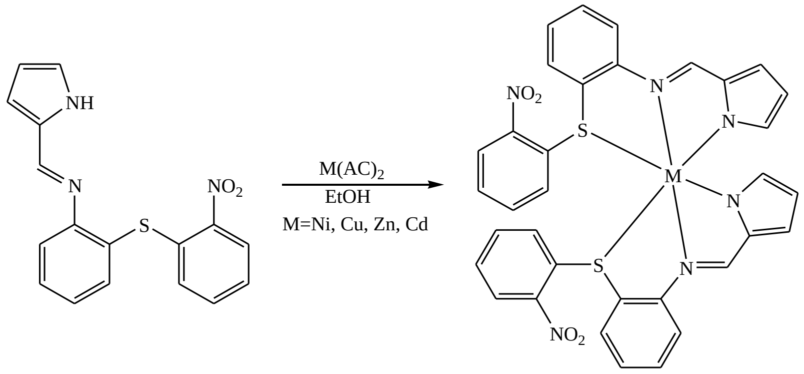
The formation of variety of metal complexes with NNS ligands, indicate the spectacular progress in coordination and bioinorganic chemistry. Schiff base complexes of transition metals containing ligand with N, S donors are known to exhibit interesting biological activity. Still, development of new Schiff bases long term administration for chelation of metal deposits [1]. Pyrrole derivatives have intensively antibacterial and antitumor activities [2].

In this work we synthesized 2-((2-nitrophenyl)thio)aniline from 1-chloro-2-nitrobenzene and 2-aminothiophenol. Then NNS Schiff base ligand prepared by reaction of 2-((2-nitropheyl)thio)aniline with Pyrrole -2-carbaldehyde. Ni(II), Cu(II), Zn(II) and Cd(II) Schiff base complexes of this ligand were synthesized. 2-((2-nitrophenyl)thio)aniline and NNS Schiff base ligand were characterized by IR, ^{1}H and ^{13}C NMR and Mass spectrometry and the synthesized complexes characterized by IR, UV-Vis, X-ray crystallography, elemental analyses and conductivity. The results show that the ligand is coordinated to metal ions through imine N, thioether S and Pyrrole N atoms (Scheme 1).



Scheme 1 Synthesis of the complexes

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Paper code: 803

N-oxide Functionalization of UiO-66 via Solvent-Assisted Ligand Incorporation: Synthesis and Cr(VI) Adsorption Studies

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Porous metal–organic frameworks (MOFs) are hybrid solid-state compounds that have attracted voluminous research efforts for applications relevant to gas storage and separation, chemical catalysis, and optoelectronic and thermoelectric devices [1]. However, many of these applications require recyclability, which is intimately tied to the stability of the corresponding frameworks in ambient conditions as well as in the presence of water. It is worth noting that only a modest fraction of the total known MOFs are both thermally and chemically stable. Among the known MOF materials, Zr-based MOFs have been intensively studied, because of their superior stability against moist atmosphere, aqueous solutions, as well as basic or acidic media [2]. The robustness arising from the kinetic inertness of the Zr–carboxylate bonds enables advanced applications in MOF systems. Solvent-assisted ligand incorporation (SALI) is useful for functionalizing the channels of metal−organic framework (MOF) materials such as UiO-66 that offer substitutionally labile zirconium(IV) coordination sites for nonbridging ligands [3,4]. Utilizing SALI, we have efficiently attached the isonicotinate N-Oxide (INO) carboxylates on the Zr_6 nodes of UiO-66. This N-oxide-functionalized mesoporous MOF, termed herein SALI-n, were studied experimentally as potential Cr(VI) adsorbent material.

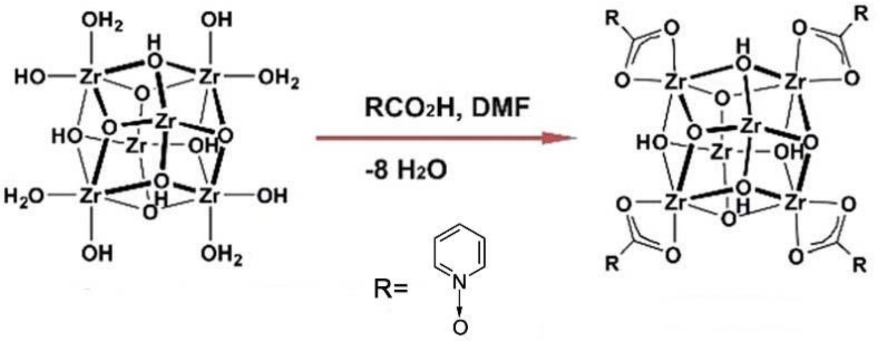

Fig. 1 Depictions of Solvent-Assisted Ligand Incorporation (SALI)

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Paper code: 809

Synthesis and characterization of cadmium sulfide nanoparticles via a solvothermal method in the presence of a new sulfur source

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Nanoparticle and nonstructural materials have attracted considerable interest in resent year these materials have found extensive use in various. filed such as high-density memory devices, laser, transistor and other optoelectronic system [1]. CdS nanostructures have been synthesized using different approaches including solvothermal or hydrothermal methods, thermal evaporation, chemical vapor approach and electrochemical deposition.

In this study CdS nanocrystals were successfully prepared using solvothermal strstegies that employed $Cd(NO_3)_2.4H_2O$ and a new sulfurizing agent from the class of thio Schiff base, N-benzylideneethanethioamide, as starting materials. X-ray diffraction (XRD) patterns, FT-IR spectroscopy (Fig.1) and scanning electron microscopy (SEM) images were used to characterized synthesized CdS [2]

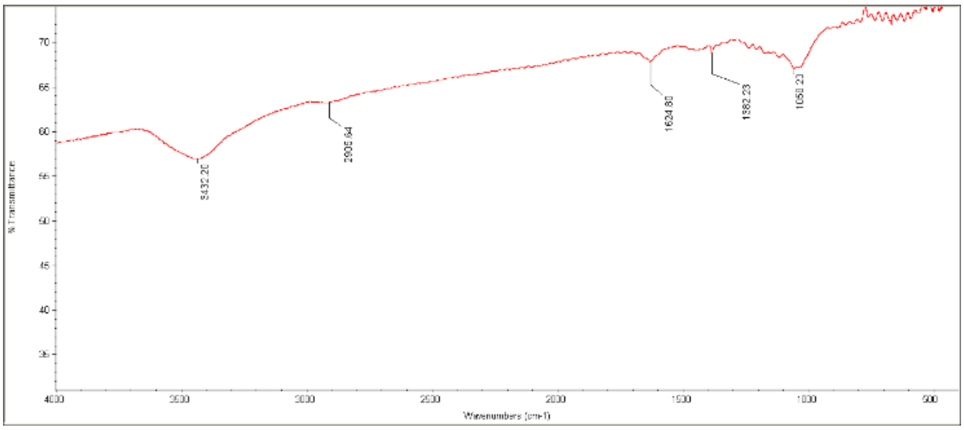

Fig.1 FT-IR spectrum of CdS nanoparticles via a as-syentheszed at 180°C for 12 h.

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Paper code: 840

Synthesis, characterization and biological activity of a new novel *cis* MoO_2 Schiff base complex

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It has been demonstrated that Schiff base ligands and their coordination compounds can be used as effective anti-malarial, anticancer, antimicrobial, antioxidant and DNA-BSA binding agents. CH=N moiety of these compounds is responsible for their biological activities that can be enhanced after complexation with metal ions. In addition to biological applications, these compounds are used in catalytic Processes and nanomaterial chemistry [1,2].

In this study, a tridentate Schiff base ligand, (1E)-1-[(2-hydroxyanillino)methylidene]naphtalen-2-one (H_2L), and its Mo(VI) complex [MoO_2(L)(MeOH)], have been synthesized and characterized using physicochemical and spectroscopic methods including molar conductivity, elemental analysis, ^{1}HNMR, UV-Vis and FT-IR. The Experimental results confirmed that the Mo(VI) central ion is surrounded by two phenolic oxygens and azomethine nitrogen of tridentate Schiff base ligand, oxo groups and methanolic oxygen. The prepared compound was also screened for antimicrobial activities.

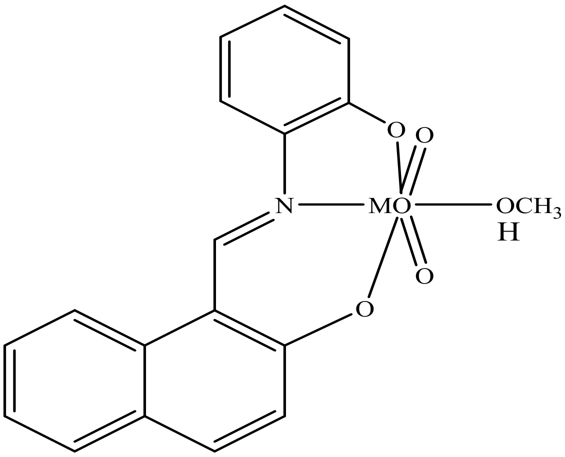

Fig. 1 Schiff base complexes Molybdenum metal (VI) with (1E)-1-[(2-hydroxyanillino)methylidene]naphtalen-2-one

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Paper code: 894

Synthesis and characterization of VO^{2+} and Mn^{2+} complexes containing a Schiff base ligand derived from Tryptamine and 2-hydroxy-1-naphtaldehyde

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Schiff bases are compounds that are usually formed by condensation reaction of the aldehydes or ketones and primary amines. The common structural feature of these compounds for discriminating of the Schiff bases is RR′C=NR″, where the R″ group represents alkyl and aryl groups that cause constancy of the Schiff base as an amine[1]. The non-bonding electron pair on the nitrogen atom in these compounds make them facility to coordinate to the metal ions and, formed one of the most important classes of complexes named Schiff base complexes [2].

In this research, we describe the synthesis and characterization of a new Schiff base ligand derived from the reaction of Triptamine and 2-hydroxy-1-naphtaldehyde and its VO(II), Mn(II) complexes. Ligand and complexes were characterized by different spectral and analytical methods (CHN analysis and, NMR, IR, UV-VIS and Fluoresce spectroscopy).

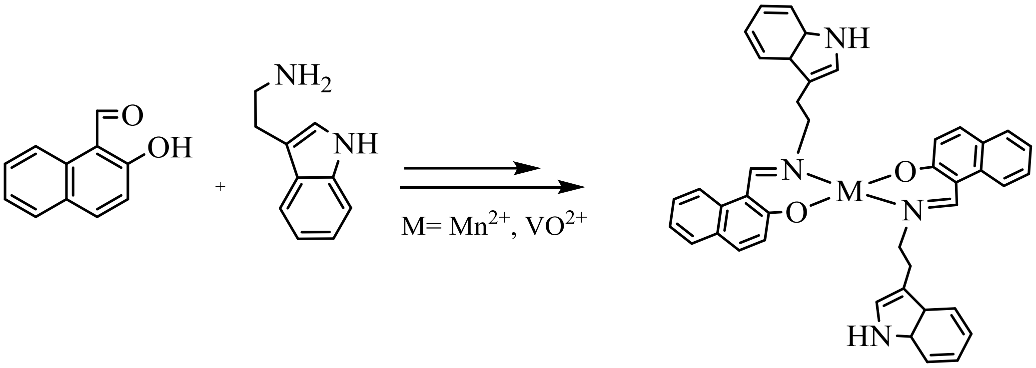

Fig. 1 The synthesis of (E)-1-((2-(1H-indol-3-yl)ethylimino)methyl)naphthalen-2-ol and its VO(II), Mn(II) complexes

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Paper code: 958

A new phosphoric triamide structure: $(CF_3C(O)NH)P(O)(NHC_6H_4\text{-}4\text{-}CH_3)_2$

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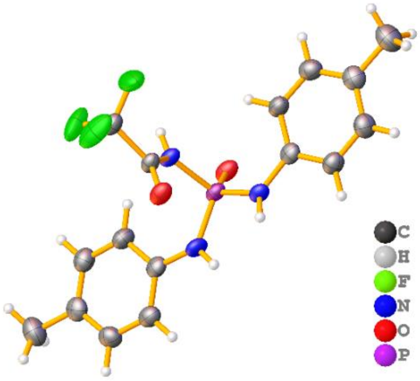
The synthesis, spectroscopic characterization (^{1}H-, ^{13}C-, ^{31}P-, ^{19}F-NMR, IR and mass) and single crystal *X*-ray diffraction analysis of $(CF_3C(O)NH)P(O)(NHC_6H_4\text{-}4\text{-}CH_3)_2$ were investigated. The compound was crystallized in the chiral space group $P2_1$ with $a = 12.4895(5)$, $b = 5.0537(2)$, $c = 13.6482(6)$ Å, $\alpha = \gamma = 90°$ and $\beta = 103.753(4)°$. The asymmetric unit is composed of one complete molecule. The P═O, C═O and P—N bond lengths and P—N—C angles are within the expected values observed for analogous structures.[1,2] The P atom has a distorted tetrahedral environment with the bond angles at the P atom within 101.9(1)° [N3-P1-N2] to 118.2(1)° [O2-P1-N3]. The N atoms bonded to P atom have mainly sp^2 character. In the crystal structure, molecules are linked *via* N—H···O═P and N—H···O═C hydrogen bonds, into a one dimensional arrangement along the *b* axis, which includes the non-centrosymmetric ten-membered ...H/N/P/N/C/O...H/N/P/O... ring motifs.



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Paper code: 1054

Packing Problem (Z′=2) in Mercuric Halide Complexes Containing the Most Stable Polymorph of Ester Ligands; Directionalized by Robust $C-H\cdots\pi_e$ Synthon

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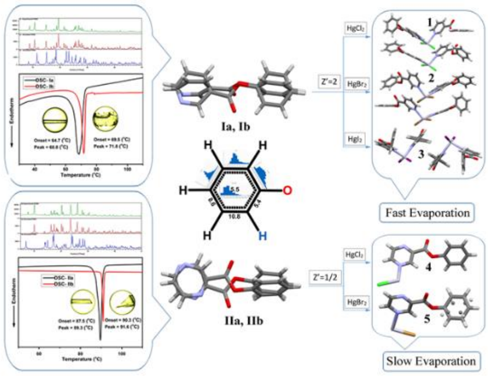
The number of formula units in the unit cell and the number of symmetry-independent units in a crystal structure are known as Z and Z′, respectively. In general, Z′ will be 1 but when it is greater than 1, the situation referred as a packing problem in crystallography. [1] The ability of a compound to exist in more than one arrangement in the solid state is defined as polymorphism and if the same molecule in two different polymorphic forms adopts clearly different conformations this is called conformational polymorphism. [2] Intermolecular interactions can determine the outcome in some part of the crystallization process since the interactive donor part of the molecule is engaged in covalent bonding. As we noted in our previous study, if one compound has two or more polymorphs, the most stable one may control derivatives of the compound. [3] In this study, with crystal engineering in mind, the organic ligands phenyl nicotinate (L_1) and phenyl pyrazine-2-carboxylate (L_2) were synthesized. For each ligand, two polymorphs were systematically obtained (Ia, Ib and IIa, IIb). For L_2 three new mercury (II) halide complexes, $[Hg(L_1)_2Cl_2]$ (1), $[Hg(L_1)_2Br_2]$ (2), $[Hg(L_1)_2I_2]$ (3) and for L_2 two new mercury (II) halide complexes, $[Hg(L_2)_2Cl_2]$ (4), $[Hg(L_2)_2Br_2]$ (5), were synthesized. All of the compounds were fully characterized using FT-IR, TGA, DSC, mass spectrometry (only for ligands), CHNOS elemental analyses, NMR, PXRD and SCXRD. Following our previous CSD study, the directionality of $C-H\cdots\pi$ interactions has also been investigated. Our results show a high tendency for $C-H\cdots\pi$ interaction but in a special way. On the basis of our observations, C−H units tend to interact with center of ring's bonds rather than the center of the ring. We named the interactions $C-H\cdots\pi_e$ (e is abbreviation for edge) and C_g (center of gravity), respectively. $C-H\cdots\pi_e$ using C_g is defined for the first time in recent study. The C_n-H_n tend to interact with neighboring C_g of C_n, even after applying the corrected parameters in the CSD search. This interaction acts as a "Lego", meaning electron deficiency for one of them can be compensated with electron withdrawing of another one. In mercuric halide complexes 1,2 and 3 (which included the most stable conformational polymorph of L_1), the $C-H\cdots\pi_e$ remains as a robust interaction and makes the high Z′ (2). Due to the different conformations for the ligands, we have formulated them as $ML'LX_2$ with different interactions in L and L′. In L_2 one of the carbons in pyridine ring was exchanged with nitrogen (pyrazine) and the packing of polymorph I (the thermodynamic crystal) was controlled by an alternative arrangement of the phenol and pyrazine rings. For 4 and 5 chemical formulas can be symbolized by $M(LX)_2$ with Z′ is 0.5 owing to the strong $C-H\cdots N$ in pyrazine ring and similar interactions for ligands in both sides (in lack of a $C-H\cdots\pi_e$ interaction).



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Paper code: 1057

Removal of malathion and diazinon from wastewater by modified iron kaolin and UV / H_2O_2

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During recent years, organophosphates due to widespread usage in agriculture constitute major pollutants of the aquatic environment and soil. Therefore, their elimination by using heterogeneous catalyst is a good manner to overcome these disadvantages. Here, motivated by this case, kaolin modified by Fe-ion exchange. The modified photocatalyst was characterized by XRD, XRF, FESEM, FT-IT and EDX technique. The catalytic activity of this system was investigated in the photodegradation of malathion and diazinon in the presence of H_2O_2 under UV irradiation. The effect of various parameters including catalyst amount, H_2O_2 concentration, pesticide concentration and time reaction on photodegradation yield was investigated. The COD experiment indicated the mineralization of pesticide. Photocatalytic degradation of dye contamination follows a pseudo-first order kinetic.

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Paper code: 1060

Removal of malathion and diazinon from wastewaters by iron-modified bentonite and UV/H_2O_2

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Pesticides are applied widely to protect plants from disease, weeds and insect damage, and usually come into contact with soil and water. Therefore, the elimination of these materials is a good manner in view point of environment [1]. In this work, we modified bentonite with Fe $^{2+}$ for Fenton reaction simulation. The photocatalyst was characterized using FT-IR, XRD, XRF, FESEM and EDX technique. The photocatalytic activity of this system was investigated in the removal of malathion and diazinone in the presence of H_2O_2 under UV irradiation. The effect of various parameter including catalyst amount, H_2O_2 concentration, pesticide concentration and time expose was studied. The COD experiment was performed for determination of degradation amount.

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Paper code: 1070

Synthesis and Characterization of Fe(II), Co(II), Cu(II) and Zn(II) Complexes Containing a New Unsymmetrical Tetradentate Schiff-base

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For decades, Schiff base moieties have been used extensively as ligands which play a key role in the field of coordination chemistry due to their ease of synthesis, stability and applications in various fields. For instance, they have been used as in biological, clinical, catalysis, analytical, and industrial systems [1, 2].

The aim of this research was synthesis of a new unsymmetrical tetradentate Schiff base ligand and its transition metal complexes such as: Fe(II), Co(II), Cu(II), and Zn(II). The ligand, N,N'-bis-(2-acetylpyridine)-3,4-diiminobenzoic acid (acpybza), was synthesized by the reaction of 3,4-diaminobenzoic acid and 2-acetyl pyridine with 1:2 molar ratio. The Schiff base ligand was characterized by elemental analysis, UV-Vis, IR, and ^{1}H NMR spectroscopic data. Then, its complexes were synthesized through the reaction of the ligand with the desired metal ions. The complexes were investigated and characterized by thermal analysis, molar conductance, magnetic susceptibility measurements, IR, and UV-Vis spectral data, as well. The results of our investigations clearly stated to the $[ML](X)_2$ formula for all of the complexes. The results of magnetic properties of the complexes revealed that cobalt complex has a low spin square-planar structure, but the Fe(II) complex form a distorted structure.

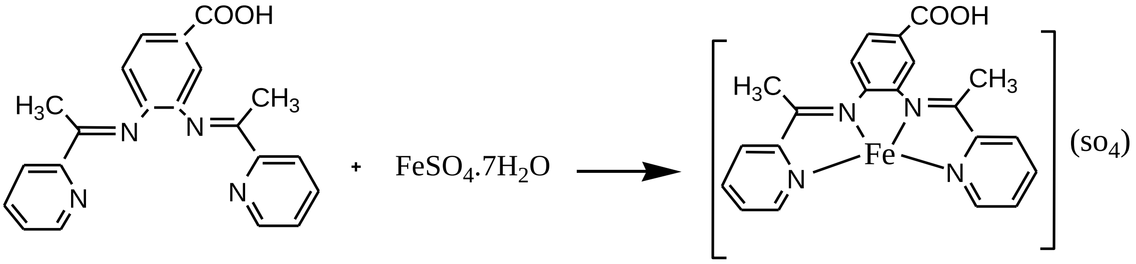

Fig. 1. Synthesis of Co(acpybza) complex.

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Paper code: 1075

Competitive Adsorption of Metal Pollutants on Modified Silica gel

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Today, absorbents have the most important role in chemical refinement of industrial Swages. Silica gels provides an excellent surface for preconcentration of various materials including metals from aqueous systems. Silica gels can be modified chemically using organic precursors producing organically modified silica.

In this work we considered competitive adsorption on modified silica between 6 intermediate and an alkaline metal, to know which one of them will be in lower concentration in primal applied solution.

At first step silica gel was chemically activated then its surface was modified using 3- chloro propyle three methoxy silane, after washing with toluene and letting it to dry, it was reactionized with 2- amino thio phenol to produce the solid product 2- amino thio phenol, attached to Silica chloropropyle (AMPTMS) [1].

We used this adsorbent for comparing absorption of different metals in binary metal aqueous solutions. Appearing new absorption bands in AMPTMS spectrum compared to other materials that we have used shows producing of a new and more complicated absorbant.in figure 2. Absorption band in 521.43cm^{-1} is belonged to C-S stretching, strong bands in 2818.08 cm^{-1} & 2883.82 cm^{-1} are belonged to symmetric and asymmetric stretching's of C-H. Finally, the weak singlet band in 3336.14 cm^{-1} is related to secondary Amines that results in "chlorine in silica chloro propyle is substituted by Amine group in 2-amino thio phenol".

The standard stock solutions of Fe^{3+}, Cd^{2+}, K^+ were prepared by dissolving appropriate amounts of corresponding nitrate salts in deionized water. The pH of metal solutions was about 6 & standard stock solutions of Co^{2+}, Cu^{2+}, Ni^{2+}, Zn^{2+} was prepared by dissolving appropriate amounts of corresponding nitrate salts in tris buffer. The pH of metal solutions was adjusted to a desirable value of 7.4 by this buffer.

For considering absorption of each metal in binary solutions, one was made with a standard concentration that mixed with 0.1 gr absorbent. Then this mixture shaked for 2 hrs, after filtration amount of adsorption on absorbent earned by atomic absorption spectrometer and flame photometer device

Final amounts are shown in below:

Table 1. Average adsorption for each metal in all solutions

	Cadmium	Zinc	Nickel	Iron	Cobalt	Copper	Sodium	**Average adsorption**
Cadmium	-	17.08	36.92	78.13	43.14	15.65	29.03	**36.66**
Zinc	23.98	-	33.5	1.71	26.21	46.2	7.57	**23.20**
Nickel	33.21	6.37	-	7.61	2.73	19.23	25.14	**15.72**
Iron	93.75	83.7	98.12	-	99.5	97.62	99.27	**95.33**
Cobalt	20.94	7.86	6	13.89	-	17.21	32.32	**16.37**
Copper	77.75	86.30	3.43	97.62	6.12	-	77.5	**58.12**
Sodium	31.58	31.58	23.82	9.86	8.31	26.92	-	**22.01**

The sequence below shows different metal ions according to the absorption intensity by the adsorbents.

Iron > Copper > Cadmium > Zinc > Sodium > Cobalt > Nickel

Iron's adsorption is higher than other ions in solutions. This method is suitable for separation of it from aqueous solutions, and relatively is good for separation of Copper ions.

High adsorption for Copper may be resulted from heterogeneous occupying of d orbitals in E_g. therefor Copper is a good acceptor for unpaired electrons on Sulfur in adsorbent.

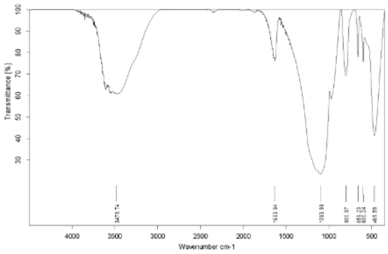

Figure1. IR spectrum of pure Silica

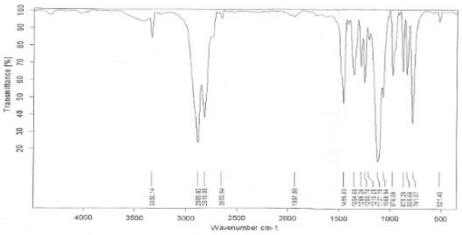

Figure2. AMPTMS

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Paper code: 1077

Graphitic carbon nitride@nickel-aluminium layered double hydroxide nanocomposites

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Through a green protocol, Ni-Al layered double hydroxides (Ni-Al LDHs) with molar ratio of 1:1, 2:1, and 3:1 were prepared in ultrasonic bath at a low temperature using hexamethylenetetramine as template. Effects of the initial reagent concentration, ultrasound illumination power, and reaction time on the shape and size of the nanostructured Ni-Al LDHs were investigated. Under ultrasonic irradiation, the synthesized nanostructures were combined with graphitic carbon nitride (g-C_3N_4) as a new nanocomposite for photocatalytic degradation of Rhodamine B (RhB) dye as a pollutant model. Field emission scanning electron microscopy (FE-SEM), powder XRD, transmission electron microscopy (TEM) and FT-IR spectroscopy were employed to characterize the Graphitic carbon nitride@nickel-aluminium layered double hydroxide nanocomposites (g-C_3N_4@Ni-Al-LDH nanocomposites). g-C_3N_4@Ni-Al-LDH nanocomposites demonstrated a more advanced photocatalytic behavior under visible light, which can be explained by the increased specific surficial area and decreased rate of the electron-hole recombination. The optimal percentage of weight for g-C_3N_4 was 40%. Our synthesized g-C_3N_4/Ni-Al LDH seem to be highly promising for future applications in different commercial fields and industries. Moreover, they are applicable for photodegradation of other organic pollutants.

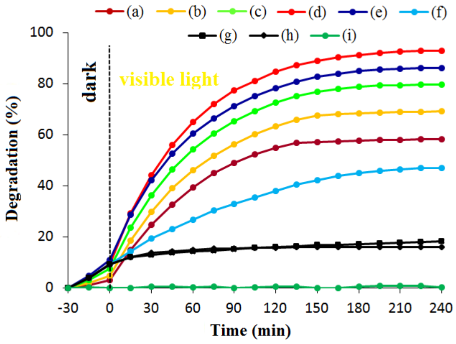

Fig. 1 Photocatalytic activities of g-C_3N_4/Ni-Al LDH nanocomposites.

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Paper code: 1082

Synthesis and Characterization of an Unsymmetrical Tetradentate Schiff Base and Its Co(II), Ni(II), Cu(II) and Zn(II) Complexes

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Schiff base compounds synthesized by condensation reaction between ketones or aldehyde moieties and simple amine groups. The resulted imine is capable to coordinate the transition metal ions. These compounds are known as catalysts, biological active sites, etc. [1-3].

In this research an unsymmetrical tetradentate Schiff base of 1- ((1*E*) -((*E*) -1- ((1*H*-pyrrole -2-yl) methylene amino) naphthalene-8-ylimino) methyl) naphthalene -2-ol (H-pmanmn) ligand and its Co(II), Ni(II), Cu(II) and Zn(II) complexes were synthesized. In these complexes, the Schiff base ligand coordinated via the imine N, amine N and phenolic O atoms. The ligand and complexes were investigated and characterized by FT-IR, UV-Vis, ^{1}H-NMR spectroscopic data, magnetic susceptibility and conductivity measurements, thermal and elemental analysis. The Schiff base structure was confirmed by elimination of carbonyl and appearance of imine peaks in FT-IR spectrum. The results show that Co(II) and Ni(II) have five coordination structure, where Cu(II) and Zn(II) complexes form four coordinate structures. The results of conductivity effects exhibit all the complexes are non-electrolytes.

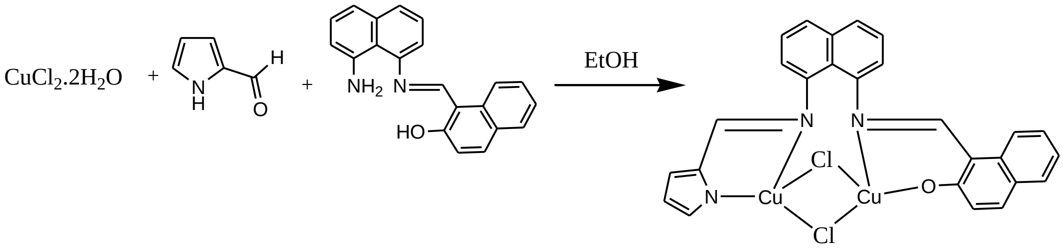

Fig. 1. Synthesis of [Cu_2(pmanmn)Cl_2] complex.

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Paper code: 1110

Mo(VI) Schiff base complex immobilized on graphene oxide nano‐sheets as an efficient, selective and reusable catalyst for epoxidation of olefins

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Heterogenization of homogeneous catalysts onto solid supports has been studied because of the long catalytic lifetime, easy separation, thermal stability, high selectivity, and easy recyclability [1]. For the heterogenization of homogeneous catalysts, which suffer from drawbacks such as deactivation, difficult recovery and difficult recycling, graphene oxide (GO) is a convenient and efficient supporting material [2].In this work Mo(VI) tetradentate Schiff base complex was covalently immobilized onto chemically functionalized graphene oxide (GO) using 3-aminopropyltriethoxysilane as a coupler. The resulting heterogeneous catalysis has been characterized by FTIR, XRD, SEM, DRS, TGA, and inductively coupled plasma-atomic emission spectroscopy (ICPAES). Catalyst was used for the selective epoxidation of alkenes using *tert*-butyl hydroperoxide as oxidant. This catalyst is efficient for oxidation of cyclooctene with a moderate 100% selectivity for epoxidation with 98% conversion in 30 min. The recycling experiment results indicated that the catalyst was highly stable and maintained very high activity, and selectivity even after being used for five cycles.

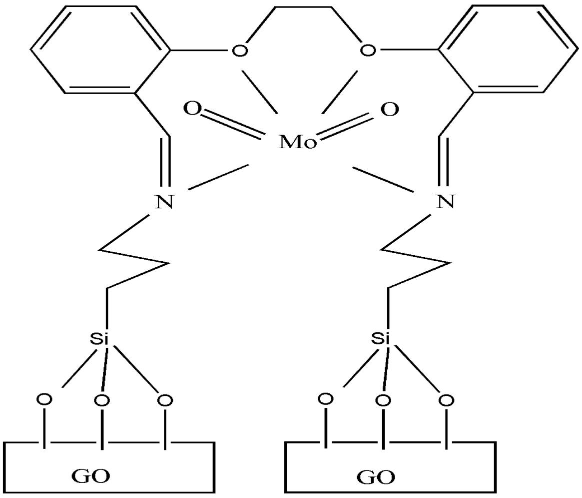

Fig. 1 Structure of Mo(VI) Schiff base complex immobilized on graphene oxide.

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Paper code: 1130

Purposeful molecular design of inorganic-organic hybrid architectures based Keggin-type polyoxometalates: luminescence properties and Monte Carlo simulation studies

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Nowadays, the construction of inorganic-organic networks through crystal engineering has been the subject of much interest. Polyoxometalates (POMs), which are nanosized metal-oxide clusters and unusually effective inorganic ligands, have been widely investigated because of their distinctive topological structures and versatile applications. Due to importance of this field, a novel series of inorganic-organic hybrid materials based Keggin-type POMs and lanthanoids coordination compounds have been successfully synthesized under hydrothermal conditions. In addition, the influences of steric hindrance of organic ligands, in situ transformation of organic ligand, charge density of POM, size of the lanthanoid ions and synthetic conditions on assembly of these POM-based hybrids have been systematically discussed [1-3]. The luminescent properties of some of these hybrids have been investigated. Monte Carlo simulation has been employed for predicting the ability of some of these hybrids to capture CH_4 and CO_2 and also to separate CH_4/H_2 and CO_2/N_2 mixtures.

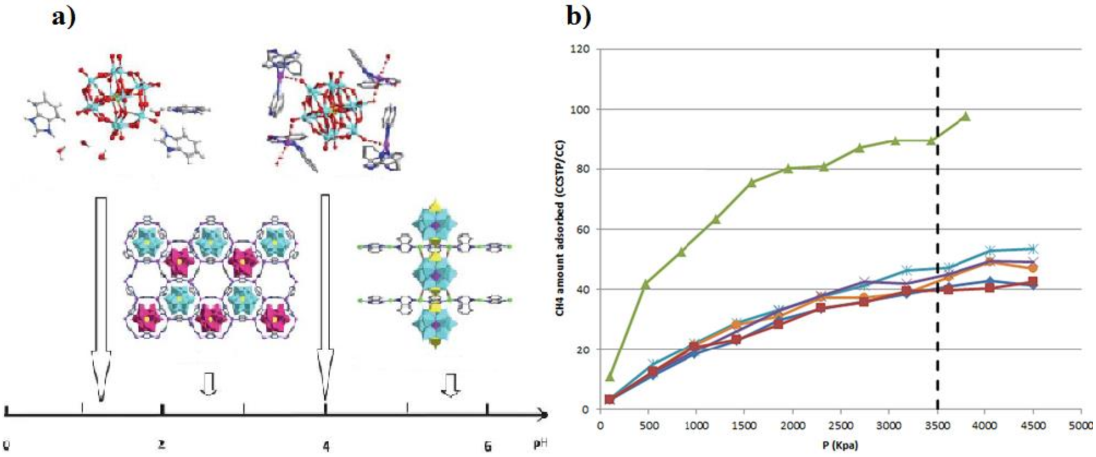

Fig. 1 a) Importance of experimental conditions in synthesis of inorganic–organic hybrid based Keggin-type POMs, b) simulated isotherms of CH_4 at 298K for some of these hybrids.

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Paper code: 1131

Structural and statistical investigation of the coordination behavior of the picolinate-based ligands using the CSD database

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For statistical investigation of the coordination modes of all complexes containing the picolinate unit, a search run on the all CSD database complexes. This study revealed that there are 33 coordination modes for this class of compounds which can be divided up into four groups including: "NO-Chelate Modes", "Two Chelates Modes", "O_2-Chelate Modes" and "Non-Chelate Modes". 92% of all the structures contain a NO-chelate ring and "(N,$O_{alcoholic}$)" mode (Fig. 1) is the most observed coordination mode (56%) in which the picolinate unit acts as NO-donor and forms one chelate ring. Also the "(N,O);O" mode (Fig. 2) is the second most common mode of the CSD analogues (20%). In another comparison, the percentage of bridged and non-bridged structures was calculated. The data revealed that the picolinate unit commonly forms a non-bridged structure (87%). The picolinate unit can bridge 2−5 metal centers. In most cases the carboxylic moiety is deprotonated during the complexation process (94%), however deprotonation of the nitrogen atom in the pyridine ring is very rare (1%).

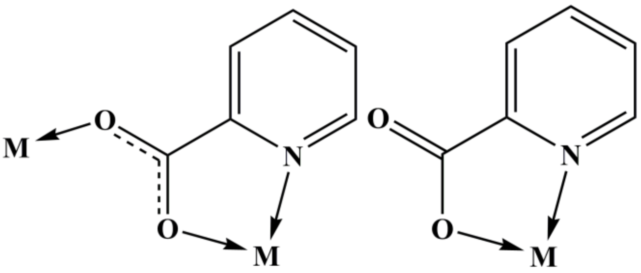

Fig. 1 Common coordination modes of the picolinate-based ligands.

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Paper code: 1183

Two single-enantiomer (R and S) Amidophosphoesters

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The compound $(C_6H_5O)_2P(O)[NHCH(CH_3)(C_6H_5)]$ exists in previously published papers, with together its melting point, elemental analysis and selected mass spectrum peaks, and with no sign of the type of $NHCH(CH_3)(C_6H_5)$ fragment as R, S or racemic. Here, the crystal structures of $(C_6H_5O)_2P(O)[NH(+)CH(CH_3)(C_6H_5)]$ and $(C_6H_5O)_2P(O)[NH(–)CH(CH_3)(C_6H_5)]$ are reported. The compounds are named as diphenyl (R-(+)-α-methylbenzylamido)phosphate, (I), and diphenyl (S-(–)-α-methylbenzylamido)phosphate, (II). In both structures, the chiral one-dimensional hydrogen-bonded architectures, along [010], are built from NH…OP interactions; however, they are mirror images of each other. The assemblies of these compounds include the non-centrosymmetric graph-set motif *C*(4) and the compounds crystallize in the chiral space group $P2_1$. Figure 1 shows the assembly of the structure (II), for a typical example. For each molecule, the two C_6H_5O groups bonded to phosphorus are different in NMR media (monitored by ^{1}H and ^{13}C NMR). For both compounds, the phosphorus signal exactly appears at –0.81 ppm (DMSO-d_6), in a calibrated condition (concentration, temperature).

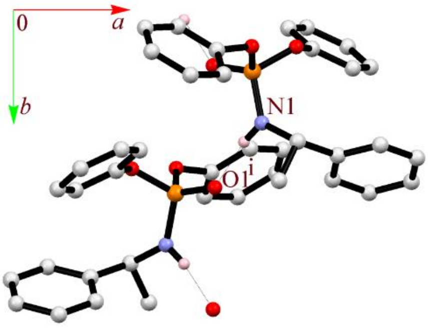

Fig. 1 A partial view of crystal packing of (II) showing the linear hydrogen bond pattern along the *b* axis. The N—H...O hydrogen bonds are shown as dotted lines. The C-bound H atoms have been omitted for clarity.

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Paper code: 1184

Preparation of sodium and potassium doped $LaCoO_3$ perovskite as adsorbent for wastewater treatment

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A perovskite group of materials (ABO3) has a wide range of applications due to their structural diversity, adaptability including exceptional physical and chemical properties. They can accommodate around 90% of metallic elements of the periodic table at positions A and/or B without destroying the matrix structure. These materials have been extensively explored for their magnetic, optical, catalytic and electrical properties. Thermal stability and catalytic properties enable them to serve as promising candidates for the control of environmental pollution. The methods of synthesis greatly influence the catalytic properties of perovskites. They have been exploited as oxidants, reductants and photocatalysts due to their enhanced catalytic properties. In addition to catalytic uses, the role of perovskites has also been explored for sensing and adsorption of various aqueous and gas phase species. Lanthanum cobaltite perovskite ($LaCoO_3$; LC) was prepared by the sol-gel method and then calcined at various temperatures (500°C, 700°C, and 900°C). Subsequently, sodium and potassium species were doped in $LaCoO_3$ structure ($La_{1-x}Na_xCoO_3$; LNC, and $La_{1-x}K_xCoO_3$; LKC). Obtained products were characterized by various analytical techniques; X-ray diffraction, FTIR spectroscopy, SEM, ICP, and Brunauer–Emmett–Teller surface area. All samples were tested as adsorbents for removal of congored from water; the results showed that sodium and potassium doping did not promote the adsorption amount of congored. Obtained results were interpreted by using ZPC analysis data.

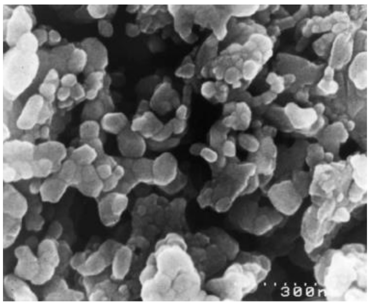

Fig. 1 SEM micrograph of the $LaCoO_3$ perovskite oxide powders at 700 ˚C prepared by the sol-gel method.

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Paper code: 1187

Synthesis of Ni-Al LDH by co-precipitation method and its application in removal of dyes

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The pollution of rivers and lakes by textile dyes has resulted in a series of environmental problems with serious consequences for fauna and flora. Approximately 100,000 kinds of dyes are available worldwide with annual production exceeding 1,000,000 tons. During dye production and the dyeing process, about 15% of all dyes are disposed of in wastewaters, primarily due to incomplete fixation of the dye onto the fabric. Adsorption processes have been extensively studied for the removal of dyes from textile wastewaters [1]. Recently, layered double hydroxides (LDH), also known as hydrotalcites, have been widely used as adsorbent for various applications due to their unique anion exchange capability [2]. LDH can be described by the general formula $[M^{II}_{1-x}M^{III}_{x}(OH)_2]A^{n-}_{x/n}\cdot mH_2O$, abbreviated as, $[M^{II}\text{-}M^{III}\text{-}A]$, where M^{II} and M^{III} are divalent and trivalent metal cations A^{n-} is the intercalated anion with n−electrical charge, and m denotes the number of interlayer water molecules [1]. The LDH structure scheme is displayed in the following figure [3].

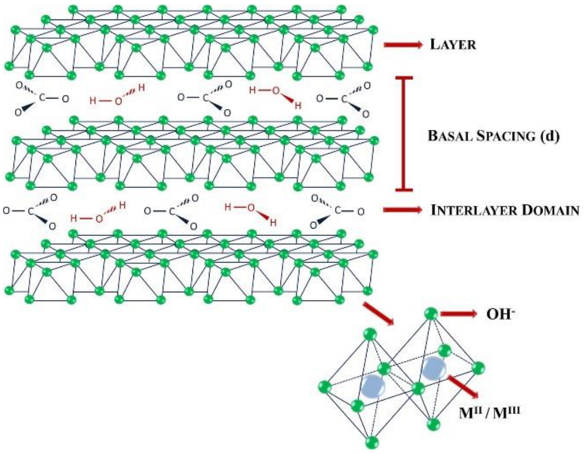

Fig. Structure scheme of Layered Double Hydroxides (LDH).

In this project, Ni-Al LDH was synthesized and the adsorption performance was evaluated by the removal of dye. Ni-Al LDH was successfully prepared by co-precipitation method. For characterization, various techniques including XRD, FTIR and SEM were used. The XRD pattern shows the characteristics peaks of the LDH as literature, FTIR with the corresponding peaks of O–H of H_2O and C–O of carbonate and SEM with the morphology and size of particles.

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Paper code: 1188

Synthesis and identification of a Zr-MOF with carboxylate linker

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Metal–organic frameworks are a new class of advanced porous materials, which have several important characteristics, such as highly periodical, diverse and designable structures, high porosity, unique and modifiable pore surface, as well as framework flexibility [1].

Metal-organic frameworks (MOFs) are a class of porous crystalline materials composed of organic linkers and inorganic nodes. For the past decade, they have been extensively studied because of their extraordinary porosity that makes them suitable for catalysis, gas separation, sensors, biomedical science, and supercapacitors. In particular, robust MOFs with strong coordination covalent bonds, such as those between metal atoms and carboxylates, are of interest. In this context, Zr-based MOFs, such as UiO-668 (nominal composition: $Zr_6O_4(OH)_4(BDC)_6$; BDC = benzene-1,4-dicarboxylate) featured zirconium oxide cluster (Zr_6O_8) secondary building unit (SBU) are known for their high mechanical, chemical, and thermal stabilities [2].

In this research, $ZrCl_4$ and benzene-1,4-dicarboxylate (BDC) as linker were used in various solvents (Dimethylformamide, ethanol, distilled water) by mechanochemical method. The characterization of the obtained MOF was conducted by XRD, FTIR and SEM.

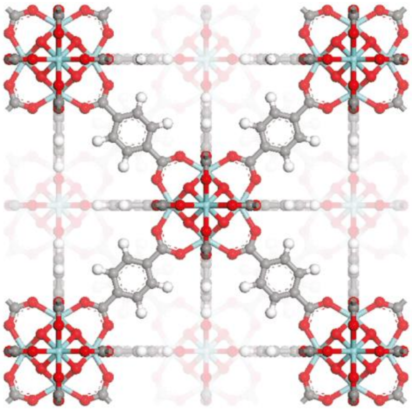

Fig. 1 Depiction of Zr-MOFs with benzene-1,4-dicarboxylate (BDC) linker.

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Multidisciplinary

Paper code: 16

Effects of surfactant, ratio of Cd: surfactant, amount of reductant and time reaction in the sonochemical synthesis of CdSe nanostructures

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A sonochemical method was used for the synthesis of CdSe nanostructures, in the presence of surfactant and reductant. The solution was irradiated with an ultrasonic horn for 30 min under air atmosphere. The resultant precipitate was dispersed in distilled water and ethanol, and then dried under vacuum. Effects of the type of the surfactant, ratio of Cd:surfactant, amount of reductant and time reaction was investigated on the morphology, particle size and properties of the products. XRD pattern, SEM and TEM images and PL spectrum were used for the characterization of the products. XRD results showed that product is CdSe. With increases in the concentration of hydrazine, the crystallinity of the products was increased and with the elongation of reaction time, the crystallinity was decreased. With the exchange of TGA to CTAB, the crystallinity was decreased. In the presence of TGA, agglomerated particles were formed. When CTAB was used, products were nanoparticles with nearly even distribution, average diameter of nanoparticles was about 50 nm. SDBS is not a good surfactant in the current experiment. When SDS was used, the products were in nano-size [1]. PL spectrum of CdSe showed that emission maximum of CdSe is located at 549.5 nm, that a blue shift is observed comparing with bulk CdSe [2].

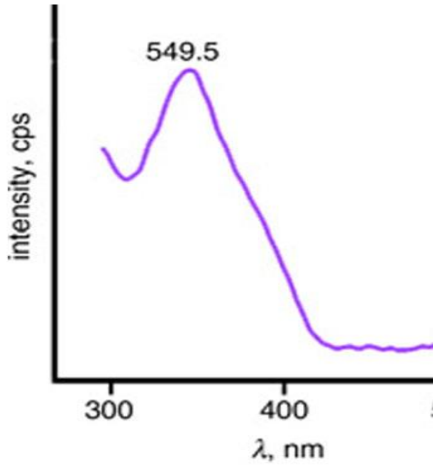

Fig.1 PL spectrum of CdSe nanoparticles.

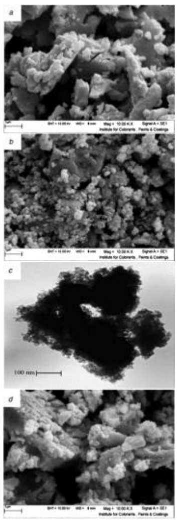

Fig. 2. SEM images of CdSe obtained in the presence of TGA for different times of sonocation.

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Paper code: 17

PbS nanostructures: thermal decomposition synthesis of [bis(thiosemicarbazide)lead(II)] precursor

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$[Pb(TSC)_2]Cl_2$ (TSC = thiosemicarbazide) was used as a single source precursor for the synthesis of PbS nanoparticles. The nanoparticles were synthesized in the presence of oleylamine and triphenylphosphine, as surfactant, at 210 ˚C. During thermal decomposition reaction, nucleation rate for the nanocrystals can reach a high value in a short time and the nuclei are wrapped by surfactant [1]. Consequently, the formed nanocrystals grow to a certain value and saturation. The effect of the surfactant is to control the size of the particles and prevent the aggregation of them. The products were characterized by using XRD. All of the XRD peaks can be indexed to the cubic PbS without obvious characteristic reflection peaks from other impurities, PbS = JCPDS No. 78-1898, with the lattice parameter a = 5.918A˚. The broadening peaks caused by the small size of PbS nanocrystals. The size of PbS nanocrystals calculated from the Scherrer formula is 35 nm. The morphology and structure of the as-prepared PbS nanparticles were investigated by SEM and TEM. Results show formation of the uniform PbS spherical nanoparticles. TEM was in good agreement with the calculated particle size from SEM, 50 nm. Also FT-IR and PL spectra of the products were investigated [2].

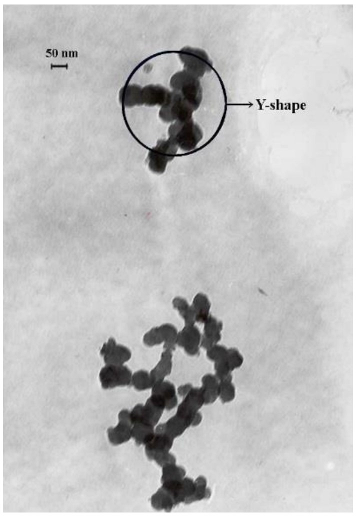

Fig. 1. TEM image of PbS nanoparticles.

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Paper code: 22

Synthesis of a superparamagnetic core-shell nanocomposite of poly(*m*-amino benzenesulfonic acid) and Fe_3O_4 and its high efficiency in solar cell

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This work reports synthesis and characterization of core-shell nanocomposite of poly(*m*-aminobenzenesulfonic acid) and Fe_3O_4 in solid-state condition. The synthesized nanocomposite (NCABS-Fe_3O_4) was characterized and its properties such as thermal, photophysical (solar cell), and magnetic were investigated. This nanocomposite was exhibited good thermal stability. According to vibrating sample magnetometry (VSM), it has high saturation magnetization of 40 emu/g at 8000 Oe and has superparamagnetic properties at room temperature. SEM and TEM images were indicated the same results and core-shell particles with 42-44 nm average size.

Polymer solar cell was prepared by NCABS-Fe_3O_4 on fluorine doped tin oxide (FTO) and aluminum electrodes. The photovoltaic cell characteristics, i.e. open circuit voltage (V_{OC}), short circuit current density (I_{SC}), fill factor (FF) were measured under simulated solar irradiation and power conversion efficiency (PCE or η) was found to be 4.24% for FTO/TiO_2/NCABS-Fe_3O_4/Al structure [1-3].

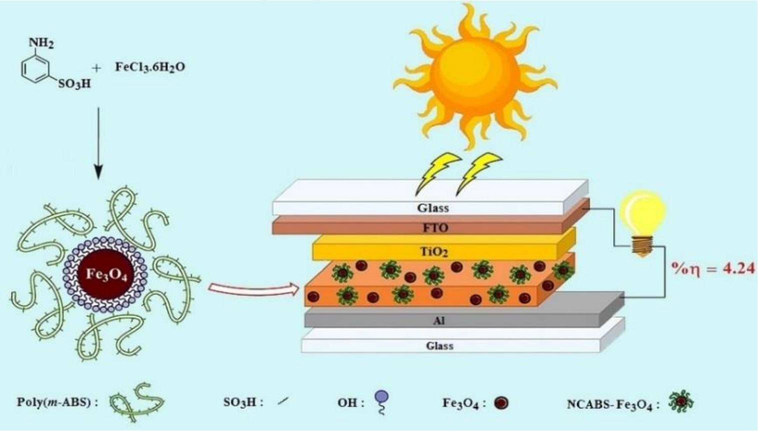

Fig. 1 The Synthesis of NCABS-Fe_3O_4 core-shells and its high efficiency in solar cell.

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Paper code: 23

Synthesis of *p*-Aminoazobenzene nanosheet via green chemistry and Study on its photovoltaic properties by preparation its solar cell

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This work reports synthesis and characterization of poly(*p*-aminoazobenzene) nanosheet in presence of Ammonium persulfate as oxidant for polymerization and in water and room temperature condition (green chemistry). The synthesized polymer was characterized and its properties such as thermal, photophysical (solar cell), morphology and crystallinity were investigated. This polymer was exhibited good thermal stability with 10% weight loss temperatures ($T_{10\%}$) in the 235 °C in O_2 atmosphere. SEM and TEM were indicated the same results and the average size of the shapeless particles was 71 nm and also the two-dimensional nanosheet shapes can be observed in some places, which are well observable with ranging in the sheet size from 150 nm to several micrometers. X-ray diffraction (XRD) measurement was conducted to examine the nature of the polymer and the sharp peak at $2\theta=14^\circ$ with high intensity and the characteristic amorphous peaks centered at $2\theta=29^\circ$ and 44° were observed. According to this pattern, the synthesized polymer is semi-crystalline in nature. polymer solar cell was prepared by poly(*p*-aminoazobenzene) on fluorine doped tin oxide (FTO) and aluminum electrodes. The photovoltaic cell characteristics, i.e. open circuit voltage (V_{OC}), short circuit current density (I_{SC}), fill factor (FF) were measured under simulated solar irradiation and power conversion efficiency (PCE or η) was found to be 1.44% for FTO/ poly(*p*-aminoazobenzene) /Al structure [1,2].

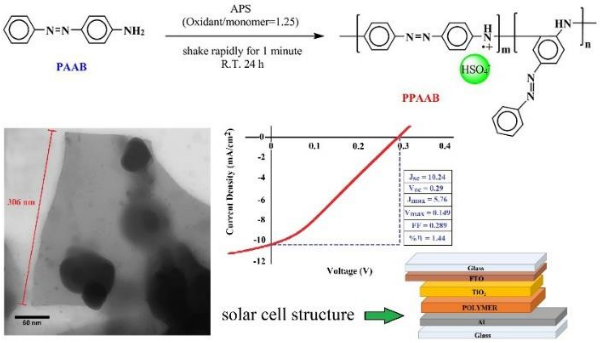

Fig. 1 The Synthesis of poly(m-aminoazobenzene) and investigation of its photovoltaic properties.

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Paper code: 28

Synthesis of 3,4-dihydropyrimidin-2(*1H*)-ones *via* Biginelli reaction using nano($BF_3/Al_2O_3/SiO_2$) as a green catalyst under solvent-free condition

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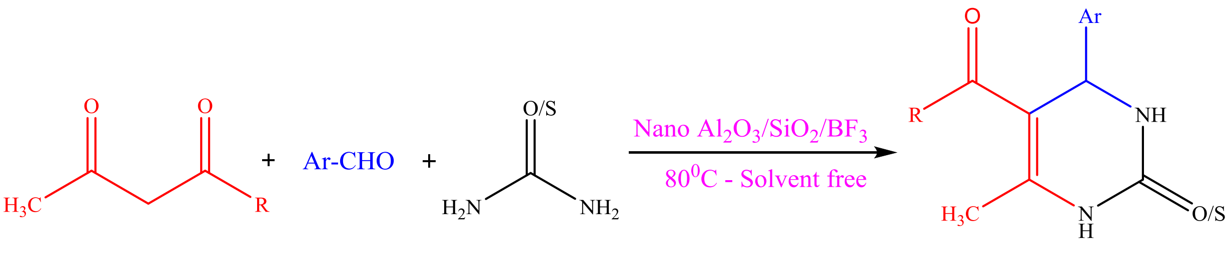
Multi-component reactions (MCRs) such as biginelli reaction are powerful strategies for the one-pot synthesis of organic compounds such as dihydropyrimidinone derivatives (DHPMs). The first biginelli-like reaction was reported by Wang [1]. Biginelli reaction involves the cyclocondensation of an aldehyde, a β-ketoester and urea or thiourea. biginelli products have potential in pharmaceutical applications such as anti-viral, anti-tumor, anti-bacterial, anti-inflammatory, anti-hypertensive and alpha antagonists [2].
Solid acid nano catalysts, which are bridges between homogeneous and heterogeneous catalysts, exhibit higher activity and selectivity than their corresponding bulk materials [3]. Heterogeneous catalysts have been applied in organic reactions in recent years. nano kaolin supported boron trifluoride is a catalyst which is reusable, cheep, readily, available, eco-friendly, versatile and efficient for promotion of many acid catalyzed organic reactions without the use of harmful solvents.
In this study, we report our results for the synthesis of 3,4-dihydropyrimidinones (DHPMs) or their analogous thioketones by a one-pot cyclocondensation of acetoacetates, aryl aldehydes and urea or thiourea using nano kaolin supported boron trifluoride ($BF_3/Al_2O_3/SiO_2$) as catalyst under solvent-free conditions (Scheme1).



1 2 3 4

Scheme1

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Paper code: 31

Removal of Pb(II) From Aqueous Solutions Using New Carboxylic Acid-containing Absorbent Polymer

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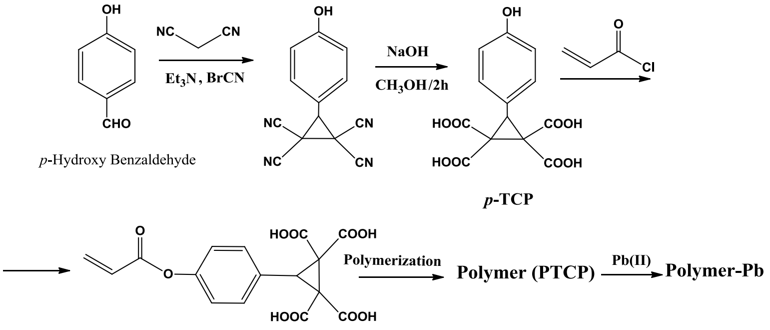
With the development of industry, heavy metal pollution has become a severe environment issue [1]. Hence, there are needed to remove from the environmental and biological samples. The different method used for their removal from aqueous solution. Among related techniques, adsorption is considered to be the most promising process due to its easy handling, high efficiency and selectivity. Therefore, the effort has been made to design and prepare new sorbent functional polymers with excellent sorption performance. In this study, we attempted to prepare new chelating polymer materials containing carboxylic acid ligands, with high sorption capacity in comparison with the similar polymers, which can be used in wastewater treatment [2].3-(4-hydroxy phenyl) cyclopropane-1,1,2,2-tetracarboxylic acid (*p*-TCP) was synthesized by new method and reacted with acryloyl chloride to preparation of *p*-(2,2,3,3-tetracarboxylic acid cyclopropyl) phenylacrylate monomer. Then the resulting monomer was polymerized by free-radical polymerization initiated with benzoyl peroxide to obtain a poly-(2,2,3,3-tetracarboxylic acid cyclopropyl)- phenylacrylate (PTCP) with multi carboxylic acid cyclopropane functionalities in the pendant group as a new polymer [3] and applied to remove Pb(II) from aqueous solution (Scheme 1). The functionalized polymer showed strong adsorption ability to the Pb (II), with the maximum adsorption capacities at pH, 5. The high adsorption rate (<50 min) was seen. The synthesized polymer and its lead chelates were characterized by various techniques.



Scheme.1 Synthesis route of *p*-TCP, PTCP and PTCP-Pb

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Paper code: 32

Chemo-phototherapy of cancer cells using gold nanocage -cored pH-sensitive thiol-ended triblock copolymer

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Light-based therapies including photothermal therapy have been validated clinically for curative and palliative treatment of solid tumors. However, these monotherapies can suffer from incomplete tumor killing [1-2]. According to these facts, gold nanocage-cored biodegradable micelles were prepared by coating gold nanocage (GNC) with synthesized pH -sensitive thiol-ended triblock copolymer [poly (acrylic acid) -b-poly (N,N dimethyl amino ethylmetacrylate) -b-poly (ε-caprolactone)-SH; PAA-b-PDMAEMA-b-PCL-SH]. Furthermore, the anti-cancer drug methotrexate (MTX) was conjugated onto the gold nanocage-cored micelles (GNC@ polymer) by the electrostatic force and the nanocomposites formed were named GNC@ polymer-MTX. The in vitro therapy effect was comprehensively evaluated among free MTX, GNC@polymer, and GNC@ polymer–MTX, with or without near- IR light irradiation to improve curative effect of GNC@ polymer–MTX led by the combination of chemo -photothermal therapy

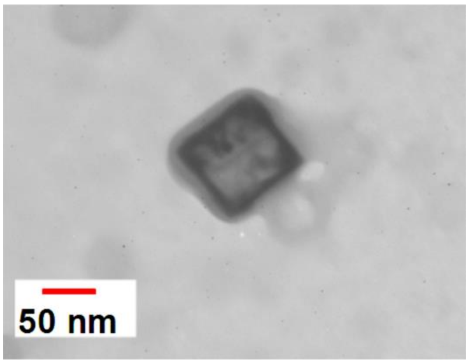

Fig. 1 TEM image of gold nanocage -cored pH-sensitive thiol-ended triblock copolymer

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Paper code: 37

A new approach for silane curing metallocene-based polyethylene-octene copolymers by Monosil and Sioplas processes

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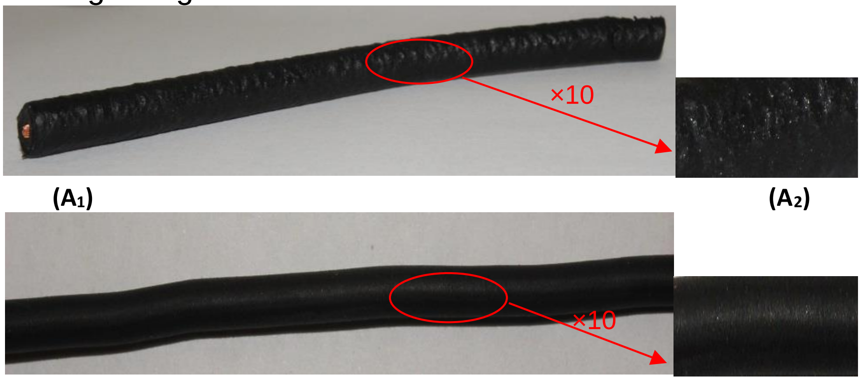
The silane grafted compound need to be storage under approprate conditions in order to be avioded from any premature crosslinking reactions, which is a necessary requirement for re-extruding the silane grafted compounds and producing the final-shaped articles. Therefore, with the aim of selecting an approprate silane grafting process, Monosil or Sioplas, the effect of dibutyltin dilaurate (DBTDL) as catalyst on the melt flow index (MFI) of the silane grafted compounds was invesigated. The results showed an MFI of 6.4±0.1 g/10 min for the silane grafted compound obtained from the Sioplas process, but, the MFI of 1.9 g/10 min which was obtained due to the presence of the catalyst in the Monosil process indicated that this method is not a promising process for silane grafting.



(A_1) (A_2)

(B_1) (B_2)

Figure 1. Effect of pre-crosslinking of silane grafted compound on the product appearance. Monosil process (A_1 and A_2) and Sioplas process (B_1 and B_2). A_1 and B_1 have a resolution of 5184×1114 pixels; A_2 and B_2 have a resolution of 295×181 pixels.

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Paper code: 65

Modification of Natural Clinoptilolite Zeolite with Iron Oxide Magnetic Nanoparticles and Sodium Sulfide Salt for Removal of Heavy Metal Cations such as Lead, Cadmium, and Manganese

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In this study, the efficiency of natural clinoptilolite zeolite modified with iron oxide magnetic nanoparticles and sodium sulfide salt in the removal of three heavy metals including lead (Pb), cadmium (Cd), and manganese (Mn) was investigated. All of the measurements were carried out by atomic absorption spectrometry. The modified zeolite was characterized by FTIR, SEM, and XRD techniques. The effects of various parameters on adsorption process such as initial concentration of metal ion, contact time, adsorbent dosage, and pH have been studied.

According to the obtained results, the removal efficiencies in the optimized conditions for Pb, Cd, and Mn were 98%, 92%, and 75%, respectively. The adsorption studies confirmed the potential recyclability of the modified zeolite. The results of the current study have indicated that the modified clinoptilolite zeolite can be used as an efficient and inexpensive absorbent for the removal of heavy metals in aquatic environments.

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Paper code: 72

Selective and mild oxidation of sulfides to sulfoxides with H_2O_2 catalyzed by copper(II) asymmetrical tetradentate Schiff base complex

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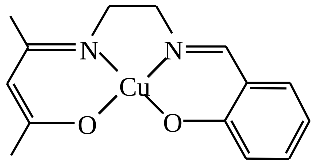
Selective oxidation of sulfides to sulfoxides without any over-oxidation to sulfones is a challenging research interest in synthetic organic chemistry, partly because of the importance of sulfoxides as intermediates in biologically active compounds [1]. Among all methods described so far, the oxidation of sulfides by various metal catalysts is one of the most attractive routes. Schiff base transition metal complexes, due to their easy synthesis and thermal stability, are used as catalysts in various organic reactions such as oxidation, epoxidation and polymerization of alkenes [2]. Recently, much effort has been paid to symmetrical Schiff base ligand due to the bonding of central metal ions with asymmetrical ligand in natural systems [3].

In this work, the copper(II) asymmetrical Schiff base complex (**1**) was synthesized according to published method [3]. The prepared complex **1** was successfully used as a homogeneous catalyst for selective oxidation of sulfides to sulfoxides at room temperature (Fig. 1). Good to high yield of products, use of hydrogen peroxide as a green oxidant and no by-product formation can be mentioned as advantages of this method for oxidation of sulfides.



(**1**)

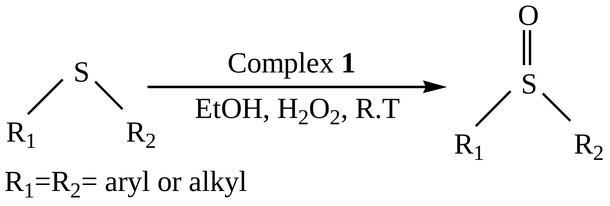


Fig. 1 Selective oxidation of sulfides catalyzed by complex **1**

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Paper code: 85

Highly Efficient Ru(II)-based Electrocatalyst for Reduction of Carbon Dioxide to Carbon Monoxide

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For the past two centuries, fossil fuels such as natural gas, oil, and coal have been essential for the production of energy and commodity chemicals. For example, around 90% of the energy produced worldwide in 2011 was derived from fossil fuels [1]. The serious problem arising from the mass consumption of fossil resources is the increase in the atmospheric CO_2 concentration. In addition, when fossil resources are utilized as chemical resources, most of the synthetic chemicals produced are finally burned and converted into CO_2 after they have fulfilled their purpose. It has recently been sounded that the increase in the atmospheric CO_2 concentration may induce severe global warming [2]. Therefore, the environmental and economic incentives to develop processes for the conversion of CO_2 into fuels and chemicals are enormous. In recent years, many polypyridyl ruthenium complexes have been widely studied for their activity in the electrocatalytic reduction of CO_2 to CO [3,4].

Herein, we report a new electrocatalyst for CO_2 reduction to CO in acetonitrile. The mononuclear ruthenium(II) complex, $[Ru(DMF)_4(PD)](BF_4)_2$, was synthesized and characterized by spectroscopic methods, cyclic voltammetry, and single-crystal X-ray crystallography. Further, the electrocatalytic activity of the Ru(II) complex was investigated for the $2\bar{e}$ reduction of CO_2 to CO in acetonitrile by cyclic voltammetry under different reaction conditions including temperature variation, CO_2 concentration, catalyst concentration, and scan rate.

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Paper code: 86

Zinc(II) Complexes: Synthesis, Characterization, Crystal Structure, and Antifungal Activity

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Metal ions play a main role in controlling the behavior of many biologically important macromolecules. Nevertheless, a metal ion alone is not sufficient to achieve the required range of functions, by changing the metal ion; the biological systems can achieve a wide range of the various functions [1]. Zinc is an essential cofactor in thousands of proteins. As one of the most prevalent transition metal cofactors in biological systems, it plays structural, signaling, and regulatory roles and is found in all six classes of enzymes [2]. Many reports on synthesis, characterization, and application of zinc complexes in various biological fields are found in the literature [3,4]. Furthermore, some zinc complexes have shown the remarkable antimicrobial activities as the antibacterial, antifungal, antioxidant, and anti-inflammatory [5].

Here, we report the synthesis, and structural characterization of some new zinc(II) complexes with N,O-chelating ligands by elemental analysis, spectroscopic techniques and single crystal X-ray structure determination. Moreover, the antifungal and antibacterial activities of these synthesized complexes were investigated against some fungi, and also some Gram-negative and positive bacteria. These complexes showed the efficient antifungal and antibacterial activities. Further, the results exhibited that the complexation of the ligands to zinc center result in the improvement of the antifungal and antibacterial properties in comparison with zinc(II) ion.

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Paper code: 87

Bio-Metal Organic Framework Nanofibers Incorporated to Polyaniline as a High-Performance Room Temperature Carbon Monoxide Gas Sensor

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Carbon monoxide (CO) is an odorless, colorless, tasteless, and hazardous gas which is notorious as invisible silent killer. Therefore, early detection of CO at maximum permissible exposure level is crucial for both environment protection and human health safety [1].

Nanomaterials such as metal nanoparticles and nano-metal oxides have been extensively used to construct gas sensors. Metal-organic frameworks (MOFs) are a class of hybrid materials comprising metal ion-based vertices and organic ligands inkers that serve to connect the vertices into two or three-dimensional periodic structures. The structures and properties of MOFs can be carefully tailored by selection of metal ion and organic linker building blocks. A remarkable property of MOFs is their intrinsic porosity, which renders them potentially useful for gas storage, separations, catalysis, and a variety of additional applications that rely on highly specific host–guest interactions [2]. Recently, Biomolecules have emerged as building blocks for constructing Metal-Biomolecule Frameworks (MBioFs). Biomolecules are structurally diverse and simple biomolecules, including amino acids, nucleobases, sugars, and others, are readily and naturally available. These features besides having different metal-binding sites and exhibiting multiple coordination modes make them excellent ligands to construct diverse structure of MBioFs [2].

In the present work, a room temperature CO gas sensor based on combination of two different nanofibers was fabricated. Polyaniline nanofibers in the presence of an amino acid based copper bio-metal-organic framework nanofibers (Cu-bio-MOF) was used as a novel CO sensing material. The crystalline structure, morphology, and composition of the prepared material were characterized by means of X-ray diffraction, Fourier-transform infrared spectroscopy, energy-dispersive X-ray spectrometer, and scanning electron microscope (SEM). The gas sensing performance of the sensor was investigated toward various concentrations of CO gas ranging from 200 to 6000 ppm at room temperature. The fabricated 2.5% Cu-bio-MOF/polyaniline sensor exhibited high sensitivity, low detection limit, fast response time, and good selectivity. Thus, the proposed 2.5% Cu-bio-MOF/polyaniline sensor is a promising candidate for a CO gas sensing nanodevice.

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Paper code: 101

Synthesis of biodegradable and highly porous conductive hydrogel based on carboxymethyl cellulose and aniline; evaluation of dye removal capability

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Today waste water treatment is an attractive challenge that encourages researchers to introduce new material with good performance. Among the developed materials, sorbent materials have more abundance because of easy synthesis, removal property with high efficiency and effortless recovery. In fact, sorption is one of the most frequently applied methods to remove pesticides, dissolved organic pollutants and other hazardous chemicals from waste water.

Hydrogels are polymer networks possessing the ability to absorb water-based fluids, swelling to form a hydrated network [1]. Moreover, Modifications of hydrogels with conducting polymers (CPs) lead to multifunctional electrically conductive materials that retain the beneficial absorption properties of hydrogels [2].

In recent years, the emphasis of science and technology is shifting more towards environmentally friendly and sustainable resources and processes; in this regard biopolymers are attractive candidates to explore for supported materials [3].

So, in the present work, it has been tried to introduce a biodegradable conductive hydrogel with high porosity by radical polymerization of aniline in the presence of CMC and radical initiator. Batch process in the pollutant removal showed that the novel conductive hydrogel has high tendency for removal of high risk dyes such as methylene blue and rhodamine from aqueous media.

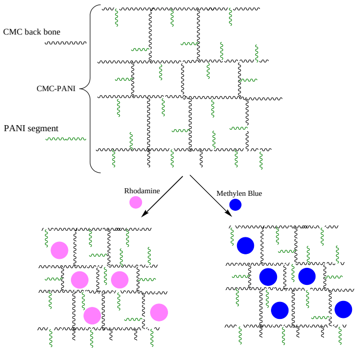

Fig. 1 high porous conductive hydrogel based on carboxymethyl cellulose and aniline

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Paper code: 104

Esterification of levulinic acid to n- Butyl levulinate using mesoporous zirconium phosphate

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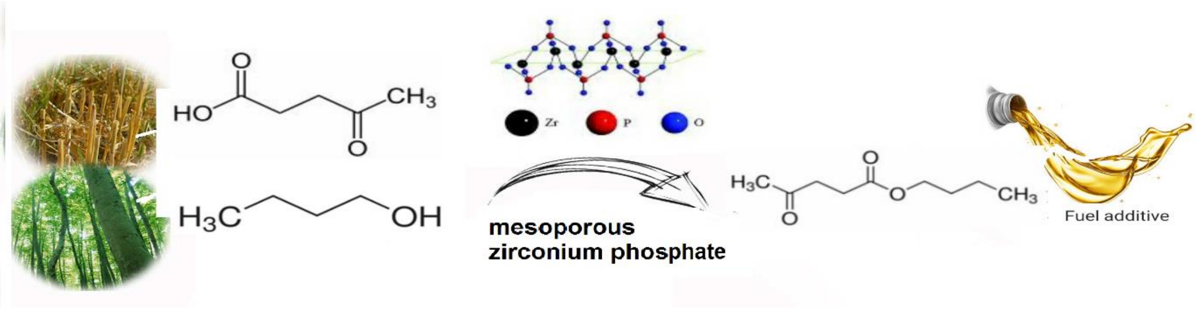
In the recent decades, there has been growing interest in the synthesis of alkyl levulinates. Among these, n-Butyl levulinate obtained by catalytic esterification of levulinic acid and n-Butanol is a versatile biomass-derived that can be used in many applications such as fragrance and fuel additives [1-4]. In this study, mesoporous zirconium phosphate was used as a heterogeneous catalyst for the production of n-Butyl levulinate from levulinic acid. The catalyst was characterized using a couple of techniques such as FT-IR, BET, SEM, TEM and ICP-OES analysis. The effect of various parameters such as reaction time, temperature, amount of catalyst, molar ratio of LA to n-Butanol were investigated. The optimum conditions for the reaction were: temperature 120, reaction time 7 hours, ratio of acid to alcohol 1:9 and 0.01g catalyst (80%).



Scheme 1: Reaction of LA esterification to butyl levulinate

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Paper code: 106

Synthesis, Biological Evaluations and DNA Interaction Studies on Trans Platinum(II) Thiolate Complexes

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The serendipitous discovery of the cytotoxicity of cisplatin and its successful use in cancer therapy since the 1970s have led to an enormous amount of research in this area [1]. One major problem with cisplatin anticancer drug is the development of cell resistance, and thus, there is a continuing need for new and highly active cytotoxic platinum compounds. Some recent work has focused on the development of *trans* platinum complexes, which were initially neglected after it was reported that *trans*-$[PtCl_2(NH_3)_2]$ is not cytotoxic [2].

We have been interested in the preparation and applications of platinum complexes containing thiolate ligands [3]. As an extension of this work, we present here the preparation, characterization, and cytotoxicity studies of *trans* platinum(II) complexes containing allyldiphenylphosphane (PPh_2Allyl) ligand as well as various thiolate ligands (Fig. 1). The cytotoxic activities of complexes have been evaluated against three human cancer cell lines: ovarian carcinoma (SKOV3), lung carcinoma (A549) and breast carcinoma (MCF-7). Also, the induction of cellular apoptosis for complexes were studied on MCF-7 cell line. Our results indicated that complexes could induce apoptosis in cancerous cells in a dose-dependent manner.

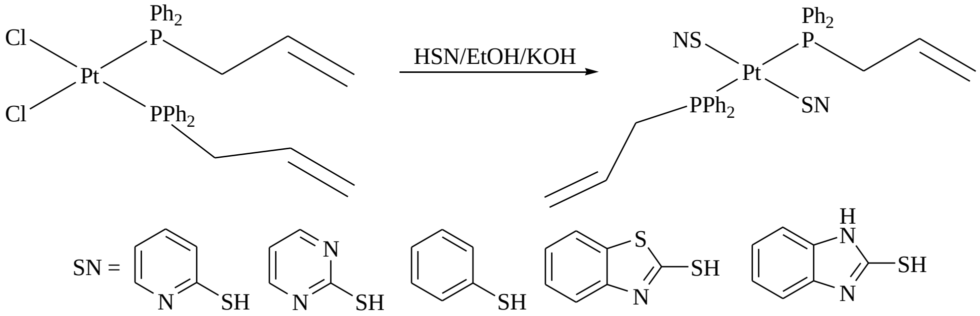

Fig. 1 Synthetic route for the formation of *trans* platinum(II) complexes.

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Paper code: 111

Design, Synthesis and Characterization of Gold(I) Complexes Containing Allyldiphenylphosphine as Improved Cytotoxic Agents

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The chemistry of gold is one of the most remarkable areas in the basic and applied chemistry research. Gold complexes have recently grown increasing attention in the design of new metal-based anticancer drugs in order to overcome the drawbacks of platinum-based chemotherapeutic agents [1]. There have been extensive studies on the therapeutic applications of gold complexes particularly antiproliferative properties against wide range of cancerous cells [2].

Here we present (Fig. 1) the synthesis, characterization and chemotherapeutic properties of allyldiphenylphosphine gold(I) thiolate complexes of [(PPh$_2$Allyl)Au(SR)], **1a**-**d**, SR = deprotonated form of pyridine-2-thiol (HSpy, **1a**), pyrimidine-2 thiol (HSpyN, **1b**), thiophenol (HSPh, **1c**), benzothiazole-2-thiol (HSbt, **1d**) and benzimidazole-2-thiol (HSbi, **1e**). The cytotoxic activities of gold(I) complexes have been evaluated against various cancer cell lines by means of the MTT assay. The results illustrated that **1a** and **1b** had the most considerable cytotoxic activities and showed the highest potency compared to cisplatin. Moreover, **1b** was found to be able to effectively inhibit the proliferation of breast cancer cells by measuring cell death via induction of apoptosis.

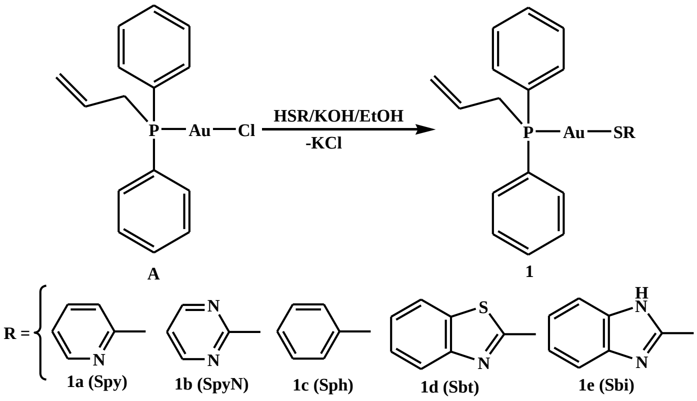

Fig. 1 Synthetic route for the formation of gold(I) complexes.

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Paper code: 124

Synthesis of novel mixed- ligand palladium (II) based on graphene and oxime: its application as a recyclable catalyst

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One of the important fields of organic chemistry is the catalyst design to improve the condition of organic reactions. Palladium (Pd) noble metal is a stable catalyst, which due to its outstanding versatility and high activity, it plays an indispensable role in organic synthesis. Functionalization of the solid supports with show chelating ligands is appearing as a viable method to adjust their catalytic efficiencies and to stabilize the metal complexes [1]. Lately, the applications of graphene oxide (GO) and graphene (rGO) have been widely investigated, by the development of metal-free carbon catalysts and the progress in graphene materials [2]. Functional groups on the GO sheets, according to availability, allow them to react to a wide range of compounds. This property of GO has highlighted it for potential applications in solid support catalysis [3]. In this paper, the palladium (II) mixed-ligand complex synthesized with reduced graphene oxides-containing tetraethoxysilane and menthone oxime and used as an efficient solid catalyst for the Heck-coupling reaction. To maintain stability and catalytic activity in the C-C bond reaction, graphene due to the available surface, as the solid support was considered. The newly synthesized nanocatalyst have beneficial properties including products easy separation, the shorter time to react, purity products (yield 79- 99 %), notably, the catalyst was reused six times without significant degradation in catalytic activity and performance.

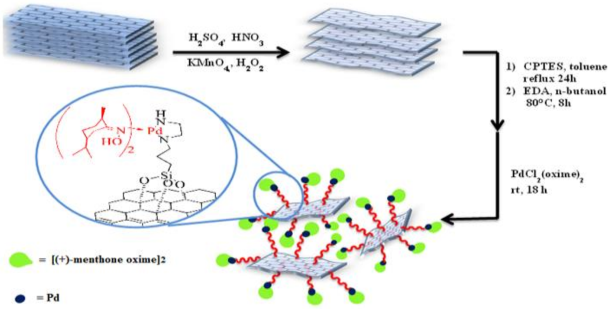

Fig. 1 Schematic illustration to prepare rGO-AATPES-Pd $(oxime)_2$ complex.

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Paper code: 132

Preparation a novel catalytic hydrogel based on biopolymers and graphene oxide containing palladium nanoparticles

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In recent years, for processes that are more environmentally friendly and the design of chemical products, the concepts of “Green Chemistry” have gained great importance. Lately, the development and application of green catalysts have possessed a large number of studies in industrial and academic groups to reduce or eliminate the use of dangerous substances [1]. The past two decades have witnessed a rapid development of hydrogels as the novel materials in both academic and industrial domains. Hydrogels are three-dimensional polymeric networks that are usually cross-linked to render the network insoluble. Also, the structural properties of hydrogels can provide in situ nanoparticle synthesis. So, the hydrogel is suitable for use as a solid support for the preparation and immobilizing of metal nanoparticles. Nowadays, polysaccharides based hydrogels such as Chitin, chitosan, starch, alginate, hyaluronic acid, and cellulose have investigated as promising materials. On the other hand, they can generate three dimensional (3D) porous structure to improve transfer and mass diffusion during catalytic reactions [2]. In this paper, we have been tried to design and synthesis of the hydrogels based on polysaccharides (chitosan NPs and dialdehyde cellulose nanowhiskers) and graphene oxide to creating a suitable solid support for adsorbing and stabilizing Pd NPs. Hydrogel composite Contains Pd NPs prepared as the catalyst was used in the Mizoroki-Heck coupling reaction and investigated its catalytic activity.

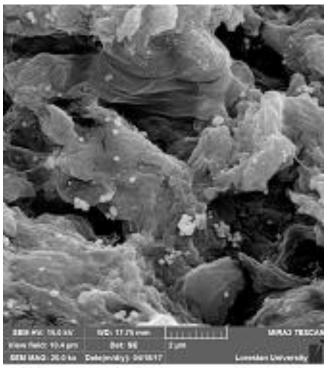

Fig. 1 SEM images t hydrogels@ Pd

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Paper code: 151

Catalytic oxidative desulfurization of model oil by TiO_2 nanotubes prepared by electrochemical anodizing

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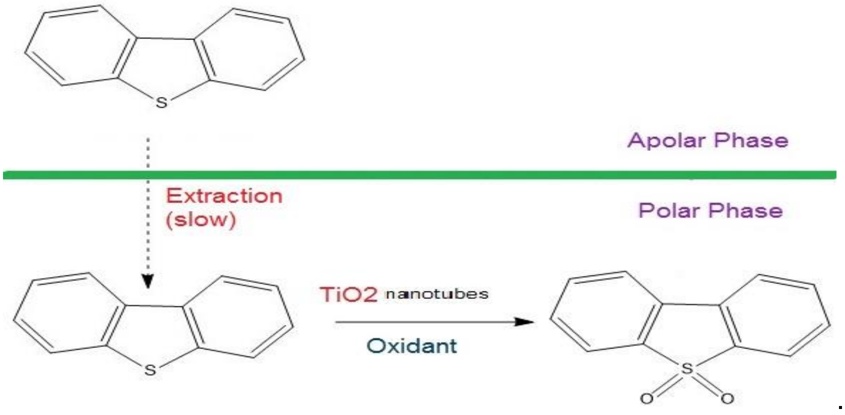
The sulfur compounds in the fuels cause acid rain and emission of SO_X in the air after fuel combustion, which are dangerous for human and environmental health. The oxidative desulfurization (ODS) process is able to deeply desulfurize aromatic sulfur compounds under mild conditions. In the ODS process, at the first stage, sulfur compounds are oxidized to the sulfones products by a proper catalyst and oxidant. Then, the sulfones are extracted from the oil phase by an extractive solvent or solid adsorbent [1-3]. In this research, the catalytic performance of the TiO_2 nanotubes prepared by electrochemical anodizing method used to removal of DBT from a model oil through ODS process. In order to identify the formation of DBT sulfone, GC-MASS analysis was used. The results indicated that the TiO_2 nanotubes exhibited excellent catalytic activity because of its unique structural and electronic properties.



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Paper code: 161

Heterogeneous activation of Oxone® by magnetic nanoparticles anchoring Schiff base complexes for water treatment

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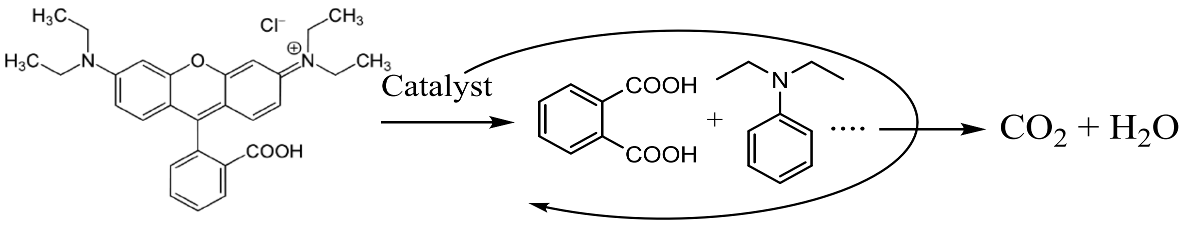
Decolorization of synthetic dyes, as potential environmental pollutants, attracted considerable attention in the past two decades. Schiff base compounds and their complexes are known as good candidates for variety of industrial applications such as pharmaceutical, magnetism and oxidation catalysis of organic compounds. In addition, they have been frequently used for removal of dyes from industrial waste water. But, there are a few studies devoted to the development of a novel approach of using Schiff base complexes as heterogeneous catalysts for degradation of various dyes [1-3].

In this work, a simple Schiff base complex immobilized coordinatively on functionalized magnetic nanoparticles and its structure was confirmed by different techniques. The heterogeneous magnetic catalyst showed an effective catalytic activity toward dyes degradation under oxidation conditions (Scheme 1). The catalyst proved to be recyclable for at least five runs while its structure remained intact. Moreover, magnetism study demonstrated that the catalyst preserved its superparamagnetic property. These benefits for such a heterogeneous system make it amenable to scalability readily, so that the method worked well in a semi scale up of 50 ppm of aqueous solution of dyes. The reactions were carried out in a 50 ml stock water solution of dye. Reaction samples were taken at regular intervals to monitor the absorbance changes of dye using a UV-vis spectrophotometer.



Scheme 1. Oxidative RhB degradation in the presence of magnetic Schiff base catalystcomplex

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Paper code: 162

Non-immobilized water-insoluble Metallosalens as efficient heterogeneous catalyst for degradation of dyes in water

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The heterogenization of homogeneous catalysts is among the main strategies employed to overcome the problems associated with the oxidative degradation of metalloporphyrins and metallosalens. Also, the catalyst may be easily separated from the reaction mixture and reused in the case of heterogeneous catalysts. However, relatively elaborate synthetic and purification procedures are required to immobilize homogeneous catalysts on solid supports. An innovative strategy is the use of non-immobilized water-insoluble coordination complexes in water. The hydrophobic/hydrophilic force drives the reaction under heterogeneous conditions. [1-3]

Industrial dye wastewater from textile and photographic industry is a principal source of environmental contamination. Large amounts of dye were released into the environment accompanied by dissolved inorganic salts, surfactants, dispersing agents, and other organics. Due to the increasing environmental pollution and the establishment of stringent standards for rejecting wastewaters, developed techniques are urgently needed to purify the industrial wastewater [4].

In this study, water-insoluble metallosalen complexes were synthesized and initially applied to activate different oxidants toward degradation of various industrial dyes. The different parameters affecting oxidative activity of hydrophobic catalysts were investigated under heterogeneous conditions.

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Paper code: 167

Highly efficient and fast co-removal of heavy metal ions and oxyanions with zeolite@layered double hydroxides core-shell heterostructure

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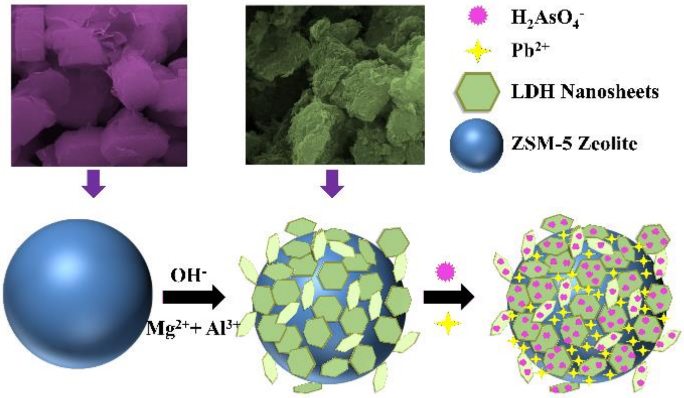
Heavy metal ions and toxic oxyanions contamination in water samples is a serious risk to the public health and other life forms on earth. In recent years, collective efforts have been channeled into removing the heavy metal ions and oxyanions from aqueous samples. Here, we synthesized Core–shell ZSM-5 zeolite@ layered double hydroxides (ZSM-5@LDH) via a simple in situ coprecipitation method. The structures of the sorbent was investigated using X-ray diffraction, scanning electron microscopy, Fourier transform infrared, Brunauer-Emmett-Teller, Barret-Joyner-Halenderm and transmission electron microscope. ZSM-5@LDH was used for the simultaneous removal of heavy metal ions (Pb(II), Zn(II), Cd(II) and Cu(II)) and oxyanions (As(V), Cr(VI), Se(VI)) from aqueous solutions. Three-dimensional ZSM-5@LDH showed promising selectivity for removing Pb(II) and As(V). The equilibrium data fitted the Langmuir sorption isotherm well, and the maximum capacity of Pb(II) and As(V) onto ZSM-5@LDH were 546.25 and 411.41 mg g^{-1}, respectively, which shows an outstanding adsorption capacity comparable to other adsorbents. The pseudo-second-order model describes the adsorption behavior towards the ions of Pb(II) and As(V) well, indicating a chemisorption process. The very high distribution coefficient (K_d) values for Pb (II) and As (V) (4.07×10^4 and 8.0×10^6 mL g^{-1}, respectively), using a V/m ratio of 2000 mL g^{-1}, place the ZSM-5@LDH at the top of materials known for such removal. As a result, this study indicates that the ZSM-5@LDH may be an ideal material for the selective removal of Pb (II) and As (V).



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175

Tandem Knoevenagel-Michael-cyclocondensation reaction of malononitrile, various aldehydes and barbituric acid derivatives using isonicotinic acid

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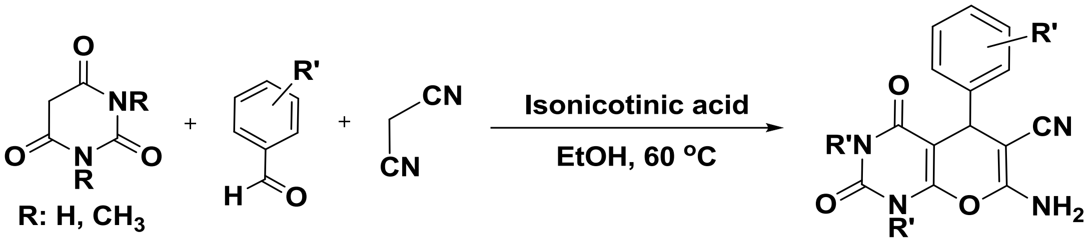
The synthesis of pyrano[2,3-d]pyrimidine dione derivatives is important due to their significant antitumor, antibacterial, antihypertensive, hepatoprotective, cardiotonic, vasodilator, bronchiodilators and antiallergic properties [1]. Also, some of them can be widely used as antimalarial, antifungal, analgesics and herbicidal materials [2,3]. Having this issue in mind, we have synthesized pyrano[2,3-d]pyrimidine dione derivatives by the tandem Knoevenagel-Michael-cyclocondensation reaction of malononitrile, various aldehydes and barbituric acid derivatives in the presence of isonicotinic acid (Scheme 1).



Scheme 1. The preparation of pyrano[2,3-d]pyrimidine dione using isonicotinic acid.

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Paper code: 178

Electrochemical Synthesis and Characterization of AgO Nanoparticles

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Silver (II) oxide (AgO), a strong oxidizing agent, is used in chemical technology and has become increasingly important in batteries [1]. AgO particles can be synthesized in two chemical and electrochemical methods. The AgO particles synthesized by the electrochemical method have a higher chemical stability compared to chemical methods, and are considered in the battery field because of their high capacity as an active cathode [2]. Until now, AgO nanoparticles were synthesized only by chemical methods and using surfactants [3]. In this research, The AgO nanoparticles were synthesized by a simple and efficient electrochemical method. This procedure was performed in a two electrode cell using aqueous sodium nitrate electrolyte, silver sacrificial anode, silver cathode, at a constant current mode and current density equal to 2.5 mA per cm^2 under room temperature. The particles were identified and characterized by fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron micrograph (SEM). The FT-IR spectrum of AgO dried powder shows a sharp peak at the frequency of 530 cm^{-1} that certifies formation of AgO particles. In the XRD pattern, four major peaks of [200], [002], [111] and [202] at 2θ positions equal to 32.4, 32.2, 34.2, 37.4 and 39.8, respectively, confirm the formation of AgO particles. The SEM micrograph (Fig. 1) shows that shape of the synthesized AgO particles is quasi-spherical. In terms of particle size, all the particles have an average particle size below 100 nm. Consequently, using this method can be synthesized AgO nanoparticles. Also, the results indicated that the shape and size of AgO nanoparticles could be controlled by varying current density and electrolyte.

Fig 1. The SEM micrograph of the electrochemical synthesized AgO nanoparticles

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Paper code: 181

Two-dimensional functionalized graphene oxide anchored TPA: $H_3PW_{12}O_{40}$ and their application for reduction of organic dyes

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This research focuses on noncovalent functionalization of two-dimensional graphene oxide. 2D geraphene oxide with controllable surface coverage and evenly distributed components on the surface is desirable for developing new supports for catalysts [1-2]. For preparation of 2D- geraphene oxide, polyvinylpyrrolidone (PVP) was used to effectively solved incompatibility and aggregation problems between GO and inorganic media and played an important role in the two-dimensional combination of GO [3]. In the following, the surface of 2D-GO functionalized with (3-Chloropropyl)triethoxysilane and *N*,*N*-dimethylbiguanide (Metformin) respectively. Finally, phosphotungstic acid immobilized on Metformin-grafted 2D-GO as acid/base bifunctional catalyst. The catalytic behavior of the prepared catalyst was investigated for the reduction of 4-nitrophenol, methylene blue and methyl orange in the presence of $NaBH_4$ as a reducing reagent at room temperature in aqueous media. The reaction was monitored easily by measuring the change in UV–Vis absorbance. The catalyst exhibited high catalytic performance without significantly reduction activity even after running ten cycles.

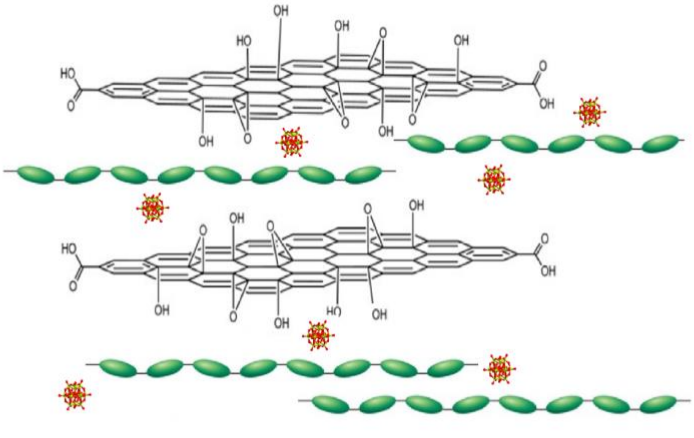

Fig. 1 Two-dimensional functionalized graphene oxide anchored TPA

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Paper code: 182

Preparation of Palladium nanoparticles from [Pd(aemptrz)Cl_2] by sonochemical method

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The 1,2,4-triazoles present antifungal and antibacterial activities and are being widely used as agricultural chemicals and as an important class of compounds for the synthesis of many pharmaceutical drugs [1].

The preparation and characterization of nanosized materials is an important issue in basic science research as well as in industrial applications, as they have their own characteristic electronic, optical, and catalytic properties greatly different from the bulk materials.
Palladium oxide-plays a central role in many industrial applications and In comparison with other materials, palladium oxide thin and ultrathin films have some advantages at gas sensor fabrication [2]. In this study, nano-structure of [Pd (aemptrz) Cl_2] (1) was prepared by a sonochemical method. The new nano-structure was characterised by scanning electron microscopy, X-ray powder diffraction, IR spectroscopy and elemental analyses. PdO nanoparticles were obtained by calcination of compound 1 at 600° C under air atmosphere and were characterised by X-ray diffraction (XRD), TG-DTA, FT-IR and scanning electron microscopy (SEM).

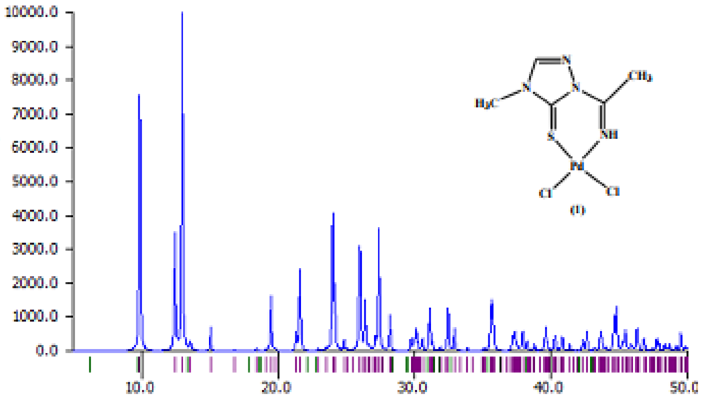

Fig. 1 XRD Pattern of [Pd(aemptrz)Cl2]

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Paper code: 189

Theoretical study on adsorption of methane molecule on nanostructured functionalized graphene with hydroxyl and epoxide

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In the present work, density functional theory was employed to analyze the effect of functional groups on the adsorption behavior of CH_4 in nanostructured functionalized graphene (G). Methane which is abundant in earth is found to be an energy carrier [1] and high use of it would result in the reduction of greenhouse gas emission. It is well known that graphene and derivatized forms of graphene offer applications as gas sensors [2].

Two oxygen-containing functional groups such as hydroxyl(OH) and epoxy(O) are applied to modify the graphene surface to clarify the role of a functional group of graphene on the gas adsorption strength. Wood et al demonstrated binding of CO2 and CH4 to model zigzag graphene nanoribbons edge-functionalized with COOH, OH, NH2,H2PO3,NO2, and CH3, while we investigated adsorption of methane molecule on hydroxyl and epoxide on the basal plane of graphene. The interaction mechanism of CH_4 with G(OH) and G(O) was demonstrated by using DFT calculation at the special level of B3LYP/6-31G*. The optimized structures of CH_4 on G(OH) and G(O) were shown in Figure 1. The adsorption energies (E_{ads}) for CH_4 on G-OH and G-O are -3.85 and -3.55 kJ/mol, respectively. Based on the calculated adsorption energy, it can be concluded that the interaction between the gas molecule and the functionalized graphene is weak. Furthermore, values of E_{ads} does not considerably change upon functional groups, indicating the type of functional group has not a significant effect on interaction of the Methane and nanostructures.

Also, the quantum molecular descriptors are reproduced with the DFT scheme for the gas molecule, the functionalized graphenes and studied complexes. The chemical potential (μ) can be calculated as follows:

$\mu=(E_{LUMO}+E_{HOMO})/2$

As can be seen, the chemical potential values of nanomaterial before and after adsorption of the gas molecule are negative; hence, all considered structures are stable [μ G(OH) = -0.199 ev, μ G(O) = -0.140 ev, μCH_4/ G(OH)= -0.199 ev, μ and μCH_4/ G(O)= -0.140 ev]. Moreover, the values of HOMO–LUMO energy gap are G(OH) =0.064 ev Eg G(O) =0.114 ev, CH_4/ G(OH)= 0.064 ev and CH_4/ G(O)= 0.114 ev respectively, indicating that the adsorption of CH4 has no significant effect on the electronic properties of the functionalized graphene.

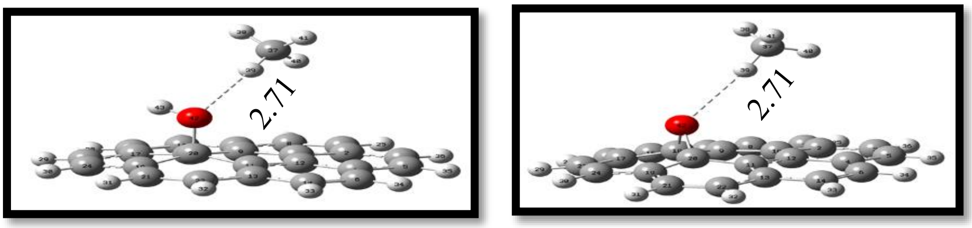

Fig 1. Optimized geometries of CH4 with G(OH) and G(O)

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Paper code: 195

Synthesis and Characterization of Nanozirconia via Interaction of Zirconium (IV) with Oxamid under Solvothermal Conditions

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Over the past two decades, various methods have been developed for the production of nanoparticles, which can be produced use of a variety of sol-gel, micro-plasma and hydrothermal methods with or without ultrasound [1]. Hydrothermal synthesis can be defined as a method of formation and growth of particles by chemical reactions and solubility changes of substances in a sealed heated aqueous solution above ambient conditions [2]. In this study, zirconia nanoparticles were synthesized from the zirconium(IV) oxynitrate in the presence of oxamide under hydrothermal condition and subsequent calcination of product. The product was characterized by TG-DTA, FT-IR, XRD and SEM analysis. Badylete was detected as the only phase of ZrO_2 after hydrotreacting at 200°C and is not changed after calcination at 600°C. A gel, however, is formed under hydrotreating at 100°C. A xerogel is formed upon drying of the gel, converting to a cubic nano-zirconia upon calcining at 600°C. Crystallite size was calculated to be about 15-20 nm for the both phase (Sherrer formula). Particle size is observed to be about 20 nm in the SEM image. Results show that the hydrotreating temperature is a critical parameter of the formation of the crystalline phase.

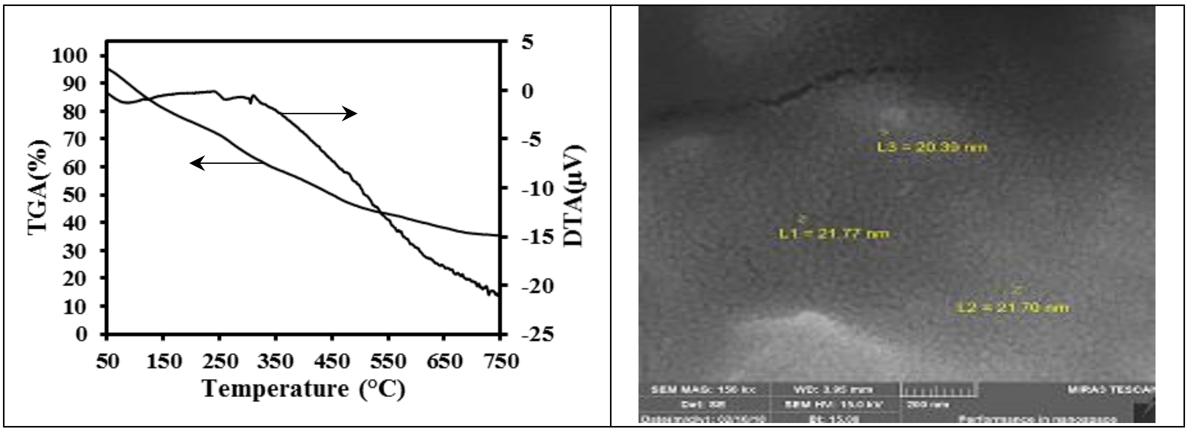

Fig. 1: TG-DTA and SEM pattern of xerogel and calcined xerogel (at 600°C).

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Paper code: 202

Structural Features of B-site Substituted Nano-Lanthanum Manganite

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In this study, $LaMn_{(1-x)}Fe_xO_3$ nanoparticles with $x = 0, 0.5$, and 1 were synthesized via citrate method [1]. Samples were studied by thermal gravimetric/ differential (TG/DTA) analysis, infrared spectroscopy, X-ray powder diffraction (XRD) and SEM characterizations. The structural characterization using commercial Xpert package and Fullprof program are witness for a structural phase transition in manganese replacement with iron. The structural analysis shows a rhombohedral toward cubic phase transition upon replacing of Mn by Fe in the form of $LaMn_{(1-x)}Fe_xO_3$. The influence of Fe substitution on the crystal structure can be described by a tolerance factor $[t=r_a+r_O/\sqrt{2}(r_B+r_O)]$ for estimation of deviation from the ideal structure. As a result, in Fe-substituted sample, t increases and rhombohedral structure transforms toward cubic structure, having higher symmetry [2]. Compared to the manganese, a more affinity is observed for the lanthanum toward iron for the cubic perovskite phase formation of $LaBO_3$ (B: Mn or Fe) [3].

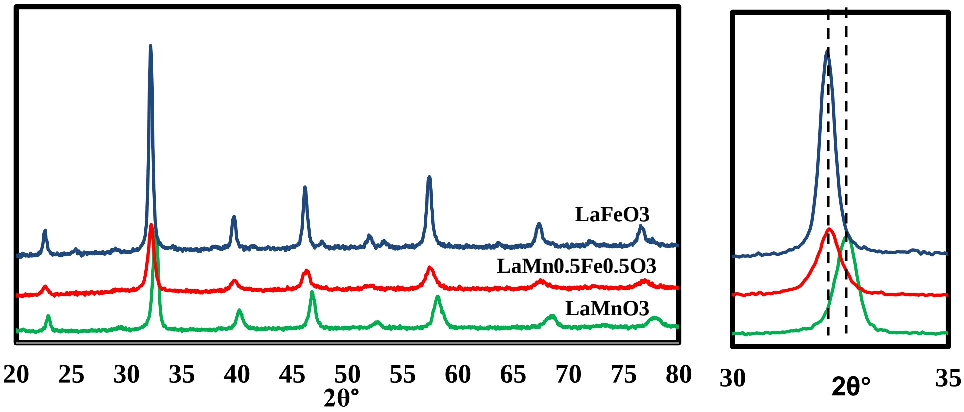

Fig. 1 XRD patterns of prepared samples.

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Paper code: 204

Deep Eutectic Solvent Copper salt as a green catalyst for the acetylation of various alcohols, phenols and amines

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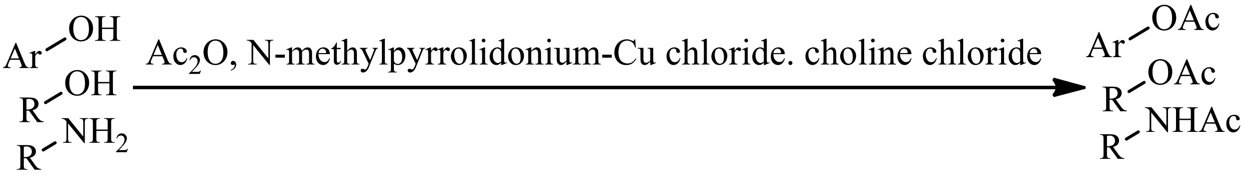
N-methylpyrrolidonium-Cu chloride based deep eutectic solvent (NMPCuClDES) was synthesized. This DES was characterized by XRD, FT-IR and NMR techniques for their surface area, surface acidity, crystallinity and functionality. The catalytic activity of DES was determined in acetylation of various alcohols, phenols and amines with acetic anhydride. The reaction conditions were optimized by varying the parameters such as molar ratio of the reactants, reaction temperature and amount of the DES. The DES catalyst can also be reused for acetylation at least for five reaction cycles without any appreciable loss of catalytic activity. The acetylation of alcohols, phenols and amines is one of the most important reactions. This reaction used for transformations in organic synthesis, especially in the synthesis of natural compounds and biological activity compounds [1]. The protection of such functional groups are often necessary during the course of various transformations in a synthetic sequence, particularly in the construction of polyfunctional molecules such as nucleosides, carbohydrates, steroids and natural products [2]. These reactions were carried out using acetylating agent and inorganic acids catalysts such as chloride acid or $AlCl_3$, BF_3. An important disadvantage of most existing methodologies is the use of high acidic, high temperatures, stoichiometric amount of catalyst, long reaction times and low yields. Therefore, introduction of new methods and catalysts for the preparation of esters is still in demand. The present method has the additional advantages of mild conditions, high yield, easy separation and environmentally friendly catalysts.



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Paper code: 219

A highly stable and very active heterogeneous Pd nanocatalyst in the O-arylation of phenol or C-O cross couplings

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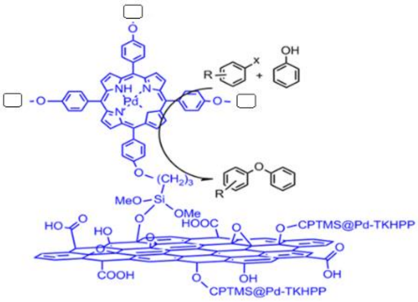
An efficacious and reusable heterogeneous Pd Porphyrin nanocatalyst with high potentials in catalysis was prepared and characterized. The Pd Porphyrin nanocatalyst exposed excellent exertions and reusabilities in aqueous phase processes including the O-arylation of phenol or C-O cross coupling. The superior utility of Pd Porphyrin nanocatalyst in catalysis was elucidated by the broad scope of the reactants, mild reaction condition and the excellent yields (95-98%) of the reaction products. This Pd Porphyrin nanocatalyst was characterized by energy dispersive X-ray spectroscopy (EDX), X-ray diffraction spectroscopy (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier-transform infrared spectroscopy (FTIR), and ICP analysis. All of these manners confirm the nanocatalyst was built.[1]



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Paper code: 224

Nano-BF_3/cellulose as a biodegradable catalyst for the synthesis of highly functionalized tetrahydropyridines

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Tetrahydropyridines (THPs) have been the subject of considerable synthetic efforts because of their potent pharmacological properties including antimalarial [1], and anticancer [2].

Nowadays, chemists prefer to use natural catalysts that can be decomposed in the environment. Cellulose as a biopolymer and biodegradable material can be used as support in preparation of different catalysts. In this work, cotton was chosen as a cheap and readily available source for synthesizing of nano-cellulose [3].

Nano-BF_3/cellulose is a solid acid and biodegradable catalyst that was prepared via reaction of nano-cellulose and BF_3. The structure of this catalyst was studied by FT-IR, FESEM, TEM, XRD, EDS, TGA, XRF and BET techniques.

In this research, the synthesis of highly functionalized tetrahydropyridines has developed via a five component reaction of aldehyde, amine and ethyl acetoacetate using nano-BF_3/cellulose under solvent-free conditions (figure 1). The structures of obtained products were identified by FT-IR, ^{1}H-NMR and ^{13}C-NMR. Some advantages of this protocol are high to good yields, environmentally benign, easy work-up and moderate reusability of the catalyst.

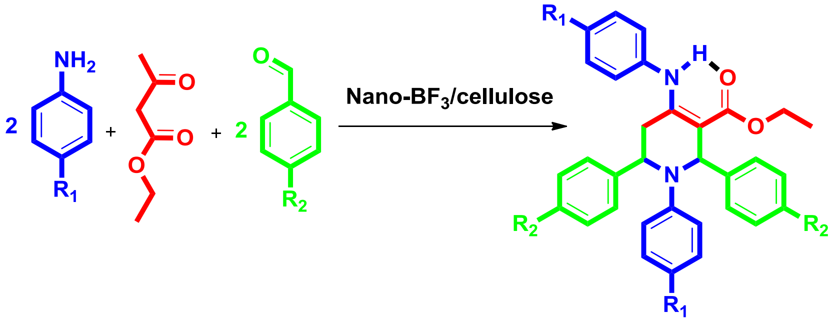

Fig. 1 Synthesis of tetrahydropyridine derivatives in the presence of nano-BF_3/cellulose

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Paper code: 226

Synthesis of highly substituted dihydro-2-oxopyrroles using Fe_3O_4@nano-cellulose-OPO_3H as a novel bio-based magnetic nanocatalyst

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Economically importance and environmentally benign features of magnetic nanoparticles (MNPs) have put them under chemical spotlight [1]. Cellulose, as a renewable and naturally abundant biopolymer, is one of the most ideal coating layers for Fe_3O_4 NPs because it not only stabilizes the nanoparticles in solution but also enjoys free OH groups for functionalization purposes [2].

2-Oxodihydropyrroles as an important class of heterocycle compounds have wide biological activities such as herbicidal, antitumor, antibiotic, antimalarial and anti-HIV [3]. In this study, Fe_3O_4@nano-cellulose-OPO_3H (Fe_3O_4@NCs-PA) was synthesized as a new magnetic bio-based nanocatalyst and characterized by FT-IR, FESEM, XRD, TGA, VSM, EDX, XRF and BET. This catalyst was successfully applied to the synthesis of 2-oxo dihydropyrrole derivatives *via* the four-component reaction of dialkylacetylenedicarboxylate, aldehyde, and amines.

The present procedure is a green and environmental friendly approach that offers many advantages including high yield, easy work-up, simple recovery and reusability of the catalyst.

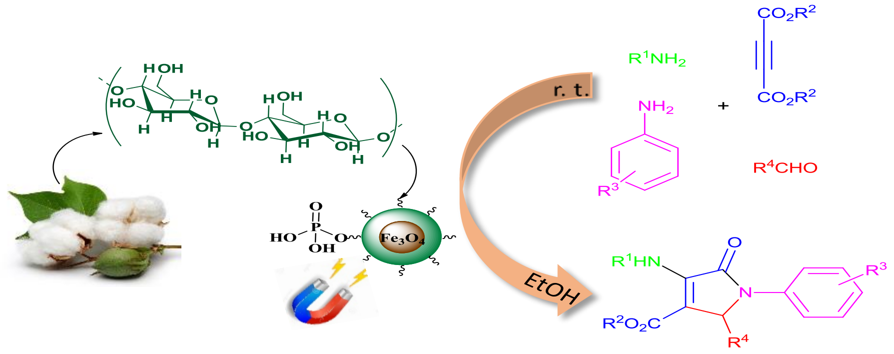

Fig. 1 Synthesis of 2-oxo dihydropyrrole derivatives in the presence of Fe_3O_4@NCs-PA.

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Paper code: 227

Application of $Fe_3O_4@SiO_2/TiCl_3$ NPs for the synthesis of quinoxaline derivatives

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Quinoxaline derivatives are an important class of nitrogen-containing heterocyclic compounds that have received abundant attention owing to their significant role in pharmaceutical industry [1].

Nowadays, magnetic nanoparticles (MNPs) have been preferred as the catalyst support [2] because of their advantages such as small size, great surface areas and activity. These nanoparticles can be easily separated from the reaction medium by an external magnet without using extra chemicals [3].

In the present study, $Fe_3O_4@SiO_2/TiCl_3$ NPs was prepared and the structure of this catalyst was studied by FT-IR, FESEM, TEM, XRD, XRF, EDX, TGA, BET and VSM techniques.

$Fe_3O_4@SiO_2/TiCl_3$ NPs was used for the synthesis of quinoxaline derivatives through condensation of 1,2-diamines and 1,2-dicarbonyl compounds at room temperature under solvent-free conditions. The structures of obtained products were identified by FT-IR, ^{1}H-NMR and ^{13}C-NMR.

We can point out simple and mild experimental procedure, short reaction time and high yields of the products as the advantages of this method.

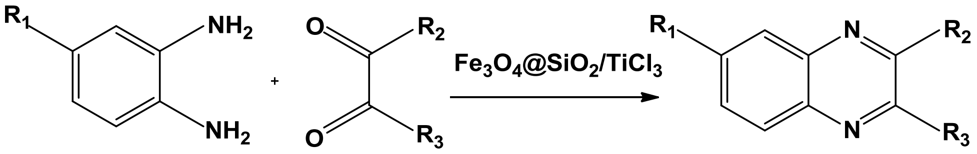

Fig. 1 Synthesis of quinoxaline derivatives in the presence $Fe_3O_4@SiO_2/TiCl_3$ NPs.

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Paper code: 228

Green Synthesis of Pyrano[2,3-*c*]pyrazoles and Spiro[indoline-3,4´-pyrano[2,3-*c*]pyrazoles] Using Nano-silica Supported 1,4-Diazabicyclo[2.2.2]octane as a Novel Catalyst

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Pyrano[2,3-*c*]pyrazoles have attracted considerable interest in organic synthesis because of their wide application in medicinal and pharmaceutical chemistry [1]. In addition, spirooxindoles are unique core structures found in pharmaceuticals [2] and natural products such as Spirotryprostatin (A & B), Pteropodine, Marcfortine B and Glesemine [3].

In this research, nano-silica supported 1,4-diazabicyclo[2.2.2]octane (nano-SiO_2/DABCO) as a novel heterogeneous catalyst was prepared and fully characterized by FT-IR, FESEM, TEM, EDX, TGA/DTA, XRD, BET and elemental (CHN) analysis. This basic nanocatalyst was successfully applied for synthesis of pyrano[2,3-*c*]pyrazole and spiro-2-oxindole derivatives *via* a one-pot four-component reaction at ambient temperature.

Simplicity, easy work-up, high to excellent yields, short reaction times, ease of recovery of the catalyst and green nature of this protocol make it appealing.

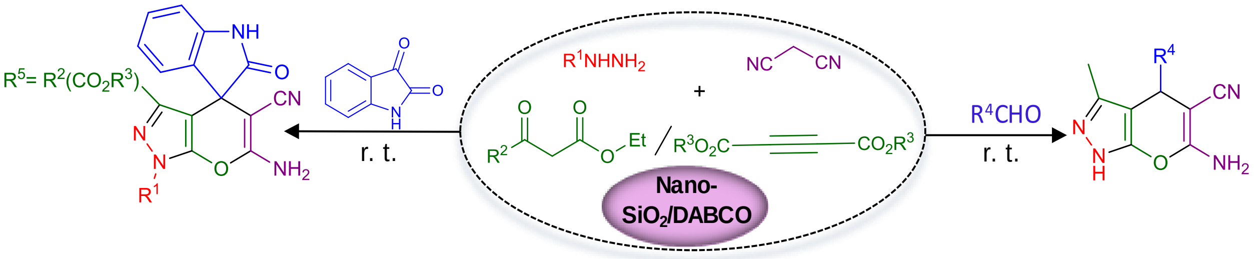

Fig. 1 Synthesis of pyrano[2,3-*c*] pyrazole and spiro[indoline-3,4´-pyrano[2,3-*c*]pyrazoles] derivatives using nano-SiO_2/DABCO.

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Paper code: 273

$RuCl_2$(p-cymene)$]_2$ complex immobilized on reduced graphene oxide for the synthesis of carboxylic acids from alcohol dehydrogenation

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For developing high performance of graphene-based nanocatalysts, dispersibility of graphene sheets in matrices and interfacial interaction are challenging due to the strong tendency of agglomeration and surface inertia of graphene. Here we report an efficient way to functionalize graphene nanosheets with 1,4-Diaminobenzene on their surfaces, to attain the functionalized graphene by diazonium treatment following reduction of graphene oxide with hydrazine hydrate. In the following amine-grafted reduced geraphene oxide reacted with 2,4,6-trichloro-1,3,5-triazine and sodium ethanediamine respectively. Finally ruthenium complex $RuCl_2$(p-cymene)$]_2$ immobilized on modified reduced geraphene oxide. Prepared catalyst applied for the synthesis of carboxylic acids from alcohol dehydrogenation for this purpose, catalytic assays were performed in a round bottom flask, using 1 equivalent of alcohol, 1equivalent of cesium carbonate, catalyst and 10 mL of solvent for 24 hours at 100 °C. Yields and conversions were determined by GC analysis.

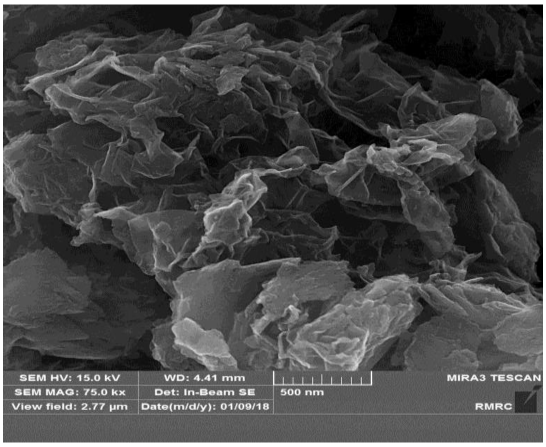

Fig. 1 SEM image of $RuCl_2$(p-cymene)$]_2$ complex immobilized on reduced graphene oxide

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Paper code: 250

Synthesis of perimidines in the presence of Fe_3O_4@nano-cellulose/BF_3 as a super paramagnetic nanocatalyst

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Nanocelluloseas as light weigh, nontoxic, accessible and low price material [1] is generally produced from partial hydrolysis of cotton. Magnetic nanocelluloseis prepared from reaction of nanocellulose with $FeCl_3$ and $FeCl_2$ in a simple reported procedure. Fe_3O_4@nano-cellulose/BF_3 as a new super paramagnetic nano catalyst is prepared from supporting of BF_3 on magnetic nano cellulose. The structure of nano catalyst was suggested by FT-IR, VSM, XRD, XRF, EX, FESEM, TEM and TGA techniques. This nano catalyst is removed from reaction medium by an external magnet.

Perimidines constitute an important class of natural and non-natural products. They have attracted great attention in synthetic organic chemistry for several reasons, including biological activities, pharmacological applications such as analgesic, antitumour, antiviral, antipyretic, antiparkinsonian, antirheumatic, antifungal, and optoelectronic properties [2, 3] .

In this investigation, perimidines were synthesized in excellent yield by condensation of aldehydes and 1,8-diaminonaphthalenein the presence of Fe_3O_4@nano-cellulose/BF_3. The FT-IR, ^{1}HNMR and ^{13}CNMR spectra confirmed the structure of compounds.

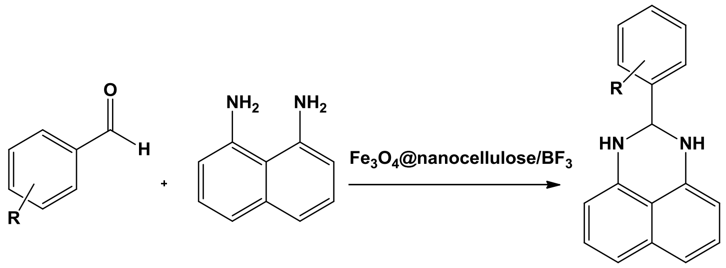

Fig. 1 The synthesis of perimidines in presence of Fe_3O_4@nano-cellulose/BF_3

This approach offers many advantages such as good yields, short reaction time, easy workup, inexpensive and efficient catalyst.

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Paper code: 254

Preparation and application of kaolin-based magnetic nanocatalyst for the synthesis of 4*H*-pyrimido[2-1-*b*] benzothiazole derivatives

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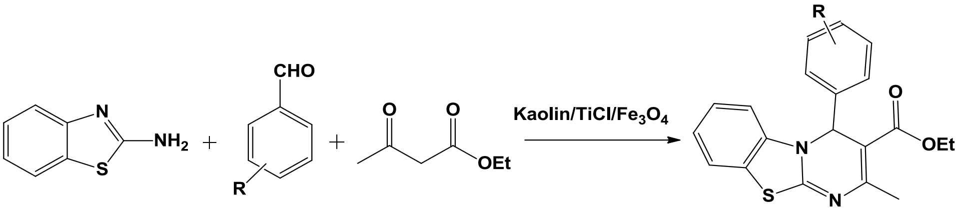
4*H*-Pyrimido[2,1-*b*]benzothiazole derivatives are an important category of fused heterocycles due to their wide range of potential biological activities such as anti-tumor, anti-allergic,anti-inflammatory, anticonvulsant,and antimicrobial activity [1, 2].

Kaolin is a rock rich in kaolinite clay, which is very cheap and abundant and has diverse uses in the industry. Kaolinite is a clay mineral, part of the group of industrial minerals, with the chemical composition $Al_2Si_2O_5(OH)_4$. It is a layered silicate mineral, with one tetrahedral sheet of silica (SiO_4) linked through oxygen atoms to one octahedral sheet of alumina (AlO_6) octahedral [3].

In this investigation, Kaolin/$TiCl_4$/Fe_3O_4 was synthesized and characterized by FT-IR, XRD, TGA, FESEM and EDS techniques. 4*H*-Pyrimido[2,1-*b*]benzothiazolewasprepared *via* three-component reaction of 2-amino-benzothiazole, aldehyde, and β-ketoester in the presence of Kaolin/$TiCl_4$/Fe_3O_4. The structure of products were confirmed by FT-IR, ^1H NMR and ^{13}C N MR spectra.



Reusability, eco-friendly and thermalstability are some advantages of this no expensive efficient catalysts. Short reaction times, high yields, simplicity of operation and easy work upare some ofadvantages of this method.

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Paper code: 257

One pot synthesis of five substituted tetrahydropyridines using nano-$Al_2O_3/BF_3/Fe_3O_4$ as a highly efficient nano-catalyst

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The five-substituted tetrahydropyridines and their derivatives have an interesting class of pharma actives [1] such as anticancer [2], antibacterial [3] and anti-hypertensive [4] activities. Because of these potent pharmaceutical properties of the tetrahydropyridines chemistry, a faster, milder and more ecofriendly methods accompanied with higher yields is needed [5].

Although the homogeneous catalysts are efficient but separation of them are so difficult. An important advantage of heterogeneous catalysts is that they can be easily separated and reused from the reaction. For this reason, one pot multicomponent reactions of aromatic aldehydes, anilines and β-keto-esters under solvent free conditions were studied in the presence of nano-$Al_2O_3/BF_3/Fe_3O_4$ catalyst. This nano-magnetic catalyst is easily isolated at the end of the reaction by using an external magnet without any filtration.(Fig1)

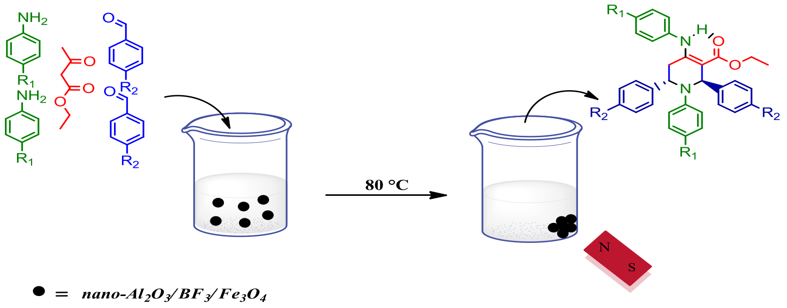

Fig. 1 Synthesis of THPs catalyzed by nano-$Al_2O_3/BF_3/Fe_3O_4$

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Paper code: 266

Synthesis of two Cd(II) based metal–organic frameworks : sonochemical synthesis aspect and applications

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Synthesis of nanoscale MOFs has also been attractive [1]. Ultrasound irradiation is one of the simplest and most effective methods for preparation of nano or microstructures MOFs [2]. In this simple, fast and green method molecules undergo a chemical reaction because of powerful ultrasound radiation (20 KHz–10 KHz).

Nano plates of two Cd(II)-based metal–organic frameworks, $[Cd_2(oba)_2(4\text{-}bpdb)_2]_n.(DMF)_x$(TMU-8) and $[Cd(oba)(4,4'\text{-}bipy)]_n.(DMF)_y$ (TMU-9) were synthesized via sonochemical reaction by using various time and concentrations of initial reagents and power of irradiation and characterized by scanning electron microscopy, X-ray powder diffraction and IR spectroscopy. Moreover, the effect of triethylamine on speed of nucleation during the synthesis was investigated. Thermolysis of these MOFs at 550 ˚C under air atmosphere yields CdO nanoparticles.

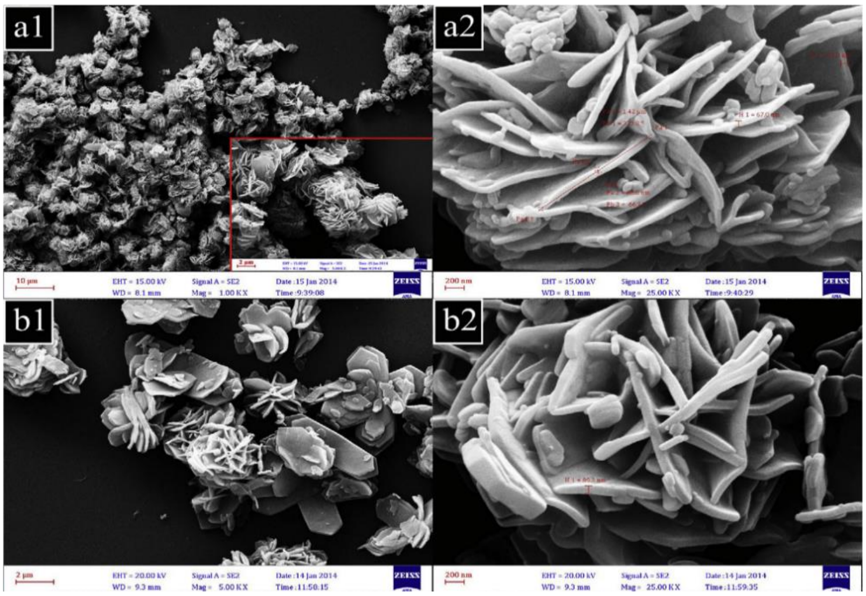

Fig. 1 FE-SEM images of nano-plates of TMU-8 synthesized by sonochemical reaction with concentration of [0.025] M of reagents and sonication time of (a) 30 min, (b)60 min

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Paper code: 269

Synthesis and characterization of DCC supported on magnetic nanoparticles: a highly active and recyclable catalyst for the synthesis of polyhydroquinolines

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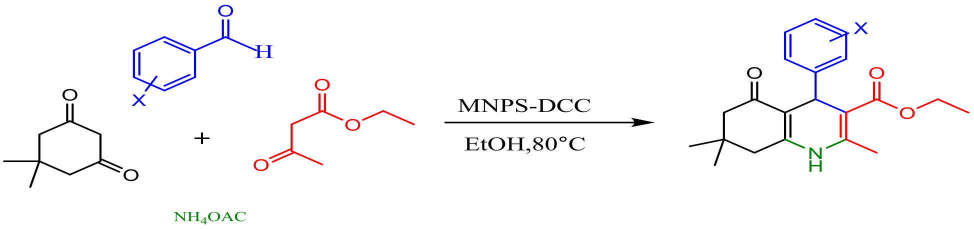
Magnetic nanoparticles are efficient, readily available, high-surface-area resulting in high catalyst loading capacity and outstanding stability heterogeneous supports or catalysts. Among the various magnetic nanoparticles used as the core magnetic support, Fe_3O_4 nanoparticles are arguably the most extensively studied because of their simple synthesis, low coast, and relatively large magnetic susceptibility [1].

Heterocyclic compounds, especially nitrogen-containing heterocycles, have attracted profound attention in modern chemistry science because they play a key role in the fields of natural products, medicinal chemistry and materials chemistry. In recent times, a lot of attention has been focused on the synthesis of polyhydroquinoline derivatives, because they are well-known as Ca^{2+} channel blockers, and have emerged as an important class of drugs for the treatment of cardiovascular diseases [2]. In continuation of our studies on magnetic nanocatalysts, herein, we investigated the synthesis of polyhydroquinolines in the presence of MNPS-DCC as a recyclable and green magnetic nanocatalyst under EtOH solvent at 80°C (scheme1).



Scheme1

This method offers several advantages including high yield, short reaction time, simple work up procedure, ease of separation, and recyclability of the magnetic nanocatalyst without significant loss of their catalyst efficiency.

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Paper code: 274

Synthesis of glucose optical biosensor nanocomposite based on tragacanth gum biopolymer

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A hydrogel based on tragacanth gum (TG) biopolymer consisting of synthetic crosslinker has been employed as a biosensing platform via encapsulation of enzyme bioreceptors (e.g., glucose oxidase) and fluorescent reporters (e.g., CdS quantum dot) [1,2]. Enzyme and quantum dot (QD) were physically immobilized within the hydrogel matrix. By using atomic force microscopy and scanning transmission electron microscopy, a three-dimensional network that physically hybridized with QDs and encapsulated enzyme bioreceptors with a minimal leakage has been observed. The prepared hydrogel has been used successfully to the detection of analyte such as glucose by using a photoluminescence quenching of the hybridized QDs.

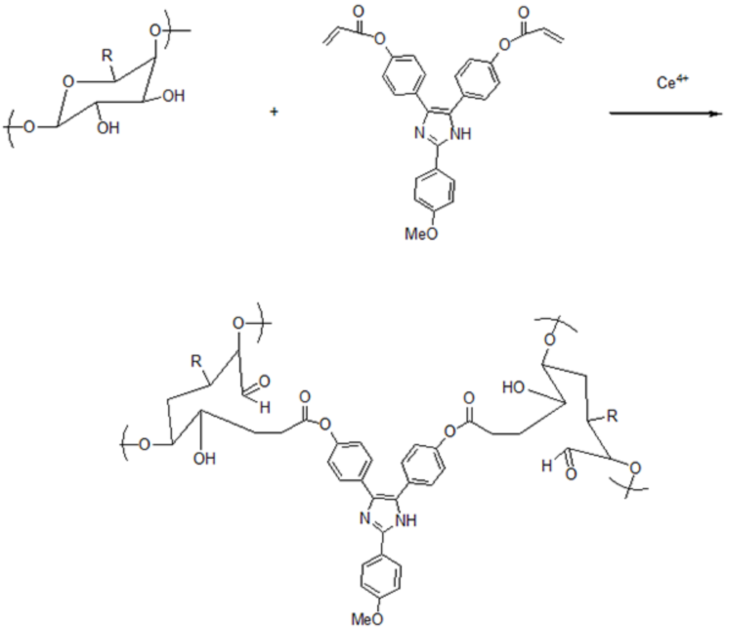

Fig. 1 Preparation of hydrogel.

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Paper code: 278

Green synthesis and antibacterial activity of rosemary (*Rosmarinus officinalis*) assisted superparamagnetic iron oxide nanoparticles

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Magnetic nanoparticles exhibit many interesting properties that can be exploited in a variety of applications such as biomedicine. In this study, superparamagnetic iron oxide nanoparticles (SPIONs) were prepared using a rapid and green method by reduction of ferric chloride solution with *Rosmarinus officinalis* water extract as the reducing and stabilizing agent. Further the antibacterial effect of iron oxide nanoparticles was evaluated against four pathogenic bacteria. Rosemary plant (*Rosmarinus officinalis*) were collected from Ferdowsi University of Mashhad Farm, washed thoroughly with distilled water, and dried overnight in 40 °C. The extract was prepared by mixing 20 g of the rosemary fine powder with 100 mL distilled water and heated at 60 °C for 30 min[1]. The crude extract was filtered with filter Whatman 42 for future use. SPIONs were prepared by mixing 25 mL of $FeCl_3.6H_2O$ solution (50 mM) with 50 mL of rosemary extract at 80 °C for 1 h under constant stirring at 1800 rpm. Changing color of solution from yellow to dark brown was an indication for NPs biosynthesis. The biosynthesized SPIONs were purified and further characterized by UV-vis spectrophotometry, X-ray Diffraction (XRD) analysis, Fourier Transform Infrared Spectroscopy (FTIR) and vibrating sample magnetometer (VSM). Antibacterial properties were evaluated against *Escherichia coli, Pseudomonas aeruginosa*, *Bacillus subtilis* and *Staphylococcus aureus* by standard broth microdilution method [2]. The results showed that the SPIONs had a cubic structure with the crystallite size of about 17.51 nm, and the maximum absorbance at 270 nm. The FTIR spectra of prepared iron oxide NPs under different conditions exhibited peak at 570 cm^{-1} assigned to Fe-O stretching vibration mode. Also, the prepared iron oxide NPs had superparamagnetic property with saturation magnetization of 39.64 emu g^{-1}. The results showed that prepared nanoparticles have moderate antibacterial activity against both Gram positive and Gram negative pathogenic bacterial strains.

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Paper code: 287

Synthesis of novel Pd nanoparticle on Fe_3O_4@ZrO2/5-amino-1,3,4-thiadiazole-2-thiol and its application for reduction Organic Dyes

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Among these heterogeneous catalysts, magnetic nanoparticles (MNPs) have attracted much attention due to their unusual magnetic, physical, surface chemical and catalytic properties [1]. Because of interesting structural features and high levels of catalytic activity associated with these materials, their applications have extended to almost all possible fields of science ranging from medicine to rocketry and organic synthesis [2,3]. However, the specific surface area and thermal stability of pure ZrO_2 is low and it shows weak catalytic activity in a number of chemical transformations. To increase the catalytic performance of zirconia-based catalysts, several procedures have been used by introducing various metals oxides, where upon zirconia acts as a support for the preparation of the solid catalysts. In this article, A novel Nano catalyst was synthesized by covalent immobilization of 5-amino-1,3,4-thiadiazole-2-thiol on the Fe_3O_4/ZrO_2 core shell surface. In the following palladium ions grafted to hydrophilic organic fragment of modified Fe_3O_4@ZrO_2 and reduced to Pd nanoparticles by NaBH4 as a reduce reagent. The synthesized Pd nanoparticles can be employed as a magnetically recycled catalyst for the reduction of 4-nitrophenol, methylene blue and methyl orange in the presence of NaBH4 as a reducing reagent. The synthesized catalyst exhibited high catalytic activity. Moreover, synthesized catalyst could be readily recycled and reused several times without significant loss of activity.

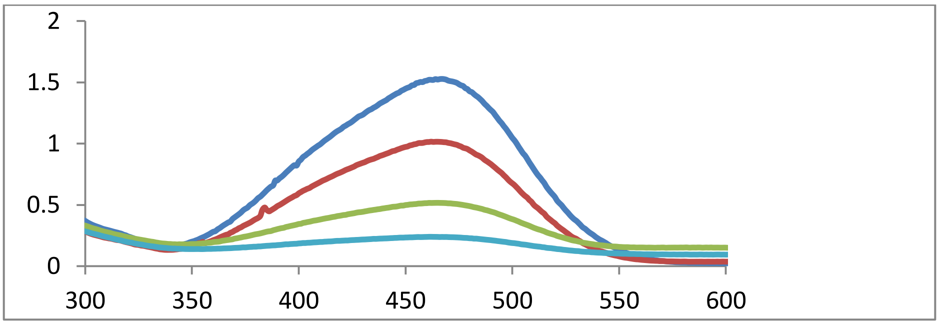

Fig. 1 UV/VIS absorbance of methylene blue.

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Paper code: 294

Synthesis of hydrogel beads based on tragacanth gum and graphene oxide through radical polymerization: study of Ca^{+2} and Mg^{+2} removal from drinking water

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Water is an essential resource for the survival of all living organisms.in this research ,we try to remove heavy metal ion from drinking water.In this study , the structure of the tragacanth gum (GT) as a natural polymer has been modified through polymerization of 2-acrylamide-2-methylpropane sulfonic acid (AMPS) and then its nanocomposite has been prepared with graphene oxide nano sheet (GO).

In the preparation of hydrogel, glutar aldehyde (GA) has been used as crosslinker in different weight ratio with the monomer. The prepared of hydrogel beads were used for adsorption of metal ion such as calcium and magnesium ions in drinking water.

The effect of experimental condition such as pH, time ,amount of adsorbent, and concentration of metal ion on the adsorption capacity were investigated and the best bead determined.

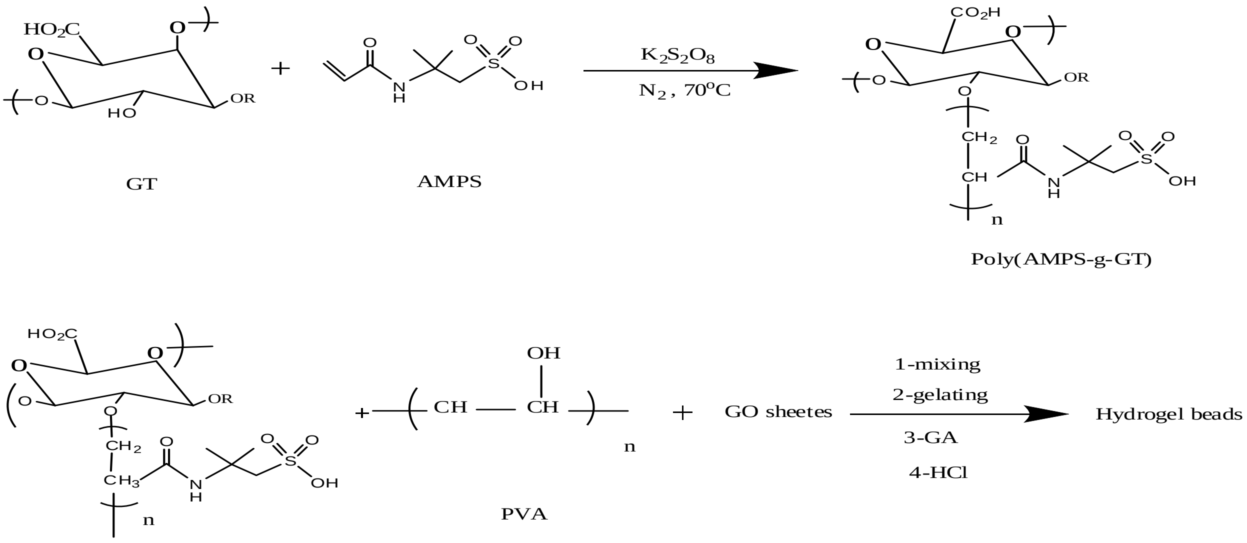

Fig. 1 General scheme of preparation of hydrogel beads in the presence of graphene oxide and poly vinyl alcohol

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Paper code: 295

Curing of DGEBA with MF resins in impregnated and laminated Paper and investigation of the kinetic parameters with DSC and FTIR methods

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In this study, the curing reaction of an epoxy system consisting of a diglycidyl ether of bisphenol A (DGEBA) and Melamine formaldehyde (MF) resins as curing agent was investigated during non-isothermal cure reaction by the Kissinger, Ozava and Isoconversional equations. Kinetic analysis of the curing reaction in different ratios of DGEBA/MF was studied by Differential Scanning Calorimetry Technique (DSC) and some parameters such as degree of conversion, pre-exponential factor and activation energy were determined by this method.

The results were compared to those obtained for the same epoxy systems using Fourier Transform Infrared (FTIR) analysis. From the infrared spectra using a peak-height method that was based on the ratio of the characteristic to reference absorbance peak, the degree of conversion and rate constant at different isothermal temperatures were calculated. And also we have investigated different ratios of DGEBA/MF resins in impregnated paper by comparing the lamination quality after pressing in wood panel.

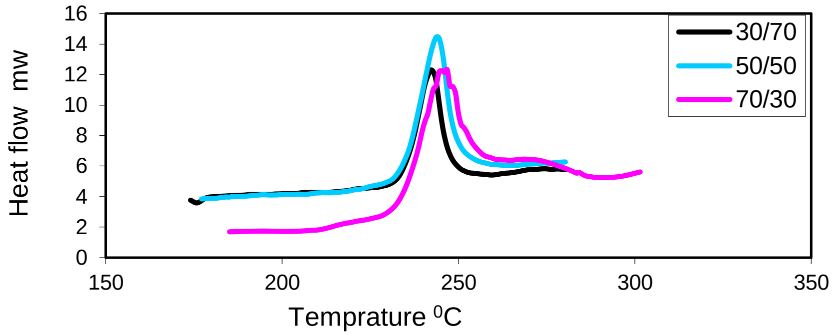

Figure1. Typical dynamic DSC thermos grams for the different weight ratio of DGEBA/MF at heating rate of 100C/min

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Paper code: 300

Synthesis and characterization of conductive star copolymer of PANI/PAA with calix[4]resorcinarene core

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Since the discovery of conducting polymers (CPs), the polymerization methods, chemical modification of these polymers, and their application fields have progressed significantly. Among them, PANI has many attractive properties such as, thermal stability, varied structure, special doping, and easy synthesis [1]. However, PANI has low solubility in common organic solvent, and poor processability [2]. The morphology of PANI influence on the physicochemical properties, and its applications. Thus, modification of this conducting polymer is important. Various procedures have been adapted to improve its solubility and processability. One method is the synthesis of PANI in star like architecture [1]. Star polymers have unique topological structures and more compact structure in solution compared to linear analogues with the same molar mass, leading to smaller sizes, and lower viscosities [2]. In this work, we described the synthesis and characterization of multiarm star-like polyaniline/polyacrylicacide from calix[4]resorcinarene as core. For this purpose, calix[4]resorcinarene was synthesized from resorcinol and butanal. In the next step, calix[4]resorcinarene converted to multifunctional Reversible Addition Fragmentation Chain Transfer (RAFT) initiator(ii), then the star polymer of acrylicacide with calix[4]resorcinarene was prepared by RAFT polymerization. Finally, aniline was polymerized at the end of the arms by radical polymerization in presence of APS. The solubility and conductivity of the synthesized polymer(iii) was improved compared to linear polyaniline.

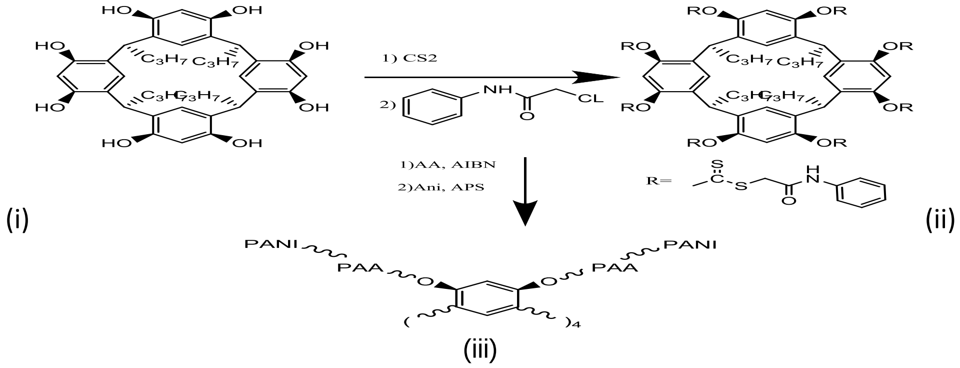

Fig. 1 conductive star copolymer of PANI/PAA with calix [4] resorcinarene core

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Paper code: 307

Synthesis and characterization of poly (aniline-co-carbazole) conductive copolymer and its carbon based nanocomposite

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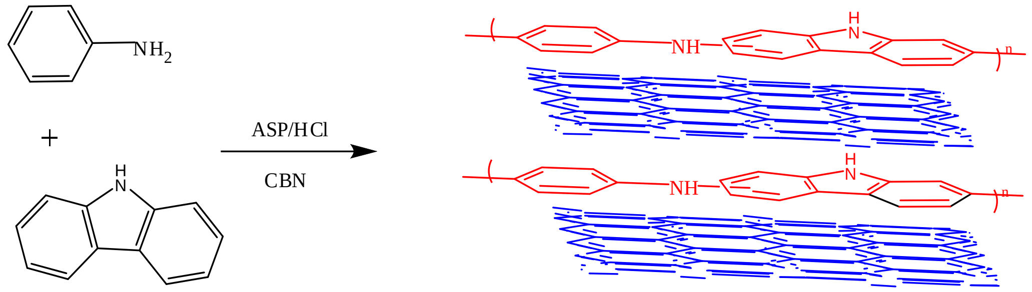
Conductive polymers are a class of materials which exhibit highly reversible redox behavior and the unusual combination of properties of metal and plastics. Among various conductive polymers, polyaniline (PANI) is a unique candidate for practical applications due to its good processability, environmental stability, low cost and reversible control of electrical properties by both charge–transfer doping and protonation [1]. Besides that, carbazole is an attractive heterocyclic compound that is an important monomer in the construction of the carbazole oligomer and polymer base material [2]. Polycabazole was studied in some aspects that showed unique properties in point of view electerical, electrochemical and optic fields [3]. However the redox sites in conductive homopolymers are not sufficiently stable during the many cycled redox processes, so conductive polymers suffer from disadvantages that include lower cycle-life and slow kinetics of ion transport [4]. Moreover, conductive polymers have low solubility in common organic solvent, and poor processability. For these reasons, the copolymer and composites of conductive polymers have been synthesized by either chemical or electrochemical polymerization.

Hence, in the present work we describe herein the synthesis of aniline-carbazole copolymer and its carbon based nanocomposites (CBN) via oxidative polymerization. Structural characterization and physical properties such as solubility, electrical conductivity, antioxidant and antibacterial activity of the materials were studied in this project.



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Paper code: 314

Preparation and design of new protic ionic liquids supported on nano-magnetite and their applications in three-component synthesis of 1-amidoalkyl-2-naphthols

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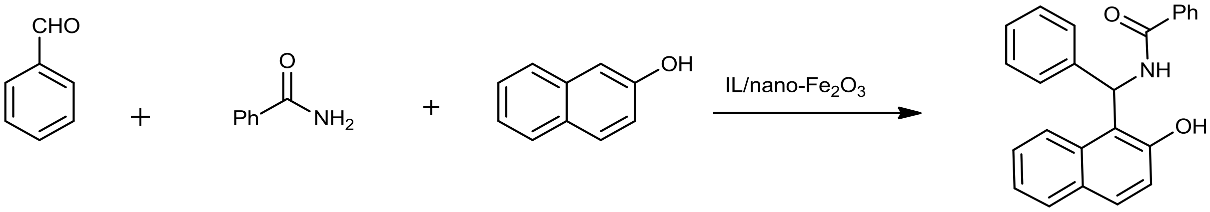
Amidoalkyl naphthols (ANs) are compounds with a variety of biological properties, that are easy converted to other active biological compound [1]. Therefore, synthesis of ANs have been developed by different methods and from different starting materials. Generally, amidoalkyl naphthols are synthesized by the three-compounds reaction of an amide or nitrile, an aldehyde, and a phenolic compound in the precence of heterogeneous and homogeneous acid catalysts [2].

Due to the limitations of some of these methods, in this investigation, amidoalkyl naphthols were synthesized modified by nano-magnetic (Mgnetic ILs) through a three-component reaction using under mild conditions. The FT-IR, ^{1}H NMR,^{13}C NMR spectra confirmed the structure of catalyst and compounds.



Non-toxicity and environmentally friendly of catalyst, short reaction times, high yields of prodocts, and easy work-up are some advantages of this developed method with magnetic catalysts.

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Paper code: 321

Synthesis of hydrogel based on poly (vinyl alcohol) for controlled drug delivery of lansoprazole according to the Farmacopeia standard

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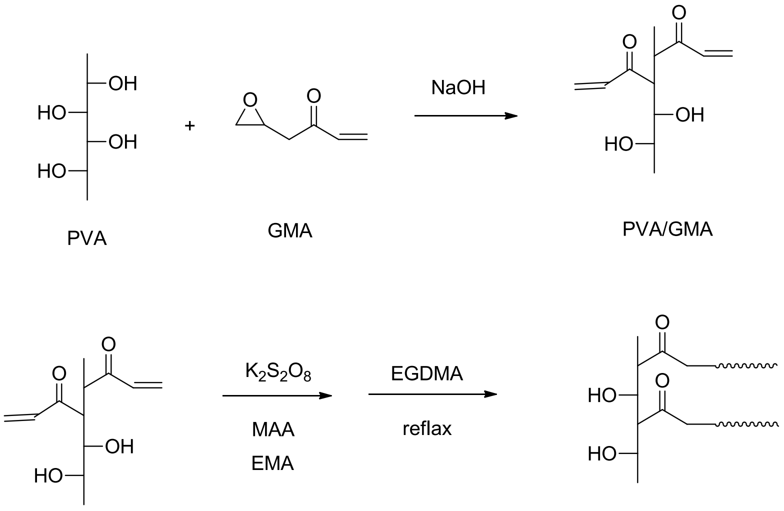
The purpose of this study is; preparation and identification of series of hydrogels based on modified poly vinyl alcohol ,GMA and acrylic monomers ,such as acrylic acid and methylmethacrylate[1]. The prepared hydrogels using different. weight ratios of these monomers to cross linking agent can affect the properties of hydrogels. After synthesis of hydrogels ,effect of several parameters such as PH,time,,temperature on the swollen behavior of them will be studied ,furthermore the effect of the percentage of the degree of gelation on lansoprazole release will be investigated[2].The prepared hydrogels act as carries for drug delivery systems providing the possibility of targeted delivery of Lansoprazole according to drug delivery conditions and through PH sensitivity.



PVA =Poly vinyl Alcohol
GMA =Glycidyl methacrylate
EGDMA =Ethyleneglycol dimethacrylate
MAA = Methacrylicacid
EMA = Ethyl methacrylate

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Paper code: 322

Synthesis and cytotoxic evaluation of poly(ethylene glycol)-coated superparamagnetic nanoparticles

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The aim of this study was to synthesize superparamagnetic nanoparticles and to investigate their cytotoxic effects on osteosarcoma cells. Fe_3O_4 nanoparticles were synthesized by the hydrothermal method and characterized by XRD, FT-IR, and zeta potential techniques. The XRD patterns of Fe_3O_4 nanoparticles showed the formation of single-phase superparamagnetic nanoparticle, and the spectra matched well with the JCPDS values (89-0691) (Fig.1). In FT-IR spectrum, the bands at 579 and 3570 cm^{-1} emerged which are related to the Fe-O and OH groups. Based on zeta potential value, fabricated nanoparticles possess negative charge surface. In order to increase the stability of nanoparticles in biological media, they were coated with poly(ethylene glycol) (PEG). Then, the cytotoxic effect of PEG@Fe_3O_4 nanoparticles on osteosarcoma cells (Saos-2 cells) was evaluated. Cells were treated with different concentrations of nanoparticles and the viability of cells evaluated using 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium (MTT) assay. The results showed that PEG@Fe_3O_4 does not have any significant cytotoxic effect on the cell growth and viability of cells up to100 µg/ml. Based on these results, PEG@Fe_3O_4 could be considered as an appropriate nanoplatform in drug delivery field.

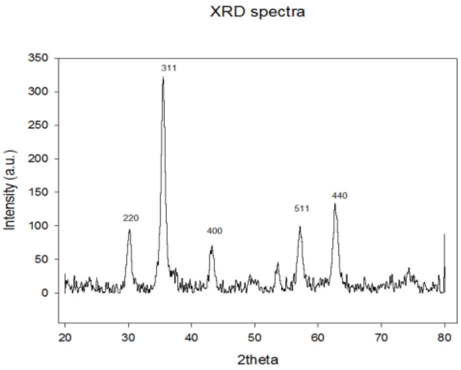

Fig. 1 XRD Spectra of synthesized nanoparticle.

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Paper code: 347

Fe_3O_4@Cu-*β*-CD nanoparticles-catalyzed synthesis of pyrazole derivatives

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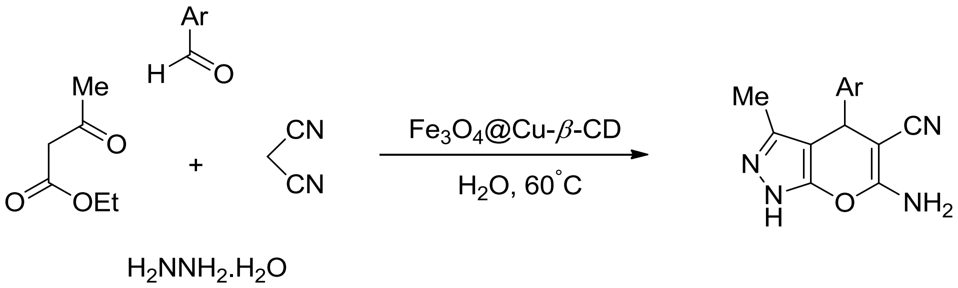
Regarding to the incrementing environmental contamination and also due to advantages of water as a solvent including environmentally safe, vast accessibility, non-flammability and cost-effective, use of such confident solvent have recently attracted the heed of chemists to its application in organic reaction [1,2]. The solubility of reactants in water boosts by using of *β*-CD through host–guest complexation. Cu nanoparticles have been recently shown to be efficient catalyst for some important reactions [3]. This paper is a report on the synthesis of the Fe3O4@Cu-*β*-CD core-shell. The cost effective and recyclable Fe_3O_4@Cu-*β*-CD nanocomposites provide an exciting new material for environmental protection applications. TEM, XRD, EDS and FT-IR were used to characterize the Fe_3O_4@Cu-*β*-CD nanocomposites. This new catalyst was used for four-component synthesis of pyrazole derivatives in aqueous solution under mild conditions (Scheme).



Scheme: Fe_3O_4@Cu-β-CD-catalyzed synthesis of pyrazole derivatives.

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Paper code: 349

Preparation of porous hydrogel beads based on calcium-ion-crosslinked gum tragacanth/graphene oxide: Swelling and drug delivery behavior

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During the past few decades, naturally derived materials have attracted much attention for development of various drug delivery systems [1]. Natural polysaccharides are preferred for drug delivery systems because of their easy availability, cost effectiveness, biodegradability and biocompatibility [2]. Preparation of ionic hydrogels with polysaccharide give interesting properties related to their polyelectrolytic nature of the structure. Bernela et al. reported ionic gelation method for synthesis of bromelain loaded tragacanth gum (katira gum) nanoparticles [3]. Composite hydrogels improve the drug encapsulation, mechanical strength, and controlled drug release with the addition of amplifying organic/inorganic fillers such as nano-clay, GO, carbon nanotubes and using blends of different polymers [4]. In this work, the objective was to prepare porous hydrogel beads from polysaccharide gum tragacanth (GT) and graphene oxide (GO) *via* ionic- crosslinking agent without using synthetic monomer The in *vitro* drug release studies from the prepared hydrogel beads exhibited significant behaviors on the subject of physiological-simulated pH values. The maximum cumulative releases were 97.62% and 42.2% at the pH values of 7.4 and 1.2, respectively.

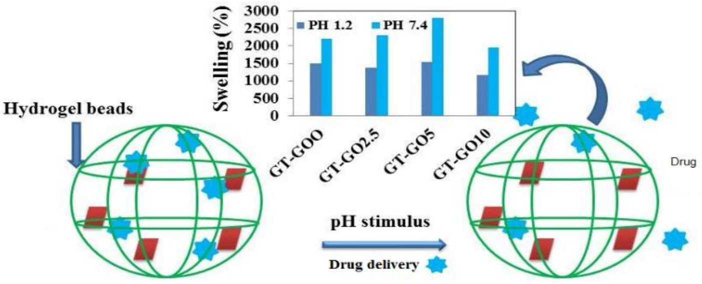

Fig. 1 Porous composite ionic hydrogel beads based on polysaccharide gum tragacanth (GT) and graphene oxide (GO).

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Paper code: 362

Fast and highly efficient removal of some cationic dyes from aqueous solutions using Sulfonated-Oxidized activated carbon

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In this study, the potentiality of Sulfonated-Oxidized activated carbon as an adsorbent for removal of Methylene Blue (MB), Crystal Violet (CV) and Thionin Acetate (Th) from aqueous solutions was investigated. The characteristics of the synthesized adsorbent was examined by FTIR and SEM techniques. Varying experimental conditions like contact time, adsorbent dosage, initial pH were studied to find the optimum adsorption conditions. The results showed that the adsorption process is too fast and after about 1 minute more than 95% of dyes were completely removed. The experimental data were well represented by Langmuir adsorption isotherm and the maximum adsorption capacities of MB,CV, Th dyes were calculated as 416.7 , 416.6 and 400.0 mg.g^{-1} respectively, which is considerably higher than the adsorption capacities of reported adsorbent in the literature. Simultaneous removal of the reported dyes was also carried out and more than 98% removal efficiency was obtained, so Sulfonated-oxidized activated carbon appears as an economical and effectual adsorbent for removal of MB,CV,Th from industrial waste waters .

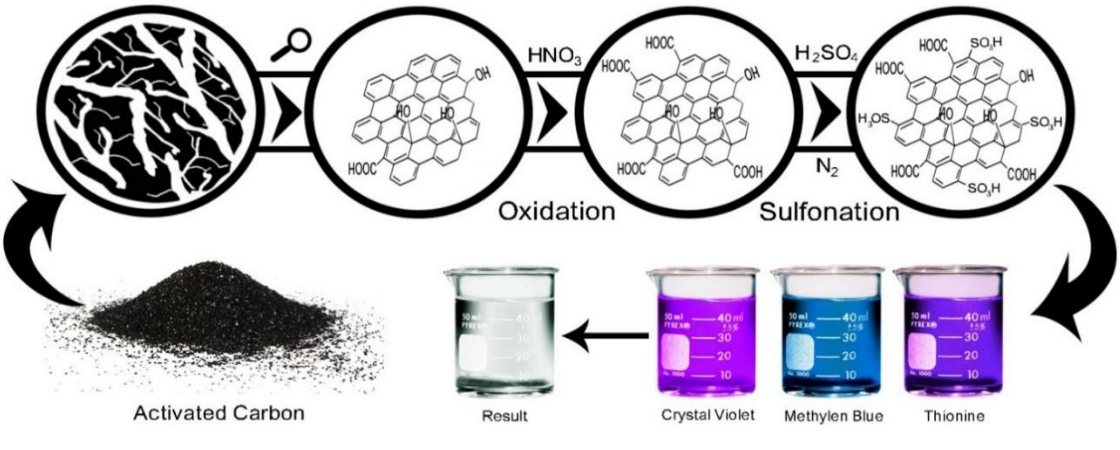

Fig. 1 Modification of activated carbon and efficient removal of Methylene Blue Crystal Violet and Thionin Acetate from aqueous solutions.

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Paper code: 371

Synthesis and characterization of wurtzite ZnS nanoparticles via solvothermal method

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Zinc sulfide has been widely studied due to it's component important wide-band-gap (3.6eV) semiconductor materials. ZnS can be prepared in various dimensional such as nanotubes, wires, rods, belts and ribbons, two-dimensional (sheet, plateles, diskettes) and three dimensional like spheres. But there are a few reports on the fabrication of ZnS only with presence thio-Schiff base ligand. ZnS can be prepared via different methods such as irradiation, solvothermal, physical evaporation and surfactant-mediated micro emulsion.
In this work a thio Schiff-base-assilsted solvothermal process has been developed to synthesize Zinc sulfide (ZnS) nanoparticles via the reaction between a metal salt $Zn(NO_3)_2.6H_2O$ and thio-Schiff base N-benzylideneethanethioamide as a new precursor (Fig. 1). X-Ray diffraction analysis and FT-IR spectroscopy were employed to characterize the obtained product. SEM images were used to investigation shape and size of synthesized ZnS. The results of this paper indicate that the shape and size of Zinc sulfide nanoplates can be controlled systematically by setting certain reaction parameters, such as the reaction temperature and duration and type of solvent. Zinc sulfide nanoparticles with different morphology and size have been successfully prepared.

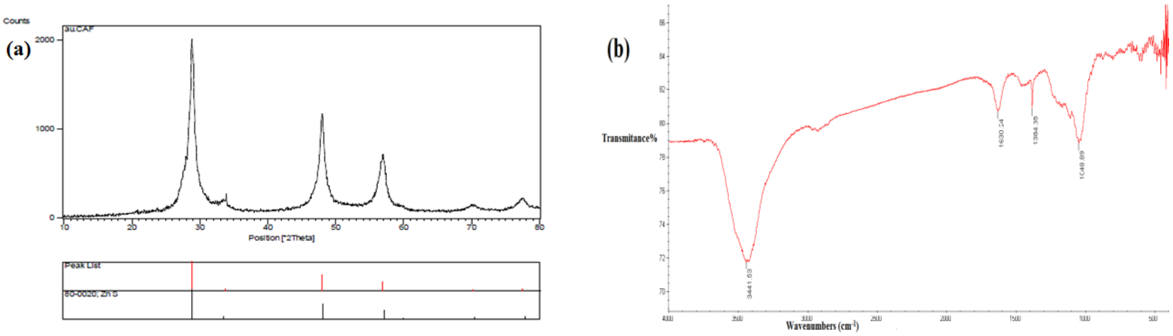

Fig. 1 **(a)** XRD pattern and **(b)** FT-IR spectrum of the ZnS particles obtained from thioschiff base via solvothermal method.

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Paper code: 374

Synthesis and Effect of (Dy, Ni) Co-doped on the Multiferrioc and Photocatalytic properties of $BiFeO_3$ on the degradation of Organic dyes

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Nanoparticles of bismuth ferrite ($BiFeO_3$) Due to their structural characteristics, the properties of multiproduct and photocatalytic properties are very important. Thus, the studies of Si nanoparticle ($BiFeO_3$) Nano silver bismuth ferrite synthesized by Dysprosium and nickel have been synthesized using the sol-gel method, and the effects of dipole substitution and nickel dispersion on its physical properties have been investigated. By diffraction spectroscopy X and IR sensors were used to identify these materials and verify the authenticity of the synthesized specimens. In the next step, the catalytic performance of nanoparticles of bismuth ferrite doped to dysprosium and nickel for catalytic removal of methyl orange color, which is one of the most important pollutants in industrial wastewaters, was investigated by UV-Vis spectroscopy and the results indicated the efficiency High nanoparticles were synthesized in the removal of methyl orange color. The effect of pH parameters, irradiation time, color concentration, and percentage of nanoparticles were optimized. Then, we investigated the photocatalytic properties of the bismuth ferrite ironized with Dysprosium with different composition percentages. $Bi_{0.94}Dy_{0.06}Fe_{1-x}O_3$(X = 0.00, 0.02, 0.04, 0.06) Based on the results obtained, the percentage of succession Dysprosium (X = 0.02) shows the most photocatalytic property. Subsequently, the nickel substitution was carried out by the bismuth ferrite. $Bi_{0.98}Dy_{0.02}Fe_{1-y}NiO_3$ (y = 0.01, 0.03, 0.05) the results indicate with the addition of nickel, the photocatalytic activity of the synthesized nano-particle increases.

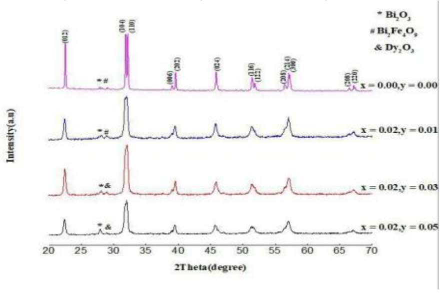

Fig. 1 results of: x-ray beam pattern, Dy and Ni co-dopped BFO

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Paper code: 376

The interaction of trypsin with one nanoparticle (CuO): Spectroscope identification

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Enzymes hold a great promise as therapeutic agents because of their unique specificity and high level of activity. Conjugation of proteins to nanoparticles has numerous applications in imaging, sensing, catalysis, delivery, therapy and control of protein structure and activity[1,2]. Therefore, characterizing the nanoparticle–protein interface is of great importance. The effect of the interaction of nanoparticles with biological macromolecules e.g., enzyme is important in biological, industrial and pharmaceutical fields of research. Some inorganic nanoparticles have been shown to act as an enzyme inhibitor which may be connected to the change of the native enzyme structure. We report the binding of a serine protease (trypsin) as a model enzyme with CuO nanoparticles. To take a comprehensive evaluation of CuO nanoparticle effect, we investigated its interaction with a serine protease trypsin by multispectroscopic techniques. The result of absorption, circular dichroism and fluorescence techniques have been demonstrated the structural changes in secondary and tertiary structure of trypsin induced by binding of CuO nanoparticles. The changes in the structure of enzyme upon binding with nanoparticles are reflected through an increasing protease activity of trypsin-CuO nanoparticles complex in comparison to the absence of nanoparticles (pure enzyme). Also we showed that thermal stability of enzyme increased with increasing nanoparticles concentrations. The thermodynamic parameters for the trypsin -CuO nanoparticles binding interaction unveil the enthalpy as well as entropy driven binding ($\Delta H° < 0$ and $\Delta S° < 0$) with an overall favorable Gibbs free energy change ($\Delta G° < 0$). The thermodynamic parameters delineate the dominate role of hydrogen bond and van der Waals interaction in the binding process of CuO nanoparticles with trypsin[3]. Enzyme activity assay gave evidence at the functional aspect to clarify the fact that CuO nanoparticle could contribute to the conformational changes and furthermore alter the function of the enzyme.

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Paper code: 387

Organic/inorganic photoconductive hybrid films based on polypyrrole-cadmium sulfide quantum dot nano-composites

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Nanostructure hybridization of conducting polymer with inorganic nano particles offers considerable advantages in polymer processing, device performance and/or tunability over standalone polymeric based devices [1]. In this work, the photoconductivity properties of the conducting polypyrrole–cadmium sulfide (PPy-CdS) quantum dot nano-composite films were studied. The soluble conducting PPy and the CdS quantum dot were separately synthesized [2, 3]. The SEM images indicated that the PPy nano particles and CdS quantum dot were synthesized successfully. After the preparation of PPy-CdS nano-composites with the different weight percent, electrospray coating method was then applied in order to deposit the mentioned nano-composite on the surface of interdigital electrodes (IDEs). This film was then connected as one resistance of a Wheatstone bridge and its photoconductivity properties were investigated while illuminating the film in the IR region (4000-400 wavenumber). Observations showed that when the film absorbed IR radiation, a current was passed through the Wheatstone bridge circuit and this photocurrent was proportional to the hybridization percentage. The current values produced by the nano-composites which are in the range between 89-117.8 µA are higher than that of the pure PPy film (70 µA).The maximum current was related to the film with 20 weight percent of hybridization. The produced photocurrent was well repeated. As a result, the prepared organic-inorganic hybrid films provide excellent photoresponsive materials which can be applied in photo detection devices.

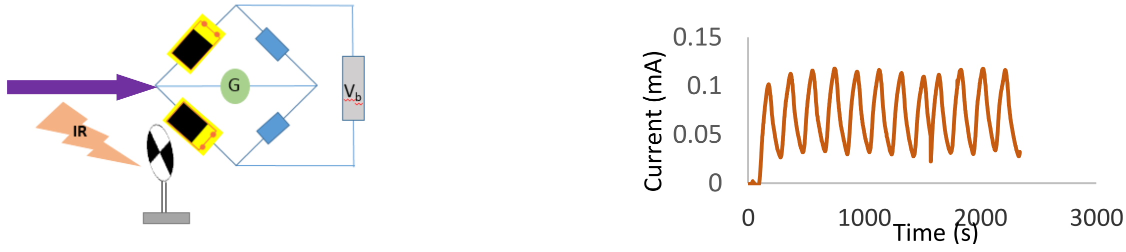

Fig. 1 A schematic view of the photoconductivity properties of PPy-CdS nano-composite film.

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Paper code: 388

Synthesized of palladium nanoparticles supported on functionalized 2D-geraphene oxide and their application in reduction of organic dyes

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In this research, Graphene oxide (GO) was first synthesized from natural graphite flakes by a modified Hummers method [1] and in a typical experiment, the obtained graphene oxide and Poly(N-vinyl-2-pyrrolidone) or PVP were added to ethanol solution for preparation of .two- dimensional GO [2,3]. In the other step, the surface of 2D-GO functionalized with 3- Aminopropyltriethoxysilane (APTES). APTES is the most commonly used alkoxysilane linker for surface modification of GO due to its terminal amino groups. In this way, one of the three ethoxy groups (–O–CH_2– CH_2–CH_3), which present in the APTES molecule breaks, then leads to covalent bonding between the APTES groups and the 2D-GO. Aliphatic amines are unstable and easily oxidize by aqueous oxidant such as metal ions solution, therefore Pd ions cannot be immobilized on the modified surface with amine groups. For solving this problem and to obtain the more active sites on the surface, during other step terminal amines group of APTES were reacted with aldehyde group of 3,4,5-Trimethoxy-benzaldehyde, which imine bond easily formed and ether functional groups coordinated with Pd ions. Finally Pd NPs synthesized by reduction with $NaBH_4$. The synthesized catalyst have been used for the rapid reduction of 4-nitrophenol (4-NP), methyl orange (MO) and methylene blue (MB) in the presence of $NaBH_4$ and shown high catalytic activity.

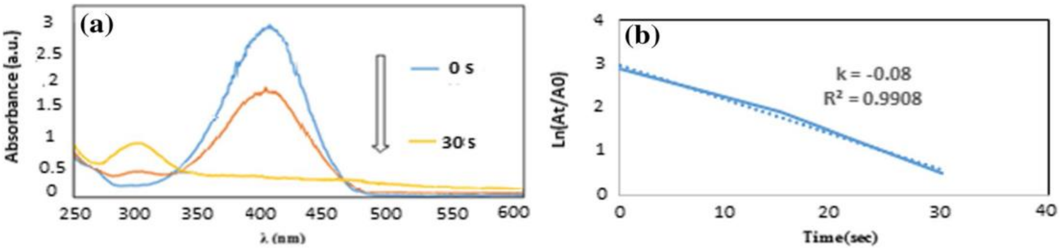

Fig. 1 Figure Time dependent UV–Vis absorption spectra of 4-NP for the reduction of 4-NP

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Paper code: 389

The Hg^{2+}/Al_2O_3 Nanoparticles for Adsorption of Thymine Nucleobase

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γ-Alumina with both acidic and basic properties is well-known catalyst for many important industrial applications. Studying the structure, reactivity and selectivity of this compound has been of great interest over the recent years [1-3]. The salts of inorganic compounds are commonly used to treatment the catalytic properties of γ-alumina. In this study, the Hg^{2+}/Al_2O_3 nanoparticles were prepared using impregnation of γ-alumina nanoparticles with mercury acetate into the solution of water/*iso*-propanol, followed by hydrolysis, washing and filtration processes. The morphology of nanoparticles was considered using XRD and FT-IR spectroscopy. The adsorption of thymine nucleobase on γ-alumina nanoparticles was investigated using UV-Vis spectroscopy.

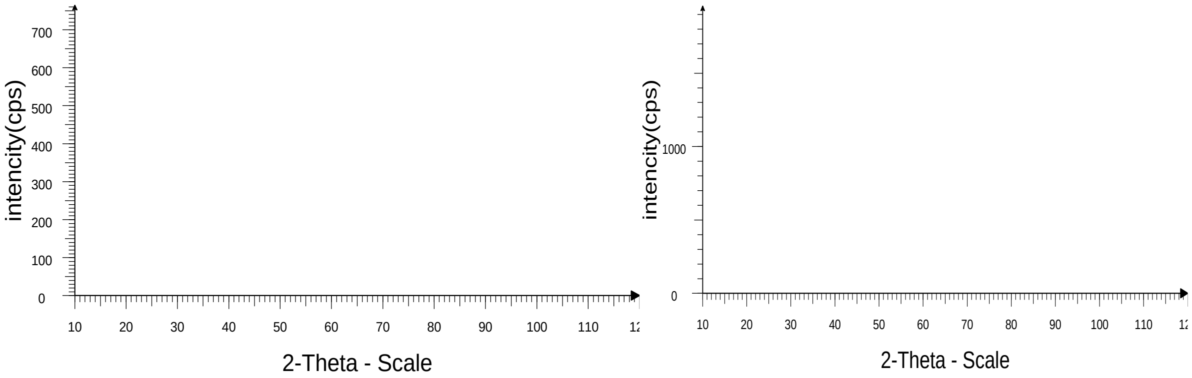

Fig. 1 The XRD patterns of Al_2O_3 (left) and Hg^{2+}/Al_2O_3 (right) nanoparticles

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Paper code: 392

Application of Chromium Tungsten/Reduced Graphene Oxide as an advanced electrode material for supercapacitors

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A composite of reduced graphene oxide (RGO) with nano-sized chromium tungstate ($Cr_2(WO_6)$) was prepared using a sonochemical method. The prepared $Cr_2(WO_6)$/RGO samples were assessed through field emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), and FT-IR spectroscopy to obtain chemical, structural and morphological information. The resulting composite ($Cr_2(WO_6)$/RGO) was evaluated as a candidate for building supercapacitor electrodes. In this line the electrochemical performance of the tested materials were studied through cyclic voltammetry (CV), galvanostatic charge/discharge, electrochemical impedance spectroscopy (EIS), and continues cyclic voltammetry (CCV). The electrochemical tests were performed using 2 M H_2SO_4 solutions as the electrolyte. The evaluations on $Cr_2(WO_6)$/RGO-based electrodes revealed the material to have a specific capacitance of 473 F g^{-1} at a scan rate of 5 mV s^{-1}, an energy density of 61 W h kg^{-1}, and a high rate capability. Continues cyclic voltammetry evaluations using $Cr_2(WO_6)$/RGO-based electrodes proved the electrodes to be capable of maintaining almost 98% of its initial SC after 4000 cycles. Based on the electrochemical evaluations the synthesized nanocomposite was proven to possess the merits of both of its ingredients.

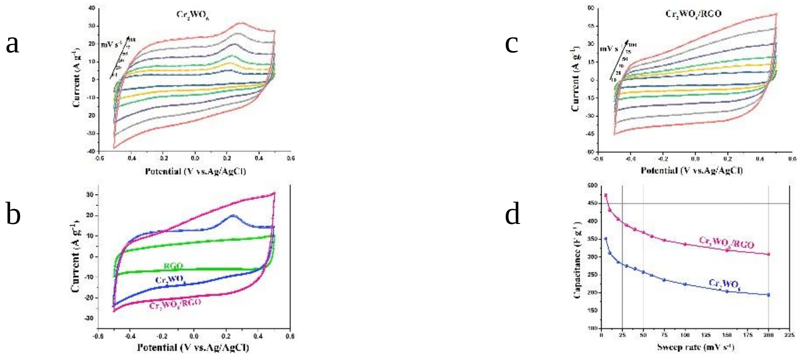

Fig. 1 (a) CVs of the $Cr_2(WO_6)$ electrode at different scan rates, (b) CVs of the $Cr_2(WO_6)$/RGO electrode at different scan rates, (c) CVs of the RGO, $Cr_2(WO_6)$, and $Cr_2(WO_6)$/RGO electrodes, at a scan rate of 50 mV s^{-1} in 2.0 M H_2SO_4 aqueous electrolyte and (d) Specific capacitance as a function of the sweep rates for the $Cr_2(WO_6)$ and $Cr_2(WO_6)$/RGO electrode.

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Paper code: 396

Catalytic activities of a novel nanofiber base on molybdenum complex/ α-Fe_2O_3

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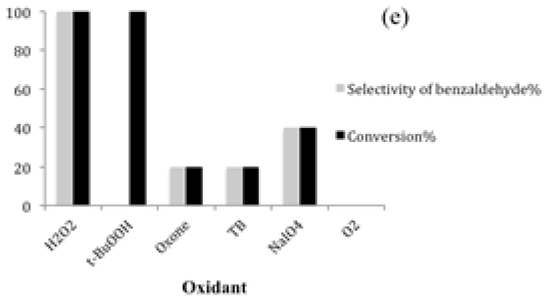
Nanocomposite compounds using metal oxides with low loading has already been proven as an effective way to produce new materials with specific properties and high performances. PVA (Polyvinyl alcohol), a synthetic water-soluble hydrophilic polymer, is widely used and studied for nanocomposites technology. Moreover,PVA has unique properties such as good thermal stability, optical properties and oxygen barrier properties. Therefore, this kind of nano-composites are widely used in filters, packaging, tissue engineering scaffolds and CO_2 membrane separation application[1]. Electrospinning is a technique using to produce fibrous. The rapidly developing technique of electrospinning has gained surging research interest since the 1990s due to its capability of obtaining nano-fibers. Enormous efforts devoted to explore applications of electrospun nanofibers, such as separation, catalysis, nanoelectronics, sensors, energy conversion/storage, and biomedical utilization[2-3].

In this work, nanocomposite PVA/α-Fe_2O_3/Molybdenum complex on 2- hydroxy naphthaldehyde was synthesized and characterized by Fourier transform infrared (FT-IR) spectroscopy, field-emission scanning electron microscopy (FE-SEM) image, energy dispersive X-ray (EDX) analysis and thermogravimetric analysis/differential thermal analysis (TGA/DTA). Catalytic application of it was investigated in the oxidation of alcohols. 100% of benzaldehyde was obtained in the presence of PVA/Fe2O3/Mo using H_2O_2 at 80°C for 7h.



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Paper code: 421

Diastereoselective three-component Mannich reaction catalyzed by prolinated MWCNTs

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Asymmetric Mannich and Mannich-type reactions are important carbon-carbon bond-forming reactions that provide access to enantiomerically enriched β-amino carbonyl derivatives.[1] These compounds are useful precursors for synthesis of β-lactams, α and ᵞ-aminoalcohols, α and β-amino acid derivatives, peroxy acetylenic alcohols/ethers, and medicinally important materials. Several strategies[2,3] are available for diastereoselective synthesis of β-amino carbonyl compounds, including organocatalysis transition-metal catalysis, Bronsted and Lewis acid catalysis, phase-transfer catalysis, biocatalysis and ionic-liquid catalysis.

Herein we report a highly anti-diastereoselective three-component Mannich reaction of aromatic amines and aldehydes with cyclohexanone in water as solvent and efficient nano organocatalyst. Reusability, easy workup, inexpensive, ready availability, short reaction time and its high diastereoselctivity 70-100% makes this catalyst an attractive alternative to the existing catalysts for the synthesis of β-amino carbonyls.

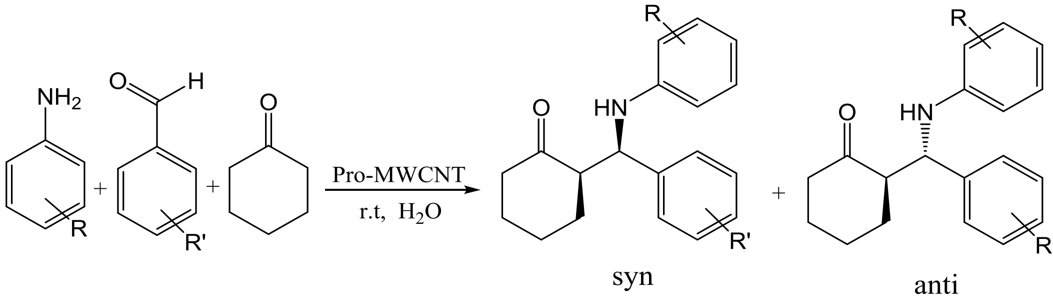

Fig. 1 Three-component Mannich reaction of aromatic amines and aldehydes with cyclohexanone

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Paper code: 424

Photodynamic Therapy Mediated Cytotoxic Activity of ZnO/HAP Nanocomposites in Human Osteosarcoma Cells under UV Irradiation

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Photodynamic therapy (PDT) is a minimally invasive therapeutic procedure that uses special drugs or compounds, called photosensitizing agents. The photosensitizers have been activated by certain kinds of lights and they can kill cancer cells selectively through the generation of reactive oxygen species (ROS) [1, 2]. ZnO is a semiconducer material that has photosensitizing effects and generates ROS. In this study, zinc oxide/hydroxyapatite (ZnO/HAP) nanocomposites were synthesized by the hydrothermal method and characterized by FT-IR and UV-visible spectroscopy. Then, the cytotoxic effect of ZnO/HAP nanoparticles on the viability of osteosarcoma cells (Saos-2 cells) was evaluated in the presence and absence of UV irradiation. MTT assay revealed that ZnO/HAP nanoparticles decreased the viability of Saos-2 cells in a dose-dependent manner; however, a significant reduction in cell viability was observed since ZnO/HAP-treated cells were exposed to UV irradiation. The phase contrast microscopic examination of the cells treated with the ZnO/HAP nanoparticles revealed growth inhibition and the typical morphological features of dead cells, however, these phenomena were significantly increased as cells treated with both nanoparticles and UV irradiation. Based on these findings, ZnO/HAP nanoparticles could be considered as a novel photosensitizer which can be employed for cancer therapy.

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Paper code: 436

Solid sorbent based on natural polymer nanosheets for removal of antibiotics from wastewater

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One of the important water contaminants is antibiotics derived from hospitals and pharmaceutical manufacturing sites. Removal of these compounds from water with high efficiency is remained a major challenge in water treatment. Several conventional methods have been used for removing these compounds from waste water but most of them suffer from high costs and energy consumption. Removing of contaminants based on solid sorbents have noticeable properties. They are effective, efficient, and economic methods for water decontamination applications [1, 2].

Solid sorbents based on natural polymers were found to be high-performance for removal of antibiotics. In this work, Magnesium oxide-chitosan-graphene oxide (MgO/CS/GO) nanosheets were successfully synthesized and used as a sorbent for efficient removal of ciprofloxacin and norfloxacin from aqueous solutions. The FTIR, BET, XRD, SEM, and TEM were used for characterization of nanocomposite and showed the layer by layer structure for this sorbent. The pH effect, adsorption kinetic, and adsorption isotherm were investigated.

The adsorption isotherm of model antibiotics well described with the Langmuir model and the maximum adsorption capacities recorded 500.20 and 430.70 mg g^{-1} for ciprofloxacin and norfloxacin, respectively. Analysis of kinetic data revealed that the synthesized sorbent followed pseudo-first-order kinetics and the maximum equilibrium was at over 150 and 100 min for the ciprofloxacin and norfloxacin, respectively. Therefore, this is introduced as a simple, economical, and eco-friendly sorbent for developing a high-performance sorbent for removal of antibiotics from wastewater.

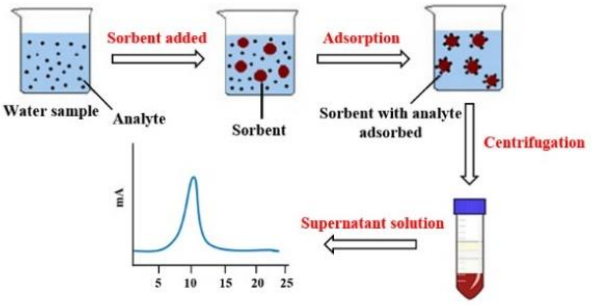

Fig. 1 The procedure of removal antibiotics with solid sorbent

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Paper code: 440

Clinical investigations of cobalt and copper complexes containing 1,10-phenanthroline-2,9-dicarboxylic acid in some cancer therapy treatments

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The design of ligands for biomedical, biological, and environmental applications and for metal ion separations, is of considerable interest, in which ligand preorganization has been an important aspect. A ligand which has the most preorganized feature is constrained compared to free ligand, and is of compatibility required for complexing with metal ions which 1,10-phenantrolene-2,9-dicarboxylic acid (H_2PDA) is of this type of ligand. Complexes involving the metal ions Co(II) and Cu(II) have many and varied applications. They have been used and screened for their antifungal and antibacterial activities. Therefore, we synthesized three complexes bearing above-mentioned ligand and 1,10-phenanthroline (Phen) as auxiliary ligand in the presence of Co(II) and Cu(II) metal ions through different techniques. Regarding our obtaining data, one can formulate the complexes as $[Co(PDA)(Phen)]\cdot EtOH\cdot H_2O$(**1**), $[Cu_2(PDA)_2(H_2O)_2]\cdot 2H_2O$(**2**), and $[Co(PDA)(H_2O)_3]\cdot 2H_2O$(**3**) were characterized by some physico-chemical methods such as elemental analysis, Infrared spectra (IR).The anticancer and cytotoxic properties of these complexes on several cancer cell lines were tested by MTT assay, flow cytometry, and TUNEL tests. Also, to compare the cytotoxicity of these complexes with common chemotherapy drugs, the cystic acidic property of cisplatin (or another anti-cancer drug) were evaluated as a positive reference and control.

$$[Co(PDA)(H_2O)_3]\cdot 2H_2O + Phen \xrightarrow[100^{\circ}C,\ 2h]{EtOH/H_2O} \mathbf{1}$$

$$Cu(NO_3)_2\cdot 3H_2O + H_2PDA + bipy + NaOH \xrightarrow[85^{\circ}C,\ 24h]{EtOH/H_2O} \mathbf{2}$$

$$CoCl_2\cdot 6H_2O + H_2PDA + Phen \xrightarrow[130^{\circ}C,\ 3day]{CH_3CN/H_2O} \mathbf{3}$$

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Paper code: 441

Catechin-conjugated hydroxyapatite nanoparticles increase Osteocalcin and Runx2 proteins in Mesenchymal stem cells

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Despite advances in stem cell biology, there are a few effective techniques to promote the bone regeneration in human bone defects after surgery in patient who suffer from osteosarcoma. One of the strategies for the regeneration of bone defects is “cell-based therapy”, using mesenchymal stem cells (MSCs). However, poor osteogenic differentiation of MSCs is an issue related to the application of these cells in “cell-based therapy”. Based on this fact, we were interested to investigate the ability of catechin-conjugated hydroxyapatite (Cat@HAP) in the induction of osteogenic differentiation Osteogenic differentiation was verified by the evaluation of intracellular content of bone-related proteins, Runx2 and Osteocalcin (OCN), by flow cytometry. After 7 days of incubation of MSCs with Cat@HAP, the content of Runx2 significantly increased at the level of protein. Runx2 contains an active transactivation domain which activates the OCN gene [1]. The expression of down-stream signaling molecule, OCN, was also evaluated at the level of protein. OCN is involved in the bone mineralization and considered as a marker for the late stage of osteogenic differentiation [2]. According to the flow cytometry data, the expression level of OCN remarkably increased in MSCs cultured for 14 days with Cat@HAP. Based on these results, Cat@HAP could be considered as an appropriate candidate for the bone regeneration along with “cell-based therapy”.

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Paper code: 446

Effect of zinc oxide nanoparticles on azo dye

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In this research, zinc Oxide nanoparticles were prepared by sol-gel technique. After preparing sol and ensure its sustainability, nanoparticles prepared by annealing from certain temperature. The structure and surface morphology were investigated by X-ray diffraction (XRD) and scanning electron microscopy (SEM) [1]. In the following Photocatalytic activities of nanopowders were performed using degradation of azo dyes. The influence of pH, time of irradiation and dye azo concentration on the photocatalytic activity was investigated. The result showed that Zinc Oxide photocatalyst cannot degradation azo dye without irradiation UV-vis and presence of all three factors Azo dye, Zinc Oxide photocatalyst and UV-Vis radiation are necessary for degradation. Figure 1 shows the XRD pattern of ZnO nanoparticles for different temperature °C. The X-ray diffraction patterns were detected with Miller indices (002), (101), and (100) indexed to the hexagonal wurtzite structure with good crystallinity. The peak intensity increase, with increase the temperature [2].

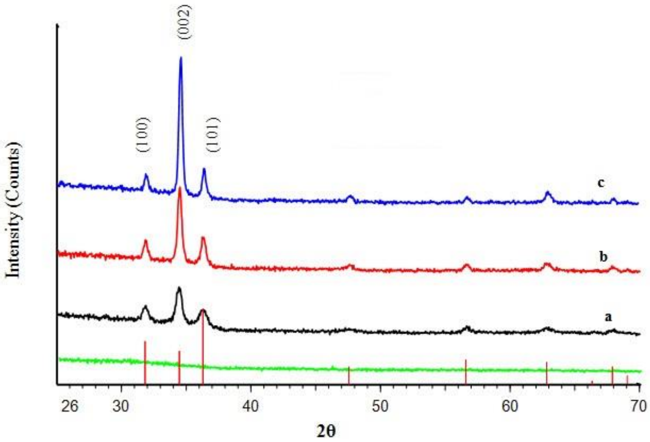

Fig.2: XRD pattern of ZnO nanoparticles annealed at 300(a), 400(b) and 600(c) °C

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Paper code: 448

Application of Horsetail and Horsetail Ash as a Novel Natural Lewis Acid Catalyst for the One-Pot Synthesis of 2-Amino-4H-Chromene Derivatives

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The present study offered an introduction of horsetail plant with its unique properties. It is a source of silica and is reported to contain active components such as phenolic acids (e.g., ascorbic acids, ferulic acids, silicilic acids, malic acids, caffeic acids, gallic acids, pectic acids and tannic acids), saponins, flavonoids, and it also contains minerals such as silicon and silicates, potassium, calcium, aluminum, sulfur, magnesium, manganese, zinc, chrome and cobalt [1]. The exposure of horsetail to a high temperature resulted in the production of the horsetail ash containing better properties and benefits rather than the horsetail itself.

One of the most common MCRs that produces an interesting class of oxygen heterocyclic compounds is 2-amino-4H-chromene derivatives synthesis, having attractive pharmacological and biological activities, such as antitumor [2]. The results have shown that both horsetail and horsetail ash could act as bench top solid acid catalytic systems. Therefore, in order to make a comparison between their catalytic activities they were each employed for the first time in the organic reaction to synthesize the 2-Amino-4H-Chromene derivatives from the reaction of dimedone 1, malononitrile 2 and aromatic aldehydes3 under solvent-free conditions (Fig. 1).

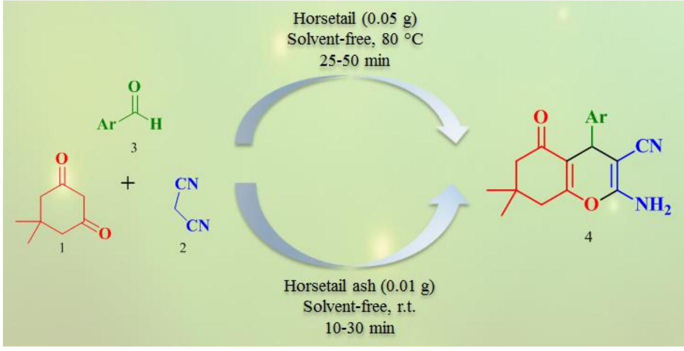

Fig. 1 Synthesis of 2-Amino-4H-Chromene derivatives catalyzed by horsetail and horsetail ash

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Paper code: 454

Synthesis of Cl-Methylated Carbon Nanotube as a 5-FU Drug Carrier

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Carbon nanotubes (CNTs) have attracted a great deal of attention in biological applications, as a promising candidate for gene therapy, bio-sensing and drug delivery [1]. Their impressive characteristics such as high surface area, enhanced cellular uptake, enable to perforate cellular membrane and elimination the side effects make them ideal nanomaterial for drug delivery carrier [2]. In addition, the drug loading capacity of CNTs can be increased by functionalization with chemical groups, in particular halogen-substituted methyl radicals. 5-Fluorouracil (5-FU) is currently in use for the treatment of colorectal cancer, breast cancer, pancreatic cancer and glioblastoma [3]. In this direction, we have carried out the experimental investigation on 5-FU loading ability of Cl-methylated carbon nanotube. The binding of CNT to 5-FU has been elucidated using FTIR analysis presented in the figure below. In this figure the FTIR spectrum of 5-FU-loaded functionalized CNT along with that of the pristine CNT and 5-FU, for comparison, are displayed. As can be seen, the pattern of 5-FU-loaded functionalized CNT shows carbonyl group, C-N stretching and bending peaks as well as disappearing C-Cl peak after reaction of 5-FU with Cl-methylated carbon nanotube in FTIR.

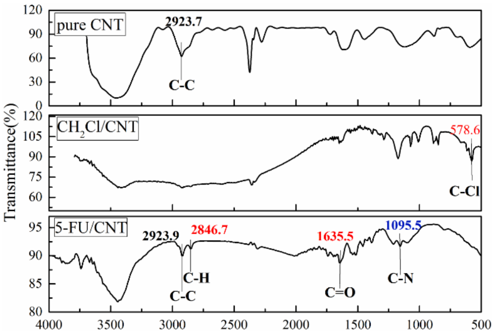

Fig. 1 The FTIR spectra of 5-FU, CNT and 5-FU loaded CNT.

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Paper code: 459

Production of electronic content for the teaching of electron quantum configuration of elements

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Teaching of drawing a quantum electron configuration to tenth secondory school students is one of the difficulty items of teaching of chemistry book by teachers. In this article, the author attempts to propose a new electronic teaching method in order to learn the quantum electronic arrangement of elements easirer. The proposed technique will facilitate ease of training for the chemistry teachers and also ease of understanding for respective students. This technique is applied by drawing a diagram based on the electron configuration developed by Boron in powerpoint software environment. The mentioned diagram is started vertically using the electron configuration of Boron and then, will continue with the simultaneous teaching of quadruple quantum numbers (downward progress), so that a diagram of orbital quantum electron configuration will be created at the end. Teaching steps of the proposed diagram in form of slideshow by powerpoint can be useful in improving learning process of students.

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Paper code: 460

Pyramid Modeling Teaching of the Quantum Arrangement of Boron Electron in Chemistry Curriculum for Tenth Secondary School

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Teaching of drawing a quantum electron configuration to tenth secondory school students in experimental or mathematical sciences in the first chapter of the chemistry book, is one of the difficulty items of teaching of this book by chemistry teachers. In the present paper, the author attempts to develop a new teaching technique of drawing of quantum electron configuration of elements. The proposed technique will facilitate ease of training for the chemistry teachers and also ease of understanding for respective students. This technique is applied by drawing a diagram based on the electron configuration developed by Boron. The mentioned diagram is started pyramidically using the electron configuration of Boron and then, will continue with the simultaneous teaching of quadruple quantum numbers (downward progress), so that a quantum electron configuration diagram will be created at the end.

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Paper code: 461

Solar light driven magnetic-photocatalyst nanohybrid and photocatalytic degradation of pharmaceutical pollutants

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Pharmaceutical pollutants substantially affect the environment; thus, their treatments have been the focus of many studies. In this regard, photocatalytic degradation of pharmaceutical pollutants in the wastewater using dispersed semiconductor nanophotocatalysts under solar light has a number of advantages such as high activity, cost effectiveness and utilization of free solar energy. However, it is difficult to recover and recycle nanophotocatalysts since the fine dispersed nanoparticles are easily suspended in waters. Furthermore, a large amount of photocatalysts will lead to color contamination. Thus, it is necessary to prepare photocatalysts with easy separation for the reusable application. To take advantage of high photocatalysis activity and reusability, magnetic photocatalysts with separation function were utilized. In this report, the solar light photocatalytic degradation of ibuprofen (IBP) as a model of pharmaceutical pollutants in water media was investigated. Two types of magnetic nanophotocatalysts (Magnetic Fe_3O_4/Bi_2WO_6 and POM-γ-$Fe_2O_3/SrCO_3$ nanohybrids) were used for photocatalytic degradation of IBP. In the case of Fe_3O_4/Bi_2WO_6 nanohybrid, high photocatalytic activity was obtained under sunlight condition with the addition of hydrogen peroxide improving the efficiency of IBP degradation. Further, the removal of IBP in the dark condition could be ignored (Fig.1 and 2). In the case of POM-γ-$Fe_2O_3/SrCO_3$ nanohybrid in comparison with the γ-Fe2O3/SrCO3, the degradation of IBP after 2-h exposure to the solar light irradiation was significantly higher for POM-γ-Fe2O3/SrCO3 nanohybrids and the degradation of IBP was enhanced by the addition of H2O2 to the air saturated solution. The photocatalytic activity and magnetization properties of this magnetic photocatalyst nanohybrid provide a promising solution for the degradation of water pollutants and photocatalyst recovery.

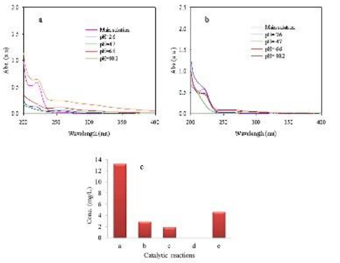

Fig.1. UV–vis spectra ofphotocatalytic degradation ofIBP on Fe3O4/Bi2WO6 at different pH after 2 h under (a) sunlight, (b) dark condition, and (c) the concentration ofIBP as a function of pH by using Fe3O4/Bi2WO6 nanohybrids under sunlight (a) initial conc., b) pH = 2.6, c) pH = 4.7, d) pH = 4.7 + 40 mL H2O2, e) pH = 6.6, amount of photocatalyst = 70 mg, initial conc. = 10 mg L1, time = 2 h).

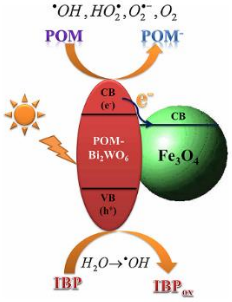

Fig.2. Schematic diagram of the photocatalytic reaction of IBP on Fe3O4/Bi2WO6 nanohybrid.

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Paper code: 462

A review on electrospun polymeric nanofibers and antibacterial wound dressing

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Wound healing is important in medicine so that the development in this area can affect a major impact on quality of patient life. Using suitable dressing is one of the effective role in wound healing. In recent years, new generation of wound dressing are developed. However, fewer dressing has complete requirement of wound healing. Recently, electrospun polymeric nanofibers is widely considered due to their unique properties in wound dressing and healing. Electrospinning has been widely used as a nanofiber fabrication technique. Polymeric nanofibers with different morphologies and dimensions can be obtained from electrospinning method. This report gives us an overview of some recent advances of electrospinning, fabrication of polymeric nanofibers and their application in wound healing. First, we briefly discuss the wound healing process then the electrospinning process and fabrication of electrospun nanofibers are investigated. Finally, nanofibers in combination with others nanomaterials and their application in wound dressing and antibacterial properties are studied.

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Paper code: 475

Polymerization and characterization of para-nitrophenol in sodium acetate medium on pb electrode

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In this work a new polymer was prepared via electropolymerization of 4-nitrophenol on lead cathode in aqueous solution acetate medium (sodium acetate). electropolymerization of para-nitrophenol carried out in a separated electrochemical cell on Pb cathode under control potential of the cathod (-1 volt). The electrochemical reduction of nitro compounds is best understood in terms of radical anions of the $–NO_2$ group [1].Under conditions of low proton availability (weak alkaline media or aprotic solvent), the radical anions are quite stable and the reduction process splits into 1-electron and 3-electron steps [2]. After four hours, the electro-product was separated and washed with DDW. The electrode-product was characterized by DSC, FT-IR, H-NMR, CV and suitable mechanism was proposed. Regarding to H-NMR spectrum, the trimeric structure of polymer is the simplest form of the electropolymerization product. It means that hexamer, nonamer, and etc. maybe were produced.

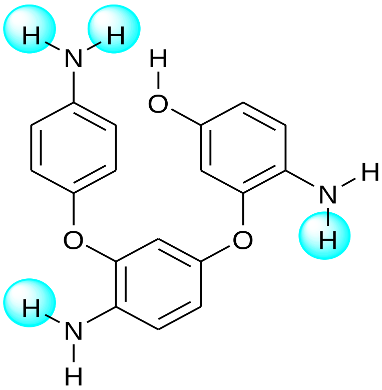

Fig. 1. the trimeric structure of polymer

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Paper code: 476

Supported molybdenum schiff base derivated from 2-aminopyridine on oxidized cellulose: synthesis, characterization, and catalytic application

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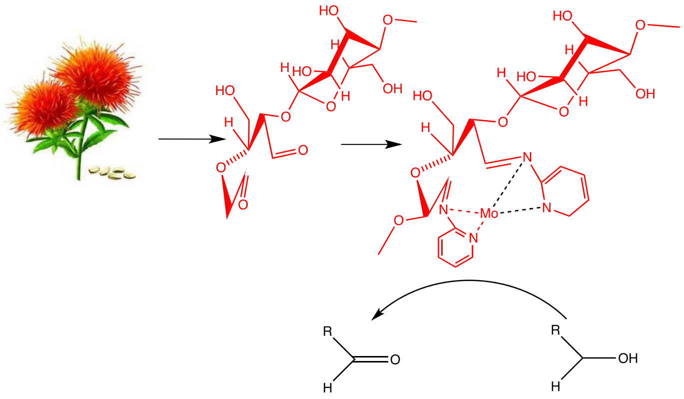
Among the natural material, cellulose is the most abundant biopolymer on Earth providing mechanical strength to plants. It has been used by humans for thousands of years as paper and textiles. Recently, the functionality of cellulose has been increased by hybridization with different materials such as different ligands and nanoparticles which it has drawn much interest in the fields of flexible electronics, biosensors, and drug delivery applications. In these micro hybrid materials, cellulose acts as an ubiquitous and biofriendly substrate for these modern applications [1-2].
Molybdenum schiff-base complex are every important material for using in medicinal inorganic chemistry due to their diverse biological and pharmacological antitumor activities. Also, schiff-bases have gained much importance in biomimetic modeling applications and designing molecular. Schiff bases are used as catalysts, intermediates in organic synthesis, dyes, pigments, polymer stabilizers, and corrosion inhibitors [3].
Herein, micro cellulose was extracted from *Carthamus tinctorius* and oxidized by sodium periodate. Molybdenum schiff base complex derivated from 2-amino pyridine was immobilized on this natural biopolymer. The catalytic properties of it were considered as a heterogeneous catalyst in the oxidation of organic compounds such as alcohols.



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Paper code: 478

Comparison of DSC curves Copolymerization of vinyl acetate- butyl acrylate with different initiators

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In this study, the DSC (Differential scanning calorimetry) curves of copolymerization of vinyl acetate- butyl acrylate in the presence of different initiators investigated. A vinyl acetate- butyl acrylate Copolymer was prepared by aqueous emulsion polymerization which contained 57 to 43 % of monomers in the presence of anionic surfactants and Potassium Persulfate (KPS), Ammonium Persulfate (APS) and AIBN initiators at 65 ° C and at 3 hours. Results show that the Tg value in different initiators are similar (Fig. 1) and copolymerization has taken place between vinyl acetate and butyl acrylate. Therefore, it is possible to use any of the initiators in this type of emulsion copolymerization.

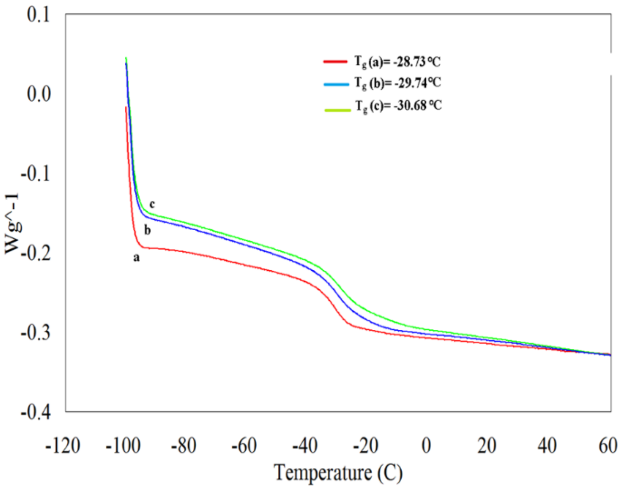

Fig. 1 DSC curves of optimized copolymer (VAc/BuA) with different initiators KPS, (b) AIBN, (C) APS.

Paper code: 480

Biological Surfactants, use in Iran, distance to global use

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Risks or negative effects of chemical surfactants has led to the creation of lower risk surfactants. Biological surfactants have been considered in this issue. These surfactants are classified in two general categories with high molecular weight and low molecular weight. Glycolipids, Fatty acids, Lipopeptides and lipoproteins are the most important low molecular weight biosurfactants and on the other hand Polymeric biosurfactants and Particulate biosurfactants are studied in a group of high molecular weight biosurfactants. In recent years significant progress have been reported in supplying and consuming products with these category of molecules. Europe, North America and Asia-Pacific respectively have had the most developments in this context. Iran Despite the progress made in the chemical surfactant industry, has not yet been able to take an effective step in the field of biological surfactants, somehow that the use of these surfactants in Iran is less than 1 percent.

Fig. 1 Global biosurfactant market share by region,2024 (value%)

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Paper code: 487

Using metal based electrochemical biosensors with nano-porous surfaces to identify phenol and phenolic compounds

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In the past few years, scientists have been looking for simple, low-cost, and rapid methods to identify and remove pollutants, including phenol and their derivatives. The electrochemical biosensors are the most widely used group of biosensors and have been the subject of fundamental research in the last few years, attention was paid to fast online capability, sensitivity, repeatability, and reliability.

The purpose of this project increase the sensitivity of phenol electrode / phenol compounds by using similar methods for the metal based electrochemical such as copper, nickel, molybdenum, and etc.

In these electrodes, nano-porous surfaces (such as nanosilicon) are used with bioreceptors such as enzymes or non-enzymes these are fixed to the surface of an electrochemical transducer by various methods such as adsorption or trapping.

In these electrochemical biosensors, the bioactive layer should be chosen in such a way as to allow to detect phenol and phenolic compounds such as bisphenol with sensitivity, high selectivity, excellent repeatability , stability and appropriate detection limit.

advanced electrochemical techniques such as rotating ring-disk voltammetry, square wave voltammetry, and pulsed differential pulse (AC or DC) have been used to produce these compound electrodes. Accordingly, in order to detect and extract these compounds, optimal experimental conditions was achieved using the chronopotentiometric or chronoamperometric techniques. The surface morphology of the modified electrode was studied by atomic force microscope (AFM) and field-emission scanning electron microscopy (FE-SEM). The phenol biosensor exhibited a wide sensing linear range from 5×10^{-8} M to 5×10^{-5} M, a lower detection limit of $3 \times 10-8$ M. The fabricated TYR/GO-COOH /GCE biosensor showd very good stability, reproducibility, sensitivity and practical usage.

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Paper code: 489

A facile and green sonochemical route for the synthesis of $CuWO_4$ nanostructure

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In this research, $CuWO_4$ nanostructure was synthesized by weak ultrasonic irradiation method at 80ºC and DI water. Sonochemistry is the research area in which molecules undergo a chemical reaction due to the application of ultrasound radiation. The physical phenomenon is responsible for the sonochemical process is acoustic cavitation [1]. In this work, we used sonochemical method which is an effective, useful, lowcost and a simple technique but it has not been used to synthesize this compound until now. $CuWO_4$ is a promising candidate for supercapacitor applications [2-3]. $Cu(NO_3)_2.3H_2O$ and $Na_2WO_4.2H_2O$ were used as reagents and the resulting precursor was calcinated at 500ºC for 2h in furnace. The product was characterized using fourier transform infrared (FT-IR), X-ray powder diffraction (XRD) and scanning electron microscopy (SEM).

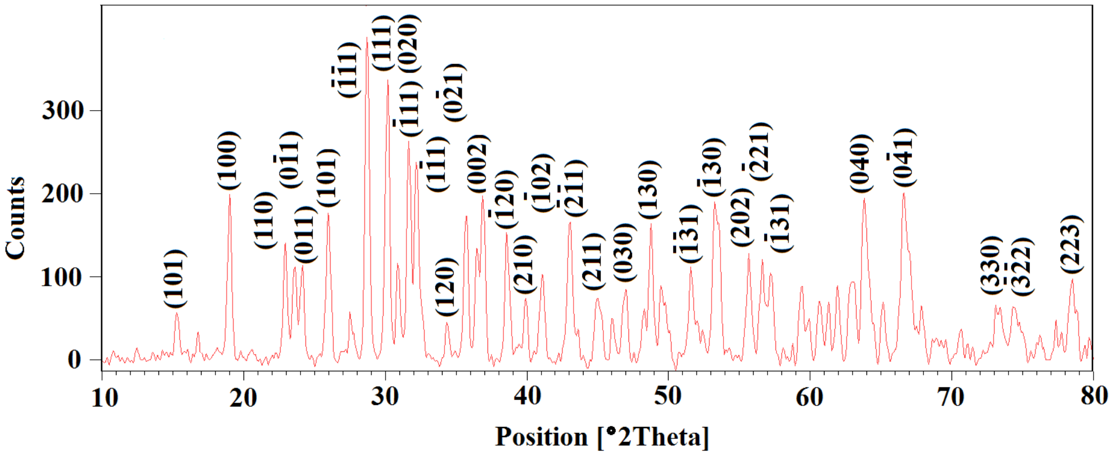

Fig. 1 XRD pattern of $CuWO_4$ nanostructure.

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Paper code: 490

A facile and green route for the preparation of $ZnWO_4$ nanoparticles

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Metal tungstates are important inorganic materials and have potential applications in some fields, such as photocatalysis, light-emitting diodes (LEDs), optical temperature sensors and cathode materials for supercapacitors [1-2]. In this research, $ZnWO_4$ nanoprticles were synthesized successfully by the reaction of $Zn(NO_3)_2.6H_2O$ and $Na_2WO_4.2H_2O$ in ultrasound bath without using any additives. The physical phenomenon is responsible for the sonochemical process is acoustic cavitation. Sonochemistry is the research area in which molecules undergo a chemical reaction due to the application of ultrasound radiation [3]. Sonochemical route is an effective, useful, lowcost and a simple method which we used for the preparation of $ZnWO_4$ nanoprticles. There is no report about the synthesis of $ZnWO_4$ nanoprticles by sonochemical process so far. The result nanoparticles were characterized using fourier transform infrared (FT-IR), X-ray powder diffraction (XRD) and scanning electron microscopy (SEM).

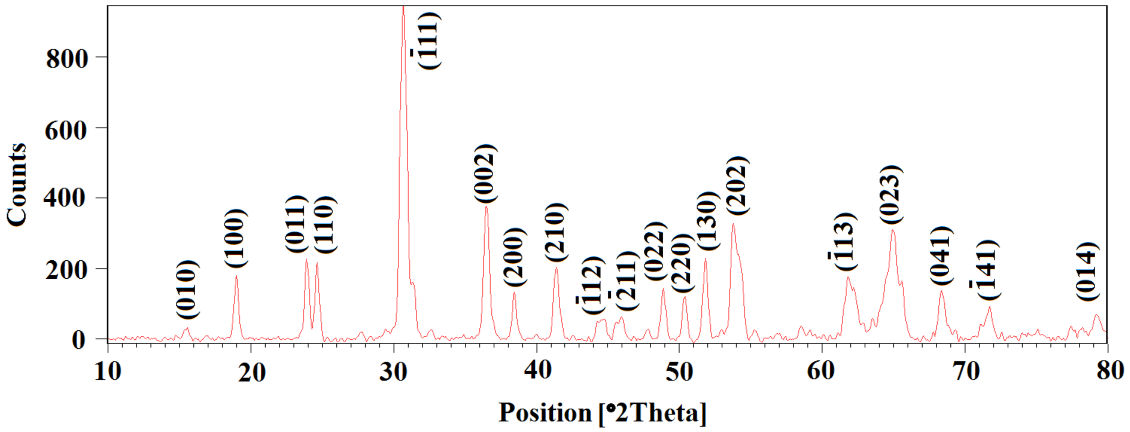

Fig. 1 XRD pattern of $ZnWO_4$ nanoparticles.

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Paper code: 499

TiO_2@ graphene quantum dots nanocomposite as an efficient photocatalyst for degradation of RB5 under sunlight irradiation

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Herein, we report the facile fabrication of graphene quantum dots (GQDs) ,TiO_2 NPs, and TiO_2@GQDs nanocomposite. TiO_2NPs with the average particle size of 8 nm, band gap of 2.45 eV, and specific surface area of 236 m^2 g^{-1} and TiO_2/GQDs nanocomposite with the average particle size of 15.60 nm and band gap of 2.23 eV were prepared by one-pot hydrothermal method. The GQDs with the average particle size of 20 nm were prepared via one-step pyrolysis of citric acid. The photocatalytic activity of TiO_2@GQDs nanocomposite was evaluated by the photodegradation of an azo dye, Reactive Black 5 (RB5) under sunlight irradiation and compared with that of TiO_2NPs, P25, and GQDs. The results showed that the complete (100.00%) photocatalytic degradation of RB5 dye was achieved by TiO_2@GQDs nanocomposite compared with that of TiO_2NPs (99.98 %), P25 (91.16 %), and GQDs (1.55 %) (Fig. 1). The photocatalytic degradation mechanism of RB5 by TiO_2 NPs was evaluated through the addition of 20 mM of different scavengers to the solution. The results showed that $OH^{\cdot}_{ads}$is the main oxidant in the photodegradation of RB5.

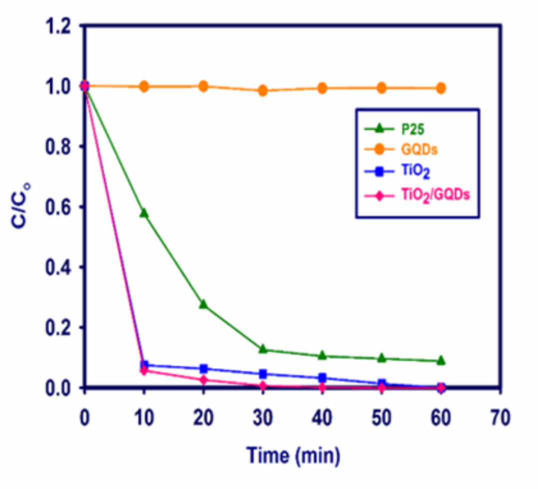

Fig. 1 Comparative studies on photocatalytic activity for P25, TiO_2 NPs, GQDs and TiO_2/GQDs against RB5 azo dye (50 ppm of dye, pH 2, dose of catalyst = 0.8 g L^{-1},

Paper code: 509

Interaction of NO gas with P-doped BNNTs: A DFT study

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Past years research demonstrated that electronic and structural properties of BNNTs can be significantly influenced by dopant atom and adsorbent [1–2]. Up to now, doping BNNTs with different types of atoms is believed to be an effective way to increase the adsorption of different compounds [3–4]. The aims of this project are to study the structural, electrical, quantum parameters, DOS, NBO, RDG and NMR parameters of the adsorption nitrogen monoxide gas on the outer and inner surface of pristine and P-doped boron nitride nanotube at different configuration models by using DFT methods at cam-B3LYP/6-31G (d, P). The calculated results indicate that adsorption NO gas on the exterior surface p-doped model are more exothermic and more favourable than pristine models. The NMR and DOS results denote that the adsorption of NO gas alter the structural, electrical and optical parameters of nanotube. With using the reduced density gradient (RDG) and atom in molecule (AIM) results, we find the nature of the bond between NO gas and BNNTs is Van der Waals type. Inspection of the quantum parameters and natural bond orbital (NBO) results reveal that the P-doped BNNTs is a good candidate to detect and adsorb NO gas.

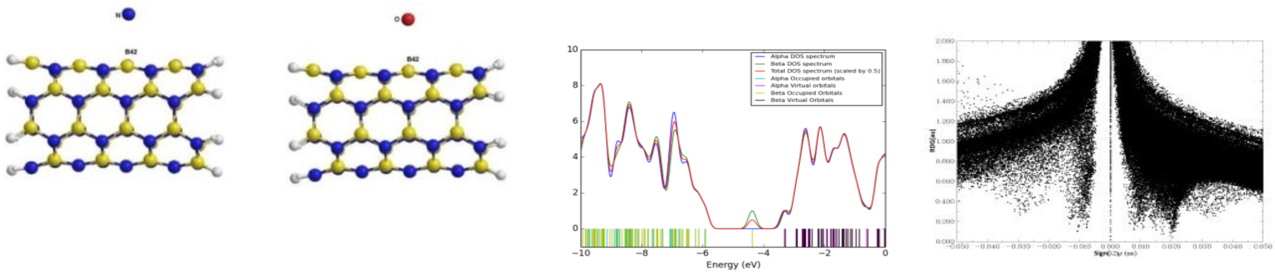

Fig. 1 The DOS, RDG and structure of optimized for NO adsorption on P-doped BNNTs.

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Paper code: 511

Solar/visible photocatalytic degradation kinetics and mechanism of RB5 dye by g-C_3N_4 nanosheets

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The photodegradation of an azo dye, Reactive Black 5 (RB5), as a model pollutant by graphitic carbon nitride, g-C_3N_4 nanosheets under visible and solar light irradiations was evaluated. The g-C_3N_4 nanosheets with the band gap of 2.7 eV was prepared by via the thermal condensation of urea. The photodegradation of RB5 dye by prepared g-C_3N_4 nanosheets was performed under different conditions including photocatalyst loading, pH, initial dye concentration, and irradiation source (Xe lamp and sunlight). Fig. 1 shows the influence of pH (3.4-9.0) on the degradation efficiency of RB5 by g-C_3N_4 nanosheets at 25 °C under 90 min sunlight irradiation. The optimum photodegradation conditions were achieved by 0.04 gL^{-1} of g-C_3N_4, 10 ppm of RB5, and pH 3.4 under sunlight irradiation.

The photocatalytic degradation of RB5 over g-C_3N_4 nanosheets under sunlight light irradiation followed the pseudo-first-order kinetics with the rate coefficient of 0.0058 s^{-1}. To elucidate which of the active species has a major role in the photodegradation of RB5 dye by g-C_3N_4 nanosheets under visible light irradiation, different radical scavengers with the same concentration of 60 mM were used. It was found that the influence of superoxide radical is the most important.

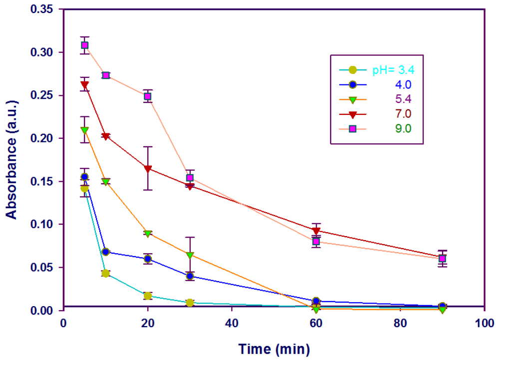

Fig. 1 Effect of solution pH on the degradation of RB5 dye by g-C_3N_4 nanosheets. (90 min sunlight irradiation, dose of photocatalyst = 0.05 g L^{-1}, 20 ppm RB5).

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Paper code: 515

Walnut Bloom Powder as a novel green sorbent for cationic dyes removal: Equilibrium, Kinetic, and Thermodynamic Studies

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3,7-bis(Dimethylamino)-phenothiazin-5-ium chloride or Methylene Blue (MB) is a heterocyclic aromatic compound, widely used in a range of different fields, especially in textile industry [1]. Most of the dyes like MB or their metabolites are toxic and some of them are considered carcinogenic for human health [2]. Therefore, it is important to treat the dye wastewater before releasing it into the groundwater [3]. In this study for the first time, Walnut Bloom (WNB) powder was used as a natural and economic sorbent for the removal of MB from aqueous solutions. This new biosorbent was characterized by scanning electron microscopy (SEM), x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and elemental EDX. The influence of various parameters such as initial dye concentration, contact time, pH temperature, and dosage of biosorbent on the remove efficiency was investigated in batch experiments. Under the optimum condition, the removal percentages achieved ~92%. In addition to Kinetics, equilibrium, and thermodynamics studies was investigated and equilibrium data and adsorption isotherms fitted well with the Langmuir model with maximum monolayer adsorption capacity of 46 mg/g. Kinetic data can be well fitted by the pseudo-second-order model, indicating a chemical adsorption. Thermodynamic data indicated that the adsorption was spontaneous, exothermic, and favorable at room temperature.

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Paper code: 516

Using ZnO-Al_2O_3 ceramic nanofibers and graphene oxide to simultaneously detect catechol and hydroquinone

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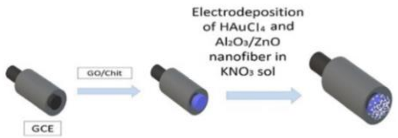
Catechol and hydroquinone are two isomers of phenolics, which are widely used in various industries such as textiles, paints, plastics, oil refineries, cosmetics, pesticides, pharmaceuticals [1]. They are highly toxic to human health [2] and have been considered as well as environmental pollutants even at very low concentrations by Environmental Protection Agency and the European Union [3]. A novel voltammetric sensor based on ZnO-Al_2O_3 ceramic nanofibers and gold nanoparticles was used for simultaneous determination of catechol and hydroquinone. Ceramic nanofibers were electrodeposited onto the mixture of graphene oxide and chitosan simultaneously with gold nanoparticle electrode-position (scheme 1). The morphology and the structure of ceramic nanofibers were characterized by Field Emission Scanning Electron Microscopy, and Fourier transform infrared spectroscopy; these techniques confirmed the presence of ZnO-Al_2O_3 ceramic nanofibers on the electrode surface. The porous structures can be used for the simultaneous detection of isomers due to their satisfied results in concurrent analytes determination; then the porosity of ZnO-Al_2O_3 ceramic nanofibers was determined using Brunauer–Emmett–Teller (BET) test. The sensor has been applied for simultaneous determination of catechol and hydroquinone which indicated good results. The limit of detection and linear ranges are obtained 3.1 and 0.5 to 40 µM for catechol respectively. For hydroquinone, there are two linear ranges, 0.13 to 1 µM and 1.5 to 56.6 µM, and two limits of detection, 0.19 and 15.0 µM respectively. For catechol, the amounts of α and ks were 0.43 and 1.12 1/s, respectively and for catechol, they were 0.35 and 0.41 1/s, respectively. The sensor storage stability was investigated and the results showed that the electrode lost about 6.9% and 8.7% for catechol and hydroquinone of its first response after 1 week, respectively.



Scheme 1. Modification of glassy carbon electrode using ZnO-Al_2O_3 ceramic nanofibers and graphene oxide

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Paper code: 527

Green synthesis of Ag nanoparticles on Fe_3O_4/HZSM-5 and its evaluation as a catalyst for reduction of organic pollutants

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Nowadays, zeolites such as HZSM-5 and natrolite have interested a considerable attention as beneficial supports and catalysts because of their high surface area, catalytic activity, thermal stability and unique cellular structural with uniform pores and channels [1]. Also, magnetic Fe_3O_4 nanoparticles and its nanocomposits have recently been gained extensive interests because of their wide use as efficient catalysts in many chemical reactions and their convenient separation from the reaction media by an easy magnetic separation [2]. Hence, combination of zeolite and Fe_3O_4 can be used for the preparation of efficient composite as a novel and unique support.

In this work, HZSM-5 and its Ag or Fe_3O_4 nanocomposites were synthesized by simple and eco-friendly method using leaf extract of *J. regia* and characterized by FT-IR, XRD, FE-SEM, EDS, BET and VSM. Reduction of Ag^+ ions and stabilization of resulted Ag nanoparticles on the surface of support are the role of plant extract. According to the FE-SEM images of nanocomposites, the average size of nanoparticles on the support surfaces was below 70 nm. The prepared nanocomposites as active catalysts were used in the catalytic reduction of organic dyes at room temperature.

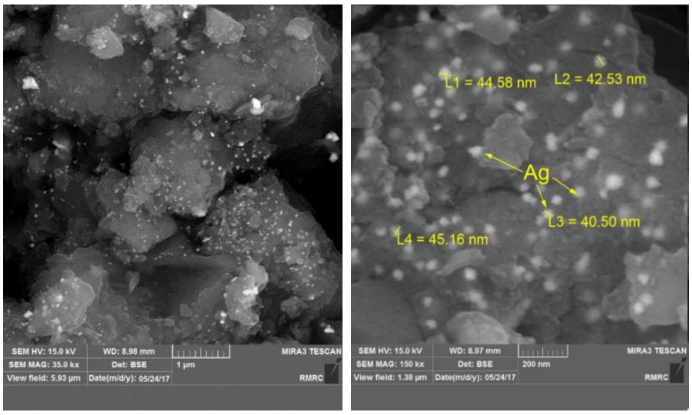

Fig. 1 **.** FESEM images of Ag/Fe_3O_4/HZSM-5 nanocomposite.

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Paper code: 528

Immobilization of Ag nanoparticles on porous carbon prepared via carbonization of red water using *Caesalpinia gilliesii* flower extract

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In recent years, carbon materials have obtained from carbonization or pyrolysis of agricultural waste products followed by chemical activation using dehydrating agents and physical activation in the presence of such as air, steam or carbon dioxide as oxidizing gases [1]. Because of singular structure, improved accessibility of active sites for reactants and appropriate electronic conductivity of carbon structures, these materials have been used as catalyst, support and adsorbents for gases or metal species.

Immobilization of metal nanoparticles on the surface of inorganic supports decreases agglomeration of nanoparticles which leads to more stability and higher reactivity of supported nanoparticles [2].

In this work, a carcinogenic waste product in the industrial unit of 2,4,6-trinitrotluene (TNT) production was converted to a stable support. The facile preparation of porous carbon and its Fe_3O_4 nanocomposite were performed by carbonization of red water and co-precipitation technique, respectively. Then, the flower extract of *C. gilliesii* was used for reduction of Ag^+ ions and stabilization of the preparead Ag nanoparticles on the surface of porous carbon and C/Fe_3O_4 nanocomposite. The as-prepared carbon nanocomposites were characterized by different methods and showed good activity in the reduction of methyl orange and 4-nitrophenol as toxic organic compounds.

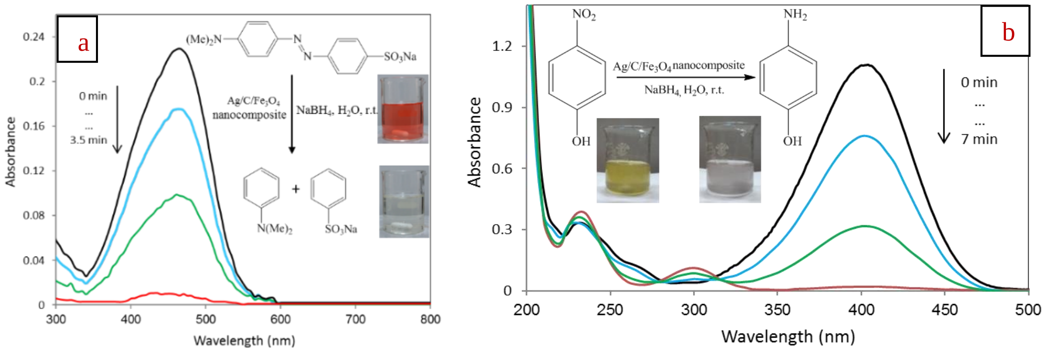

Fig. 1 **.** UV-Vis spectra of catalytic reduction of MO (a) and 4-NP (b).

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Paper code: 530

Synthesis of $SrZrO_3$ nanocomposites and their Photocatalytic property under visible light

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Nanocomposite $SrZrO_3$ were synthesized by hydrothermal method using Zirconium(IV) propoxide solution 70%wt in 1-propanol as Zr source, $Sr(Ac)_2$ as Sr source [1]. The photocatalysts was characterized by different techniques such as X-ray diffraction, Field Emission Scanning Electron Microscopy, and UV-visible diffuse reflectance spectroscopy (UV-Visible DRS). Characterization data reveal the formation of nanocrystalline $SrZnO_3$ perovskite-like composition with improved physical properties, possibly due to lower synthesis temperature used [2]. The photocatalytic properties of $SrZnO_3$ were investigated under sunlight irradiation, and $SrZnO_3$ shows higher photocatalytic efficiency than $ZnZrO_3$ for Congo Red and Rhodamine B degradation.

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Paper code: 531

Investigation on Synthesis, Characterization and Photo catalytic properties of nano Composite Perovskites $SrTiO_3$ /Zn_2TiO_4 for degradation of Congo Red

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The perovskite phase formation of nanoparticle powder of strontium titanate / Zinc Titanium Oxide was investigated. Nanopowder of $SrTiO_3$ /Zn_2TiO_4 was synthesized by hydrothermal method using the NaOH mineralizer [1]. The structure, phase formation and morphology of nanocomposite powder characterized using the X-ray diffraction technique (XRD), Fourier transformation infrared (FT-IR) spectroscopy, Energy-dispersive X-ray spectroscopy (EDX), Scanning Electron Microscope (SEM). Our results indicated that, the phase structure of the $SrTiO_3$ /Zn_2TiO_4 nanoparticles is in cubic perovskite phase. The photocatalytic activity of $SrTiO_3$ /Zn_2TiO_4 was evaluated by performing photodegradation of congo Red dye under sunlight irradiation. This study indicates the potential use of high aspect ratio (96%) $SrTiO_3$ /Zn_2TiO_4 nanoparticle for removal of congo Red pollutions [2].

References

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Paper code: 537

Morphological studies of LDPE prepared using pyridine-imine based catalysts: Effect of catalyst bulkiness and metal

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Polyethylene with special morphology, such as spherical morphology, as a raw material is interesting from industrial point of view, because it allows easy processing. Besides thermal and physical properties of polyethylene, the size and shape of polyethylene particles are considered as important features of this widely used product. Based on this, a series of pyridine-imine [N-N] ligands were efficiently prepared through the condensation reaction of ketone precursor and synthesized aniline. The ligands (L_n, n=1-3) and corresponding nickel complexes (C_n, n=1-3) were characterized and used for polymerization of ethylene in the presence of modified methylaluminoxane (MMAO) as cocatalyst. The SEM images were used to monitor the influence of different bulky ligands and metals on structural morphology of the products. A uniform morphology is observed for all polyethylene samples prepared at the polymerization temperature of 0 ^{o}C. The observed morphologies were globular clump for the polyethylene obtained in the presence of the $\mathbf{C_1}$ catalyst to sphangum moss for the $\mathbf{C_2}$ catalyst. It can also be mentioned that, with replacing of iron metal to the active center of the catalyst, the specific morphology of the polyethylene particle for $\mathbf{C_3}$ catalyst is changed to the rock-shape and single population of crystalline phase in the DSC trace was seen. However, the DSC curve of the obtained polyethylene using C_1 and C_2 showed two broad peaks, which could be attributed to clumped structure in morphology of the products shown in Figure 1.

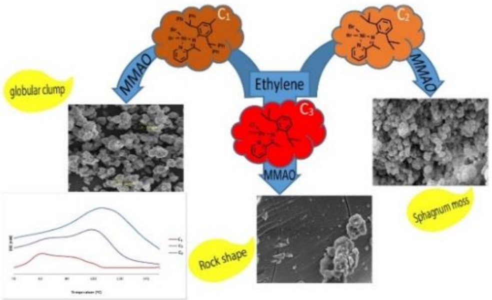

Fig. 1 SEM images of the polyethylenes produced using pyridine-imine based catalysts.

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Paper code: 538

Beneficial influence of MWCNT on the pyridine-imine catalyzed ethylene polymerization: effect of type, content and technique

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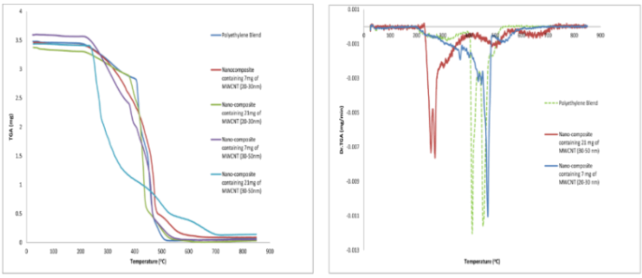
A series of low-density polyethylene (LDPE)/nano-composites containing different content and type of MWCNTs were prepared by *in-situ* polymerization and solvent evaporation techniques, and analyzed by differential scanning calorimeter, FT-IR, SEM and TGA to investigate the thermal, structural, morphological and thermal stability of the resultant nano-composites compared to the sample obtained by 50:50 molar ratio of Ni: Fe catalysts combination at the same condition in presence of MWCNT. Overall activity of these catalysts reduced (from 7.50×10^4 to at least 0.66×10^4 g of PE. mol $(Fe+Ni)^{-1}$. hr^{-1}). The produced LDPE/nano-composites were showed the lowest melting point as well as crystallinity in presence of MWCNT (30-50 nm). Whereas, the resultant sample in presence of MWCNT (20-30 nm) exhibited the lower vinyl content (0.12) than the neat polyethylene blend. Based on this analysis, the branch extent varied from 11.55 to 70.81 CH_3 branch per 1000 carbon atoms. The sample prepared by 10.50% of MWCNT (30-50 nm) were exhibited the highest onset and endset degradation temperature (217.74 and 708.71 ^oC, respectively). However, addition 2.33% of MWCNT (20-30 nm) improved the overall thermal stability of the neat polyethylene blend up to 400 ^oC. Almost, an irregular shape of morphologies was seen for the obtained samples. The samples prepared by in-situ polymerization were shown distinct shape of morphology as well as two peak of melting point in SEM images and DSC traces, respectively.



a b

Fig. 1 Thermogravimetric and differential thermogravimetric curves of the neat polyethylene blend and LDPE/nano-composites prepared by *in-situ* polymerization.

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Paper code: 546

Catalytic activity of cyclopalladated complexes derived from benzo[h]quinolinate and diphosphine ligands

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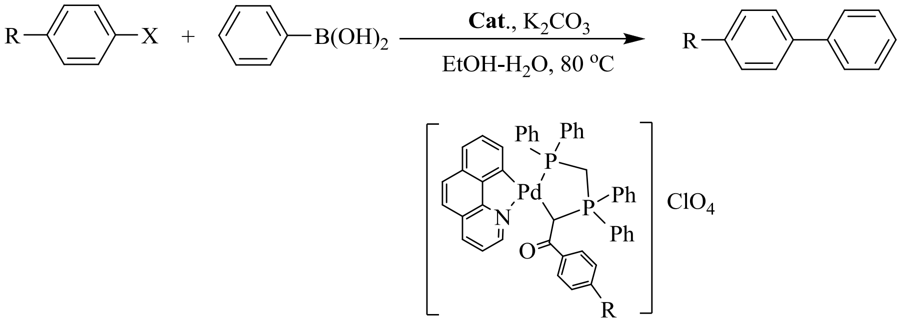
Biaryl compounds are versatile building blocks in the field of pharmaceuticals, herbicides, polymers, liquid crystals, natural products, ligands for catalysis, and advanced materials. The Suzuki-Miyaura cross-coupling reaction catalyzed by palladium complexes is one of the most important methods for the preparation of biaryls in organic synthesis [1-3]. The use of phosphines as ligands in the Pd-catalyzed Suzuki reaction provides an efficient route to the synthesis of substituted biphenyl through cross-coupling reaction of aryl halides with arylboronic acid. In the case of less reactive aryl bromides and aryl chlorides usually, electron-rich bulky tertiary phosphines are used as ligands. Here, we would like to report the simple mononuclear cyclopalladated benzo[h]quinolinate complexes with bidentate phosphine ligands, namely, $[Pd(bzq)((Ph_2PCH_2PPh_2C(H)C(O)PhR)]ClO_4$ (R = Cl ($\mathbf{C^1}$), Br ($\mathbf{C^2}$) NO_2 ($\mathbf{C^3}$) OCH_3 ($\mathbf{C^4}$) that act as an effective homogeneous pre-catalysts for Suzuki-Miyaura reaction of aryl iodides and bromides with phenylboronic acid in aqueous solution. Highly yields of corresponding product, low catalyst loadings and short reaction times are important features of these homogeneous reactions.



Cat: R = Cl ($\mathbf{C^1}$), Br ($\mathbf{C^2}$), NO2 ($\mathbf{C^3}$), OCH3 ($\mathbf{C^4}$)

Fig. 1 Suzuki cross-coupling reactions of aryl iodides and bromides with phenylboronic acid in catalytic amount of Pd complex.

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Paper code: 554

Water Vapor Removal from Gas Streams Using Nano-Structured Zeolites

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Natural gas is considered as a mixture of methane, as main component, and other gases. The presence of these gases in natural gas and others could make difficulties in their utilization in various fields such as electricity generation, vehicle fuels and energy resources. H_2O as an important impurity would cause hydrate formation and pipeline and equipment blockage as well as corrosion in the presence of acidic gases like H_2S and CO_2 [1]. There have been many reports on the investigation of dehydration of gas streams through different methods. In this regards, using adsorbents with high dehydration capacity is a promising idea. Zeolites as a key group of molecular sieves with high surface area, thermal and chemical stability and being low-cost sorbents beseem appropriate candidates [2]. To the best of our knowledge, there was not any report on evaluating the ability of nanostructured zeolite 4A in water removal from gas mixtures including methane. In this study, zeolite 4A was synthesized via hydrothermal route. The zeolitic gel underwent ageing stage during different times. Then, the milky gel was transferred into a stainless steel autoclave and put into an oven at 100˚C for certain time. The final white powder was washed with deionized water, dried and characterized using X-ray diffraction pattern (XRD) and scanning electron microscopy (SEM) techniques. As shown in Fig. 1, the cubic morphology has been obtained for the zeolite LTA crystals. Moreover, an adsorption set-up comprising a gas mixture cylinder, sorbent reactor and a humidity analyzer has been designed. It is a novel idea to gain outstanding dehydration results due to the hydrophilic nature and small particle size of as-synthesized zeolites.

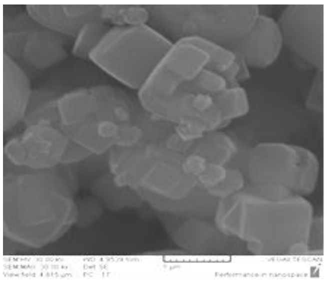

Fig. 1 SEM image of as-synthesized zeolite 4A.

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Paper code: 558

Water Harvesting from Air Using Nano-composites

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Recently, the World Economic Forum has addressed the water rarity as the greatest global risk in the near future. Among water sources distributed across the earth, only ca. 1.2% of all fresh waters (2.5%) is surface waters which 3% of its amount is present in the atmosphere. So, it seems to be necessary to investigate the novel strategies for supplying fresh water from atmosphere. In this way, appropriate adsorbents with good structural quality such as high surface area, porous framework, and high water uptake performance play incredible role [1]. Amongst various adsorbents, zeolites are well-known solids with intrinsic hydrophilic feature depended on their Si to Al ratios [2]. The aim of this study is to investigate the adsorption ability of FAU zeolite framework for water vapor adsorption from air. At First, the composite of commercial granular FAU zeolite with $CaCl_2.4H_2O$ was provided by an impregnation method. ICP elemental analysis was carried out to measure Ca^{2+} content in the pores of the zeolite; it was calculated 0.873 ppm. In addition, zeolite 13X powder was synthesized hydrothermally and its physicochemical properties were determined using different techniques such as FT-IR, XRD and SEM. The calcium-exchange process was also fulfilled for the sample the same as before. Fig.1 shows the FT-IR spectra of both commercial and synthetic zeolites. To assess the water harvesting tests from air, an adsorption set-up including a sorbent reactor, humidity analyzer and a wet air cylinder has been designed. According to the high water sorption capacity of the composite, it could be a promising idea to gain fresh water from air even at low relative humidity using the proposed adsorbent.

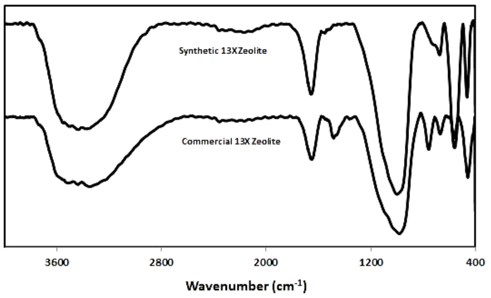

Fig.1. FT- IR spectra of commercial and synthetic zeolite 13X

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Paper code: 563

Benzimidazole based porous organic polymer: synthesis and characterization

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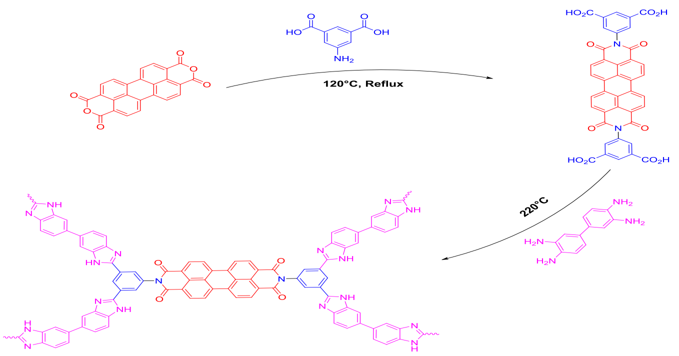
Nowadays porous structures and materials gained much attentions due to their wide variety of applications. Benzimidazole based organic polymers are a class of porous organic structures which made up of covalent bonds with mostly common elements such as carbon and nitrogen. Their high surface area and high porosity made them good choices for usage in the fields of catalysis and gas storage [1], [2]. Herein, synthesis of a novel benzimidazole based polymer were explained. Briefly, the tetraacid monomer of the desired structure was produced by known amount of perylene-3,4,9,10-tetracarboxylic dianhydride and calculated amount of 5-aminoisophthalic acid using the imidazole as the solvent under reflux condition for 6 hours (Scheme 1). Then the participated was filtered and washed several times with ethanol and for polymer synthesis, it was heated at 180 ˚C for 5 hours in the presence of diaminobenzidine in polyphosphoric as the solvent, finally, that the reaction was completed at 220 ˚C for 24 hours. The resulting red powder were washed with sodium bicarbonate. The structure of monomer and polymer was confirmed by Fourier transform-infrared spectroscopy, elemental analysis, X-ray diffraction, field emission scanning electron microscopy (FE-SEM), and thermogravimetric analysis. TGA of the synthesized polymer showed good thermal stability and FE-SEM images proof the good porosity of this novel structure.



Scheme.1 synthesis of benzimidazole based monomer and porous organic polymer.

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Paper code: 565

A phenobarbital molecularly imprinted polymer electrochemical sensor based upon a polyaniline/graphene oxide nanocomposite

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Molecular imprinting technology is a rapidly developing technique for the preparation of polymers having specific molecular recognition properties for a given compound, its analogues or for a single enantiomer. A variety of applications of molecularly imprinted polymers (MIPs) have been already investigated. Preparation of artificial antibodies, using in solid-phase extraction process, application as chromatographic stationary phases, and fabricating of selective electrochemical sensors are among these applications [1].

Phenobarbital (PB) is one of the oldest known anticonvulsant [2]. Selective determination of this compound is important because its toxic effects [3]. Furthermore, the concentration of PB in blood is critical and must be accurately controlled. The possibility of metabolization of PB in the liver is a menace for human health.

This communication intends to report the preparation of an electrochemical sensor based upon a MIP fabricated by polyaniline/graphene oxide nanocomposite. This composite was characterized by field emission scanning electron microscopy (FESEM), electron diffraction X-ray (EDX) and thermal gravimetric analysis (TGA). The prepared MIP was used for modification of carbon paste electrodes to fabricate a selective PB electrochemical sensor. Electrochemical behavior of PB on the investigated sensor and the optimization of the parameters affecting the PB determination with respect to the aqueous solution conditions and the electrode composition, were followed by cyclic voltammetry (CV). The obtained cyclic voltammograms of PB, showed a peak at about 0.2 V *vs.* saturated calomel electrode. It was shown that the anodic peak current increased linearly with PB concentration in the range of 10-100 (R^2 = 0.98) μg/L with the corresponding RSD 1.40% (for a solution of ٤٠ μg/L) and 0.٦% (for a solution of 100 μg/L), respectively. The selectivity of the proposed sensor was tested by determination of PB in the presence of relative barbiturate compounds. The developed electrode was applied for determination of PB in some real samples.

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Paper code: 578

Effect of coupling agent (malic anhydride) on polypropylene compound

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"Polypropylene (PP) is one of the most important plastics as it has an excellent balance of mechanical properties such as, melt flow, color stability, chemical residence and moisture barrier properties together with low cost" [1]. Polypropylene was reinforced with a talc ($Mg_3Si_4O_{10}(OH)_2$) additive and following to addition of a coupling agent to improve its impact strength and reduction of the price. "Talc represents one of the most useful mineral fillers which are compatible with polypropylene" [2]. Mechanical properties such as impact strength was also investigated. Due to the optimal of mechanical properties obtain, PP(90%)+Talc(10%) compound, the compound were selected, which shows a 50% drop in impact strength compared to the polypropylene itself. An optimal percentage (3%) of the malic anhydride was added to the PP (90%) + Talc (10%) compound as a coupling agent, which shows an increases (18%) in impact strength compared to the polypropylene and (100%) increases compared to PP (90%) + Talc (10%) compound (Figure 1).

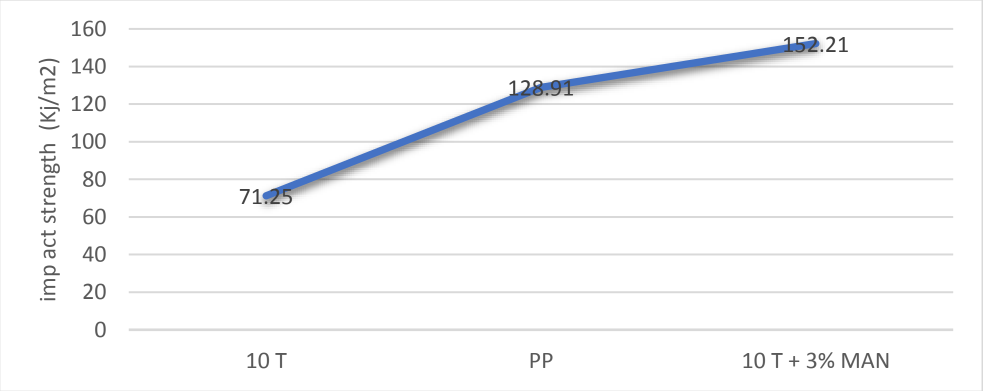

Figure 1. The effect of coupling agent on pp compound.

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Paper code: 602

Titanium Dioxide Nanoparticles: Synthesis and study of its modifying properties on acrylic paints

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The goal of this research was the optimization of the synthesis of TiO_2 nanoparticles (TiO_2 NPs) in order to use them in the paint industry. For this purpose, several processes were tested such as; reverse microemulsion, reaction between $TiCl_4$ and benzyl alcohol, sol gel method and reaction titanium esters with acid anhydrides [1-4]. In each method, by varying various factors such as pH, temperature, calcination time and other effective parameters, nanoparticles of titanium dioxide were produced and the conditions were optimized. The nanoparticles obtained from all syntheses were characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FT-IR). The titanium dioxide nanoparticles were used in the production of two types of industrial products; acrylic thermoplastic paints and acrylic water based semi-gloss paint. TiO_2 nanoparticles were being used in order to improve the efficiency and to provide new functionalities to the paints. The qualitative tests that were approved by the Institute of Standards & Industrial Research of Iran (ISIRI), and the industrial tests were carried out on the modified colors showed that the use of paints reinforced with nano titanium dioxide instead of paint containing titanium dioxide, had a significant effect on the improvement of the color properties. Nano titanium dioxide is used in paint to achievement two of good properties; photocatalytic activity and UV-protection. The combination of the photocatalytic effect, along with hydrophilic properties results in a paints' self-cleaning effect. The surface will no longer need regular cleaning as the water and dirt will no longer stick on it.

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Paper code: 606

Synthesis of 2,3-dihydroquinazolin-4(1*H*)-ones catalyzed by Fe_3O_4@nano-cellulose/$CuCl_2$ as a bio-based magnetic catalyst

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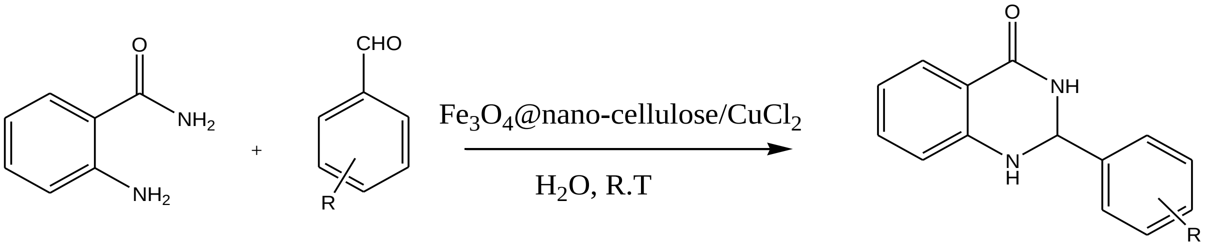
Recently biopolymers such as cellulose and starch [1-2] have been used as support for heterogeneous catalytic systems. In this context, cellulose can play a major role as a natural, biocompatible and biodegradable polymer containing free OH groups with nucleophilic character for bonding to Lewis acids. Nano-cellulose was prepared *via* partial hydrolysis of cellulose in cotton. Fe_3O_4@nano-cellulose can be obtained from reaction of $FeCl_2$ and $FeCl_3$ *via* NH_4OH in an aqueous solution of nano-cellulose in a simple procedure. Lewis acids such as $CuCl_2$ can be bound to surface OH groups in nano-cellulose for preparation of Fe_3O_4@nano-cellulose/$CuCl_2$ as a new, green, bio-based and recyclable magnetic nano catalyst. This catalyst was characterized by FT-IR, FESEM, TEM, XRF, VSM, EDX and XRD. 2,3-Dihydroquinazolin-4(1*H*)- ones are an important class of fused heterocyclic compounds which have drawn much attention because of their biological potential and pharmaceutical activities such as anti-inflammatory, antibacterial, antitumor, antimicrobial and antioxidant [3]. In this report, 2,3-dihydroquinazolin-4(1*H*)- ones can be synthesized *via* condensation of 2-aminobenzamide and aldehyde in the presence of Fe_3O_4@nano-cellulose/$CuCl_2$ in water at room temperature (Scheme 1). This protocol includes some important advantages such as short reaction times, high yields, simple methodology and easy work-up. The nano-catalyst could be recycled and reused without significant loss of its catalytic activity.



Scheme 1 Synthesis of 2,3-dihydroquinazolin-4(1H)- ones in the presence of Fe_3O_4@nano-cellulose/$CuCl_2$

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Paper code: 615

New efficient visible light photocatalyst for degradation of phenol: Nano-particle of HAP/Bi_2O_3-Ag composite

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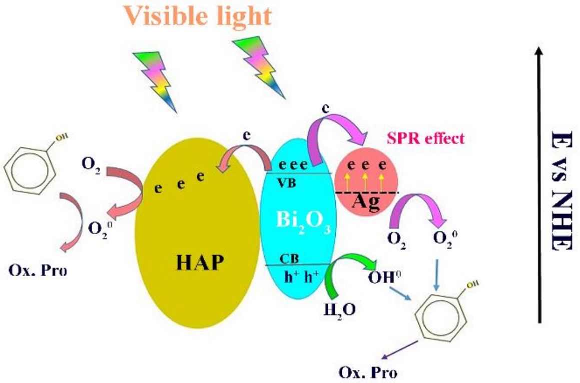
Nowadays, degradation of phenol and its derivatives was attracted due to high toxicity for human health and high stability in environment [1],[2]. In this study, we focused on preparation of new nanocomposites of hydroxyapatite (HAP) with high photocatalytic activity for degradation of phenol. In this regards, different nanocompoistes of HAP/Bi_2O_3-Ag with various mass ratios of Bi_2O_3-Ag and HAP (5:95; 10:90; 30:70; 50:50) were fabricated by simple and low cost of precipitation-hydrothermal method. The prepared nanocomposits were characterized by X-ray diffraction (XRD), FT-IR spectroscopy, and Scanning electron microscopy (SEM) equipped with Elemental analysis (EDX). The nanocomposites were used for photocatalytic degradation of phenol in aqueous solution. The prepared nanocomposites were showed higher activity than HAP and Bi_2O_3 alone. This behavior is related to hetrojunction of HAP with Bi_2O_3 semiconductor with low band gap and Ag as a plasmonic compound. The proposed mechanism of photocatalytic degradation of nanocomposite has been depicted in Scheme 1.



Scheme 1. The proposed mechanism of photocatalytic activity of prepared HAP/Bi_2O_3-Ag composite.

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Paper code: 616

Catalytic Epoxidation of Polybutadiene Rubber Using H_2O_2/CH_3COOH and Na_2WO_4

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Post-polymerization functionalization of polybutadiene and other rubbers is very interesting since it can be served to modify the properties of these rubbers. The double bonds present in the main chain of polybutadiene can be used for its functionalization and modification [1]. As one of the most well-known chemical reactions which can be performed on double bonds, epoxidation can be used to modify the properties of polybutadiene rubber. However, the yield of epoxidation of rubbers is very low for many common oxidation reagents and methods, and undesired side reactions can also occur [2]. Therefore, it is promising to develop new methods and reagents for efficient epoxidation of polybutadiene and other rubbers.

We used sodium tungestate as catalyst to improve the efficiency of epoxidation of polybutadiene rubber and increase the yield of the reaction. Polybutadiene rubber was dissolved in THF and epoxidized by H_2O_2/acetic acid as oxidant in the presence of sodium tungestate as catalyst (Fig. 1). After extraction and purification, the modified rubber was characterized instrumentally. NMR spectra confirmed epoxidation of polybutadiene rubber and no significant byproduct was detected. The results indicate that epoxidation is the main reaction performed in the mixture and no undesired side reactions occurs during the process. The epoxidation percent of the product was also calculated. It was found that the epoxide content of the product can be adjusted by controlling the experimental condition such as reactant ratios and other experimental conditions. Epoxidation was increased by increasing the amount of oxidant/catalyst system. The reaction proceeded with high yield in mild condition and epoxidized polybutadienes with high epoxidation percents up to 35% was obtained.

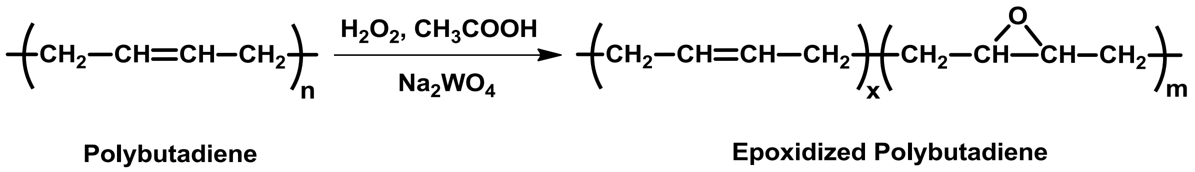

Fig. 1 Epoxidation of polybutadiene by H_2O_2/CH_3COOH in the presence of Na_2WO_4.

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Paper code: 617

Synthesis of Aldehyde-Terminated Epoxidized Liquid Polybutadiene Rubber

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Polybutadiene rubber is a synthetic elastomer with large scale applications in industry. Functionalization of polybutadiene and other polyolefins is a method to adjust their physical, chemical and mechanical properties [1]. However, preparation of functionalized polyolefins with controlled functionalities usually needs complex synthetic routs and accurate control of the reaction condition [2]. Herein, we prepared epoxide- and aldehyde-functionalized polybutadiene rubber by modification of pristine polybutadiene rubber.

Polybutadiene rubber was dissolved in THF and treated with periodic acid. Periodic acid is an oxidizing agent which first reacts with vinyl groups (double bonds) to produce epoxide rings. The resulting epoxide groups can further react with periodic acid, and aldehyde groups are formed through epoxide ring opening and subsequent chain cleavage reactions. Therefore, an aldehyde-terminated epoxidized polybutadiene rubber is obtained at the end of the reaction (Fig. 1). The structure of the product was characterized by NMR spectroscopy and the presence of epoxide and aldehyde groups were confirmed. The epoxidation percent and molecular weight of the final product were also calculated. Because of the cleavage of the polymer chain, the molecular weight of the polymer is decreased and, thus, a viscous liquid functionalized polybutadiene rubber is obtained. Aldehyde-terminated epoxidized polybutadiene rubber with controlled molecular weights and epoxidation percents could be obtained by varying the amount of oxidant and the experimental conditions. This method is also promising for functionalizing other vinyl-containing rubbers.

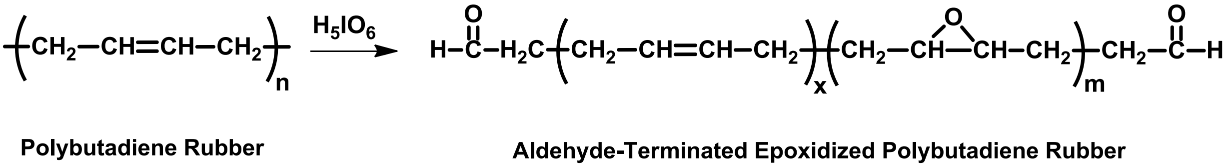

Fig. 1 Synthesis of aldehyde-terminated epoxidized polybutadiene rubber.

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Paper code: 619

A novel ligand-metal complex immobilized on magnetic graphene oxide as a magnetic nanocatalyst for the coupling reactions

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Nanoparticles are attractive candidates as solid supports for the highly active and recyclable catalytic systems. They can combine the advantages of both homogeneous and heterogeneous catalysts [1]. Superparamagnetic nanoparticles can be well dispersed in a reaction solution, providing a large surface. After the end of the reactions, the nanoparticles can be isolated efficiently from the product solution through a simple magnetic separation process [2]. Graphene oxide (GO), being an important derivative of graphene, possesses many carboxyl and hydroxyl groups, which makes it an excellent supporting matrix for growing and anchoring of nanostructured catalysts [3].

In the present study, a magnetic nanocatalyst containing a ligand for the metal ion is prepared on the surface of the graphene oxide magnetized with Fe_3O_4 as illustrated in Fig. 1. The improved Hummers' method is used to synthesize the graphene oxide from graphite powder. Then, magnetic graphene oxide (MGO) is prepared through coprecipitation of $FeCl_3{\bullet}6H_2O$ and $FeCl_2{\bullet}4H_2O$ in the presence of GO. Thereupon, MGO is functionalized with Nitrogen-containing ligand such as aminophenanthroline via amidation reaction between carboxyl groups of GO and amine group of the ligand. The latter is treated with the metal ion to generate magnetic nanocatalyst appropriate for the C–N cross-coupling of amides with aryl halides.

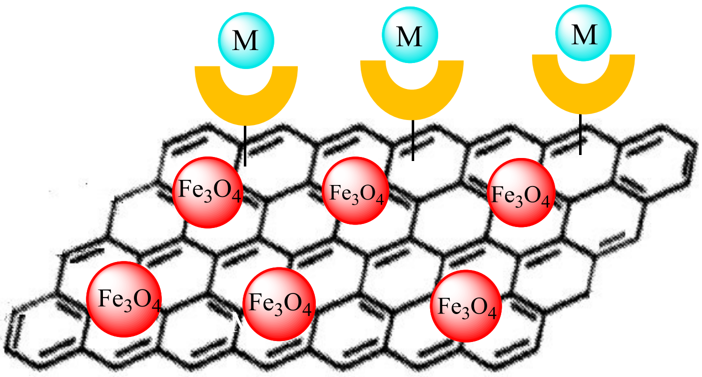

Fig. 1 Magnetic nanocatalyst based on graphene oxide

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Paper code: 622

QM study of interaction between phenolic compounds as inhibitor with active site of human carbonic anhydrase enzyme

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CO_2, bicarbonate and protons are an essential molecule and ions for many important physiologic processes occurring in all living organisms. However, the uncatalyzed rate of interconversion of such species is too slow to meet the physiological needs of most biochemical processes. This task is efficiently accomplished by the carbonic anhydrases. This superfamily of metalloenzymes possess within their active sites a highly nucleophilic metal hydroxide species, such as zinc(II), cadmium(II) or iron (II) hydroxide, depending on the class [1].

Phenol and its derivatives were reported to be a competitive inhibitor of human Carbonic Anhydrase II (hCA II). The phenolic moiety has an amphiphilic character. The presence of the hydrophobic planar aromatic ring is responsible for hydrophobic interactions (π-stacking), whereas at the same time the polar hydroxyl groups can participate in hydrogen bonding. This dual behavior allows these molecules to bind to the amino acid residues of several proteins, enzymes or receptors [2]. The inhibition mechanisms and possible structure activity relationships is presented in Figure 1. This research is going to study the mechanism of the inhibition of phenolic compounds with active form of CA (II) using DFT calculations.

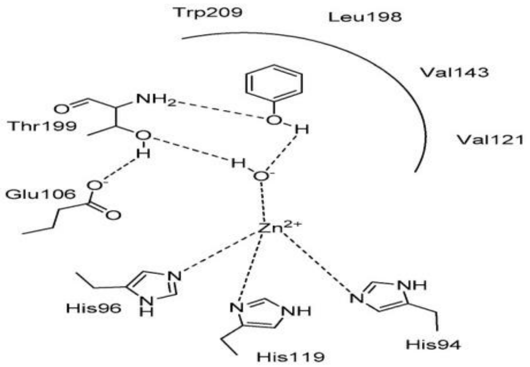

Fig. 1. Schematic representation of the binding mode of phenol within the hCA II active site

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Paper code: 628

Automated EME-DLLME Method on a disk

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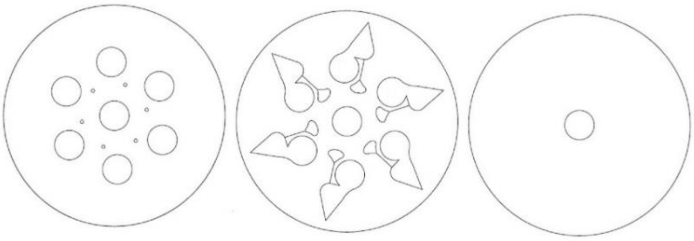
Recent developments in clinical examination have heightened the need for small and portable devices using little amount of sample. A fascinating goal of miniaturization of analytical instrumentation is the development of micro total analysis systems (µTAS) which are capable of nearly autonomous analysis of samples. Centrifugal microfluidic (CM) devices which are one of the microfluidic platforms make use of centrifugal force for flow control. These devices, which most often take the general form of compact disks (CDs), can be made portable and have very low power usage [1].

Dispersive liquid-liquid microextraction (DLLME) and Electromembrane extraction (EME) are two of the most popular microextraction techniques [2, 3]. With combination of the methods, the advantages of these methods can be utilized.

In this work we designed a centrifugal microfluidic device (CMD) to miniaturize and integrate the two popular conventional methods on a disk (as can be seen below). The device consists of 6 extracting units and each unit includes an EME chamber, a chamber for extracting solvent and chamber for DLLME and also phases separation. The analysis was performed by using a GC instrument with MS detection. To demonstrate the performance of the device, amitriptyline and its active metabolism, nortriptyline, were used. The parameters of EME method including composition of organic solvent used in porous membrane, pH of acceptor and donor phases, applied voltage, and extraction time and effective parameters of DLLME including kind of extracting and dispersive solvent and also volume of extracting and dispersive solvent were optimized. The optimal conditions of on-disk EME-DLLME were applied in human plasma, urine and saliva. Satisfactory analytical figures of merit including linear dynamic range and limits of detection in the range of 50-1000 ng mL^{-1} and 70-1000 ng mL^{-1} and extraction recoveries (38.5–28.6%) were obtained for amitriptyline and nortriptyline respectively with correlation coefficient higher than 0.9948.



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Paper code: 629

Preparation and characterization of antibiofouling PES nanofiltration membrane

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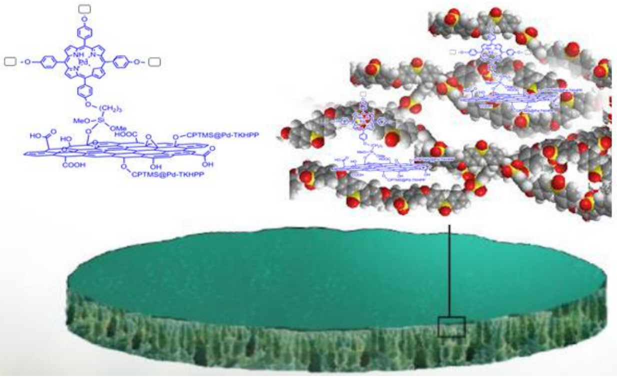
Graphene oxide/ CPTMS@Pd_TKHPP nanoparticles (GO/CPTMS@Pd_TKHPP) was synthesized that was hydrophilic functional groups such as hydroxyl group (OH^-) and carboxyl group (COOH) and phenol. Graphene oxide/ CPTMS@Pd_TKHPP nanoparticle embedded in antifouling polymer polyethersulfone (PES) mixed matrix nanofiltration membranes that was synthesis by phase inversion methods. The performance of the membrane synthesized was studied and evaluated in terms of pure water flux, hydrophilicity property, anti-biofouling behavior and dye removal (direct Red 16) properties in different percentage of the GO/CPTMS@Pd_TKHPP nanoparticle in matrix polymer membrane and the results illustrated that the GO/CPTMS@Pd_TKHPP embedded membranes had the notable improvement in pure water flux, anti-fouling resistance and dye removal capacity.



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Paper code: 631

Cu nanoparticles immobilized on modified magnetic zeolite as a new efficient catalyst for the synthesis of 1,2,3-triazoles via click chemistry reaction

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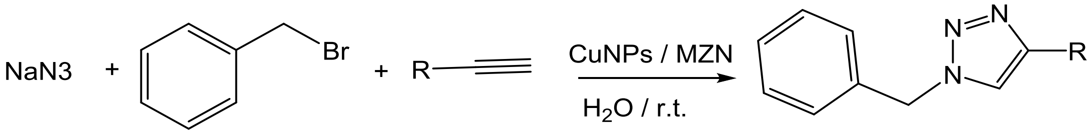
Magnetically recoverable copper nanoparticle loaded on functionalized natural zeolite (CuNPs/MZN) as an efficient catalyst was synthesized. The Fe_3O_4 magnetic nanoparticles (MNPs) were immobilized into the pores of natural clinoptilolite zeolite which were modified with linkers having amino and hydroxyl groups and then CuNPs were decorated on the surface of functionalized zeolite. The CuNPs/MZN were characterized by FT-IR, CHN, TGA, ICP, XRD, SEM,TEM and BET techniques, successfully.The activity of the prepared catalyst was tested for the synthesis of 1,2,3-triazoles via click chemistry reactions which lead to the desired products in high yields and short reaction time. The eco-friendly, low cost and efficient CuNPs/MZN were separated from the reaction mixture via a simple external magnetic field, and reused several times, successfully



R= Ph, OH-CH2-, Br-CH2-

Fig.1. The reaction between sodium azide, benzyl bromide and terminal alkyne for the synthesis of 1, 2, 3 triazoles

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6 Paper code: 32

Graphene Oxide-Supported Palladium Complex: Synthesis, Characterization and Application in Cross-Coupling Reactions

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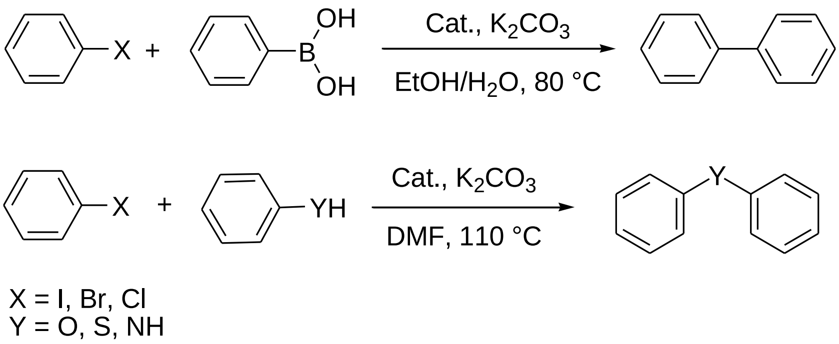
Graphene oxide (GO) possesses a number of advantageous properties, such as two-dimensional planar structure, large surface area, chemical and mechanical stability, superb conductivity and good biocompatibility [1]. Graphene oxide as a substrate for a variety of chemical transformations has been reported.

The transition-metal-catalyzed carbon-carbon and carbon-heteroatom bond-forming reactions are important fundamental transformations in synthetic chemistry [2]. Inspiring from recent developments in the field of nanocatalyst [3], herein, we report preparation and characterization of GO- supported palladium complex with terpyridin-based ligands which has also been applied as an effective nanocatalyst for the C−C, C−N, C-S and C-O bond formations via cross-coupling reactions of aryl halides. In addition, the catalyst can be reused up to four times without losing much of its activity.



Scheme 1. One pot formations of C-C, C-O, C-N and C-S bonds

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Paper code: 639

Synthesis of pressure sensitive adhesive using emulsion polymerization of core-shell technique, effect of acrylic acid monomer on Shear strength

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Pressure sensitive adhesives (PSAs) are viscoelastic materials that can adhere strongly to solid surfaces upon application of light contact pressure and short contact time. PSAs are used for many applications (e.g. tapes and labels) and can be obtained using different technologies such as emulsion [1]. "Recently, waterborne PSAs have received much attention from both industry and academia as a means for complying with environmental regulations" [2]. In this paper, different values (0.56, 1.12, 1.67 and 2.21 wt%) of acrylic acid monomer have used in the preparation of the adhesive. The shear strength of the obtained adhesive increased (from 397 kPa to 501 kPa) with increasing acrylic acid concentration from 0.56 wt% to 2.21 wt% which studied (Fig. 1). Improvement of the shear strength with addition of the acrylic acid could be due to presence of COOH polar group affected on the adhesion of the PSAs [3].

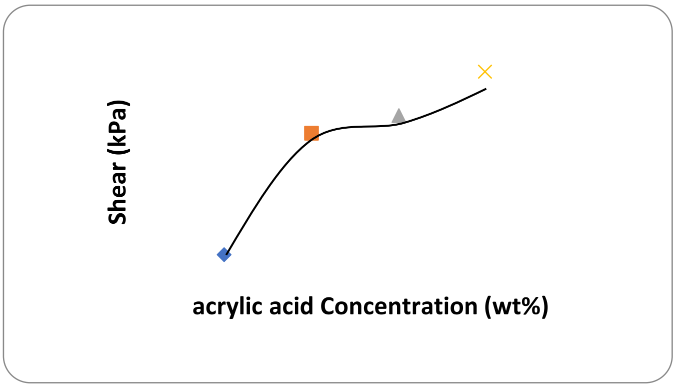

Fig. 1 Effect of acrylic acid concentration on shear strength of PSAs.

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Paper code: 651

Green synthesis of Ag/RGO nanocomposite using *Punica Granatum* peel extract and its catalytic activity for the reduction of 4-nitrophenol

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For the past few years, green synthesis of nanoparticles using plant extracts have been widely attracted, because this method provides advantages over physicochemical methods such as simplicity, mild reaction conditions, use of non-toxic solvents such as water, cost effectiveness and elimination of toxic materials [1].

In the recent years, Graphene oxide (GO) and reduced graphene oxide (RGO) are the great interests of many scientists as a new class of promising support and catalysts [2, 3]. GO is a two dimensional material which derived from graphene with a large number of oxygen containing functional groups such as epoxy, carboxyl, carbonyl and hydroxyl groups. The properties of GO include thermal and chemical stability, large specific surface area, high mechanical strength, water dispersity and good electron conductivity [4]. Therefore, GO and RGO could prevent the agglomeration of metal nanoparticles and stabilize them.

Nitrophenols and their derivatives are the most stubborn pollutants in industrial wastewaters, so the elimination of them is necessary. Many approaches have been acclaimed to eliminate 4-NP from aquatic environments, including electrochemical treatment, adsorption, and microbialdegradation. These procedures have some major limitations, including limited degradation efficiency, slow degradation rate, high costs and strict conditions [5]. The catalytic reduction of 4-NP is performed by sodium borohydride in the presence of metal nanoparticles as catalysts which is an environmentally friendly, effective, fast and simple method.

Herein, this context outlines the simple, cost effective and environment friendly protocol for the synthesis of Ag/RGO nanocomposite using *Punica Granatum* peel extract without capping agents or surfactants. The as-synthesized nanocomposite was characterized by UV-Vis, FT-IR, XRD and FE-SEM techniques. The catalytic efficiency of Ag/RGO nanocomposite was tested for the catalytic reduction process of 4-nitrophenol (4-NP) in aqueous solution at room temperature in the presence of sodium borohydride as hydrogen source. The progress of reaction was monitored using UV–Vis spectroscopy and the nanocomposite exhibited a high catalytic activity.

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Paper code: 653

Green synthesis of Ag/Fe_3O_4 nanocomposite using *Citrus sinensis* peel extract and its catalytic activity for the reduction of organic dyes

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Iron oxide magnetic nanoparticles have been widely used in many fields, which are attributed to their unusual magnetic, physical and surface chemical and catalytic properties, high stability and ease of recovery with an external magnet. Recently, the dopping of noble metals to iron oxide nanoparticles has been attracted widely because of unique multifunctional applications of hybrid nanostructures. Morever, the iron oxide nanoparticles can act as an effective support to prevent the agglomeration of metals nanoparticles [1].

For the past few years, green synthesis of nanoparticles has been widely attracted. This method has several advantages over chemical and physical synthetic methods, such as facility, safety, elimination of toxic materials and cost effectiveness [2].

Herein, this context outlines the simple and eco-friendly route for the synthesis of Ag/Fe_3O_4 nanocomposite using *Citrus sinensis* peel extract without stabilizers or surfactants. The as-synthesized nanocomposite was characterized by UV-Vis, FT-IR, XRD and FE-SEM techniques. The catalytic efficiency of Ag/Fe_3O_4 nanocomposite was examined for the catalytic reduction process of methylene blue (MB), methyl green (MG) and methyl orange (MO) in water at room temperature in the presence of sodium borohydride as reducing agent. The concentration of MB, MG and MO was used 3.1×10^{-5} M, 3×10^{-5} M and 3×10^{-5} M, respectively. The concentration of $NaBH_4$ for the reduction process of MB, MG and MO was used 5.3×10^{-3} M, 2.6×10^{-4} M and 3.7×10^{-2} M, respectively. In a typical experiment, 25 ml of $NaBH_4$ solution was added to 25 ml of dyes solution and the result was that the reduction of MB and MO was not occured after 24 h, and the reduction of MG was performed in 1 h. In the presence of catalyst and $NaBH_4$, the catalytic reduction of MB, MG and MO was completed in 127, 56 and 131 seconds, respectively. The decrease of reaction time shows the performance of nanocomposite clearly. The catalytic reduction occurs at the surface of catalyst. There were two steps of dyes reduction; (i) diffusion and adsorption of dyes to the catalyst surfaces via π-π stacking interactions and (ii) electron transfer mediated by the catalyst surfaces from BH_4^- to dyes. Ag NPs supported on the Fe_3O_4 NPs can function as the electron mediator between oxidant and reductant, and the electron transfer occurs via the Ag NPs. It suggested that the Fe_3O_4 NPs as support may play an active part in the catalysis, yielding a synergistic effect [3]. The progress of reactions was monitored using UV–Vis spectroscopy.

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Paper code: 654

Thermal Analysis and Ion Exchange Capacity of Poly (Vinyl Alcohol)-Based Membranes Modified with 2-Nitroso-1-Naphthol-4-Sulfonic Acid for Direct Methanol Fuel Cell Applications

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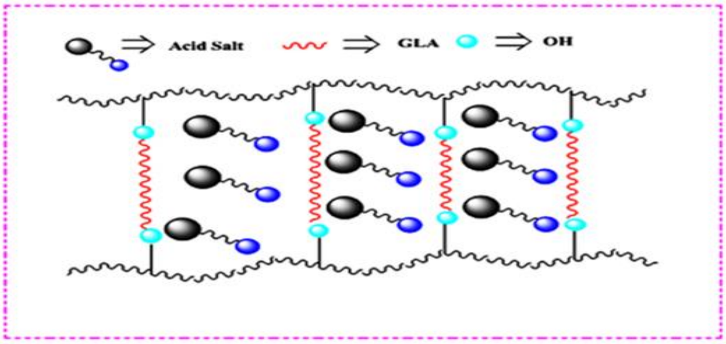
Fuel cell technologies based on polymer electrolyte membranes (PEMs) have received wide attentions in recent years [1-2]. In this study, we attempted to fabricate the novel poly (vinyl alcohol) (PVA) membranes comprising 2-Nitroso-1-naphthol-4-sulfonic acid those crosslinked by glutaraldehyde (GLA) with solutions casting method (Scheme.1). These membranes were assessed using thermal analysis (TGA), ion exchange capacity (IEC), and water uptake. It was demonstrated that ion exchange capacity and water uptake increased by increasing the acidic group content of the hybrid membranes. TGA results were confirmed that the thermal stability of the membranes improved as the acidity enhanced.



Scheme 1. Proposed model structure of the crosslinked PVA/sulfonic acid hybride membrane.

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Paper code: 656

Effect of Crosslink Density on the Characteristics of the Poly (Vinyl Alcohol) Membranes having Boromo Ethane Sulfonic Acid

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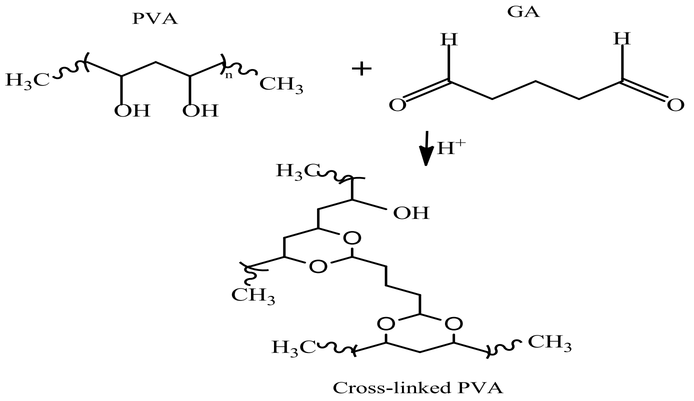
In the present study, the hybrid crosslinked membranes of poly (vinyl alcohol) (PVA) comprising boromo ethane sulfonic acid were prepared. Crosslinking modifies PVA through its hydroxyl groups, as a result creates a series of applications for this material. for example, the crosslinking of PVA can leads to water-insoluble hydrophilic vinyl alcohol which have been used for a wide range of applications. The membranes were synthesized at various concentrations of the crosslinker under acidic conditions. Various concepts of the membranes performance like methanol permeability, proton and electrical conductivities were addressed. Results showed that the degree of crosslinking is decreased due to the reduction in available volume and compression of the membrane structure [1-2]. Also, the proton conductivity of the membranes decreased as the cross-link density increased. The X-ray diffraction patterns confirmed an extension in the amorphous character of the membranes by enlarging the cross-link density. The reaction between the – OH group of PVA and the –CHO group of GA may be responsible for the observed behavior (schem.1).



Schem 1. Chemical reaction of PVA polymer with GA catalyzed by acid.

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Paper code: 676

Sol-gel synthesis of $LaFeO_3$/ZnO composite as promising photocatalyst

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Perovskite ($LaFeO_3$), zinc oxide(ZnO), and the composite of perovskite and zincoxide (ZnO/$LaFeO_3$) were prepared using sol-gel method. The prepared photocatalysts were characterized by FTIR, XRD, FESEM and UV-Vis spectroscopy analysis. Subsequently, the photocatalytic properties of prepared materials were investigated in degradation of congo red dye under visible light irradiation. The results showed that ZnO/$LaFeO_3$ composite possesses higher photodegradation ability compared to ZnO and bare $LaFeO_3$ photocatalysts.

Recently perovskite-type oxide materials have attracted considerable attention because of their useful application in many fields. $LaFeO_3$ is one of the important perovskite materials widely reported for various applications including solid oxide fuel cells, sensors, catalysts and magnetic storage/recording etc. In recent years, the LaFeO3 has attracted as a photocatalyst. $LaFeO_3$ can maximize the use of sunlight, So it has been developed as a new type of efficient photocatalyst driven under the visible light irradiation. ZnO is also considered as a promising photocatalyst because of its low price and nontoxicity, but its large band gap (3.2 eV) limits its usage as photocatalyst under sunlight irradiation.

In this work, we synthesized $LaFeO_3$, ZnO, and the composite of perovskite and zincoxide (ZnO/$LaFeO_3$) species and used them in photocatalytic degradation of congored dye.

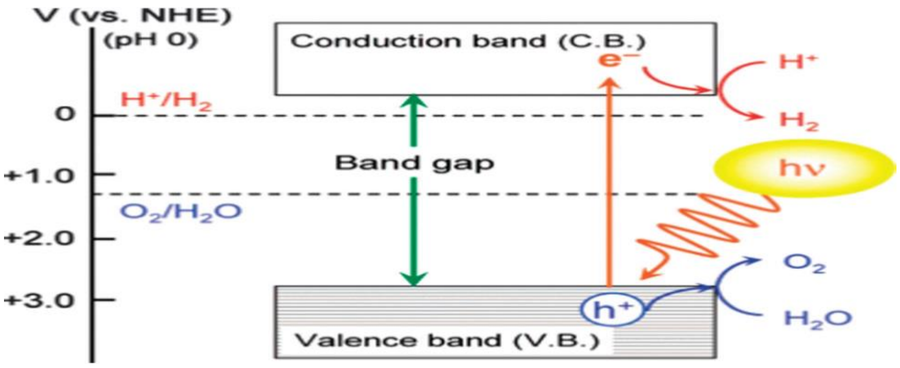

Fig. 1 Basic principle of the overall water splitting on a heterogeneous photocatalyst. Reproduced with permission from ref. 31. Copyright 2007, American Chemical Society.

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Paper code: 680

Fabrication of polyurethane rigid foam composites incorporated with phase change materials

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Phase change materials (PCMs) are a series of functional materials with storing and releasing energy properties. PCMs are able to adjust and control the environment around them through storing and releasing energy during phase change process namely, solid-solid, solid-liquid, liquid-gas and etc.

In this communication preparation and characterization of phase change materials based on encapsulated palmitic acid (PA) by the SiO_2 shell via sol-gel process is reported.

DSC results indicated that the phase change temperature of the PCM in melting and solidification process is 58.05 ^oC, and 56.97 ^oC, respectively without significant super cooling phenomena observation by having latent heats of 189.4 J/g and 258.7J/g.

In continue the prepared PCMs were used in the fabrication of rigid foam polyurethane by in-situ polymerization method.

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Paper code: 683

AgNPs–GO nano sheets for Aerobic Aqueous Oxidations of Alcohols

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Graphene-based nanosheets have attracted remarkable attention in recent years since their discovery in 2004. One of the major concerns in the area of graphene-based materials relates to the stabilization of the exfoliated sheets of graphene and GO [1]. The use of surfactants has been regarded as a highly appropriate, simple, and greener methodology for the exfoliation of GO compared with other proposed methodologies. The cytocompatibility of P123 has been studied for biological applications. Interestingly, the combination of surfactants and GO in catalytic processes has never been explored to date [2]. In this work, we propose the utilization of a surfactant combined with catalytically active Ag@GO (AgNPs–GO; NPs=nanoparticles) in chemical processes, illustrated by the selective aerobic oxidation of alcohols in aqueous media. In addition to the oxidative nature of GO, the use of the surfactant was found to improve the solubility of reactants (e.g. oxygen and organic compounds) in water, which improved the catalytic activity in the systems. In our investigations, the surface of GO was modified chemically with Ammonia and then GO sheets exfoliated by using of different surfactants such as P123, F127 and CTAB. After this step, Ag ions were loaded to the amine modified GO. Finally, Ag nanoparticles were generated via Ag ions reduction by $NaBH_4$ solution. The achieved Ag@GO sheets (AgNPs–GO) were used in oxidation of alcohols. AgNPs–GO was found to aggregate during the oxidation reaction of alcohols and, therefore, Ag nanoparticles were sandwiched between GO nanosheets. The catalytic activity was enhanced when cationic cetyl trimethylammonium bromide (CTAB) surfactant was used for exfoliation of GO sheets.

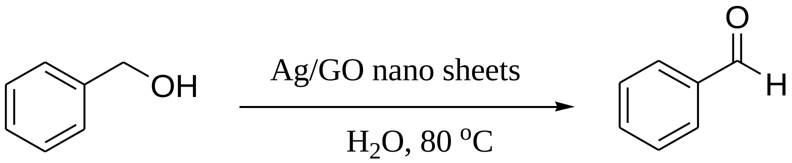

Fig. 1 Schematic pathway of reaction

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Paper code: 687

Facile Chemical Synthesis of silver Tungstates and silver Tungsten/Reduced Graphene Oxide as High Performance Supercapacitor

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Nanosilver tungstate (Ag_2WO_4) were synthesized by a chemical precipitation reaction in aqueous ambient involving direct addition of silver ion solution to the solution of tungstate reagent. Optimization of the synthesis procedure was carried out using Taguchi robust design as statistical method. In order to controllable, simple and fast synthesis of Ag_2WO_4 nanoparticles, effects of some synthesis conditions such as reagents concentrations (i.e., silver and tungstate ions), flow rate of silver feeding and temperature of the reactor on the size of synthesized Ag_2WO_4 were investigated by the aid of an orthogonal array (OA9). Chemical composition and microstructure of the prepared Ag_2WO_4 were characterized by means of XRD, SEM, FT-IR spectroscopy and UV-Vis spectroscopy. a composite of reduced graphene oxide (RGO) with silver tungstate (Ag_2WO_4) was prepared using a sonochemical method. The prepared Ag_2WO_4/RGO samples were assessed through FE-SEM to obtain morphological information. The resulting composite (Ag_2WO_4/RGO) was evaluated as a candidate for building supercapacitor electrodes. In this line the electrochemical performance of the tested materials were studied through cyclic voltammetry (CV), galvanostatic charge/discharge, electrochemical impedance spectroscopy (EIS), and continues cyclic voltammetry (CCV). The electrochemical tests were performed using 2 M H_2SO_4 solutions as the electrolyte. The evaluations on Ag_2WO_4/RGO-based electrodes revealed the material to have a specific capacitance of 534 F g^{-1} at a scan rate of 5 mV s^{-1}, an energy density of 68 W h kg^{-1}, and a high rate capability. Continues cyclic voltammetry evaluations using Ag_2WO_4/RGO-based electrodes proved the electrodes to be capable of maintaining almost 102.1% of its initial SC after 5000 cycles. Based on the electrochemical evaluations the synthesized nanocomposite was proven to possess the merits of both of its ingredients.

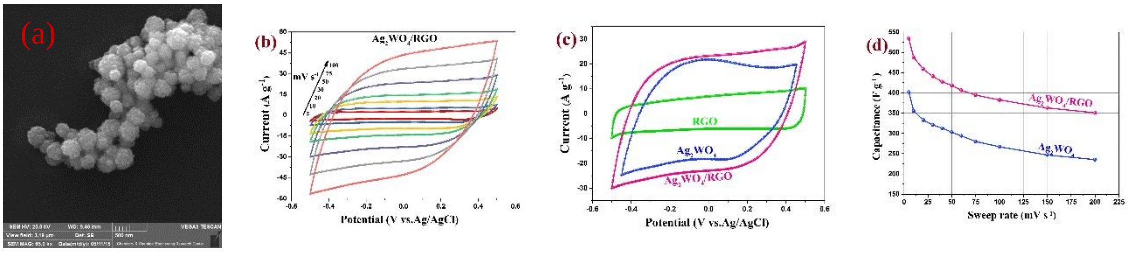

Fig. 1 (a) SEM image of Ag_2WO_4 prepared via precipitation under optimum conditions, (b) CVs of the Ag_2WO_4/RGO electrode at different scan rates, (c) CVs of the RGO, Ag_2WO_4, and Ag_2WO_4/RGO electrodes, at a scan rate of 50 mV s^{-1} in 2.0 M H_2SO_4 aqueous electrolyte and (d) Specific capacitance as a function of the sweep rates for the Ag_2WO_4 and Ag_2WO_4/RGO electrode.

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Paper code: 688

Comparison of different analytical methods for measuring salt in crude oil

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The crude oil extracted from the well contains large amounts of water and salt that forms an emulsion. Usually these emulsions lead to some problems, such as oil price devaluation, increased operating costs, corrosion and catalyst contamination in refineries. Separation of water and salt from crude oil is carried out in desalination and operation units. One of the important parameters that determines the quality of crude oil for export and use in refineries is the amount of salt in crude oil. For this purpose, several methods have been proposed to measuring the amount of salt in crude oil. [1]-[3].

In this study, two standard test methods of measuring salt in crude oil were tested and the results were evaluated. Finally, advantages and disadvantages of the methods were discussed.

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Paper code: 689

Synthesis of Dopant/hydroxyapatite/graphene oxide nano composites for dye degradation

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Nano composite Dopant/hydroxyapatite/graphene oxide n-(D/HA/GO) was successfully prepared by loading dopant hydroxyapatite onto graphene oxide sheets. Incorporation of semiconductor materials enhanced photocatalytic activity. In this work, we have synthesized samples co-doped with Zn^{2+} and Cu^{2+} as a semiconductor materials. Then Photocatalytic degradation of methylene blue was carried out using n-(D/HA/GO). X-ray powder diffraction (XRD) pattern reveals that all reflection peaks of each sample still corresponded to the HA phase and besides, there were changes in crystallinity, lattice parameters and crystal size due to the addition of dopant ions. Fig.1 shows the Field Emission Scanning Electron Microscope (FESEM) results that the prepared n-(D/HA/GO) consists of extremely thin needle-shaped composites. Also the decrease in crystal size that was associated with the increase in the surface area. The photocatalytic activity of samples was evaluated under UV irradiation, the prepared n-(D/HA/GO) composites showed a high catalytic effect (up to 70%) in the discoloration of the methylene blue solutions.

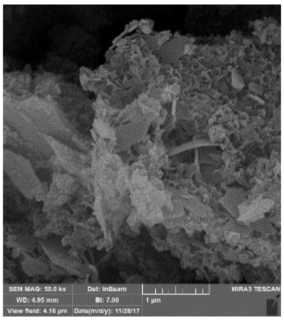

Fig. 1 FESEM images of D/HA/GO nano composites.

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Paper code: 702

Extraction and Identification of the Alkaloids in Papaveraceae Endemic Plant Resources in Iran

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Papaver somniferum L. belonging to the Papaveraceae family, grows naturally in Iran with anti-cancer and anti-HIV properties because of isoquinoline alkaloids such as morphine, papaverine, thebaine and noscapine. The aim of this study was to quality the amounts of the mentioned isoquinoline alkaloids in the samples collected from Iran[1].

Therefore, three regions were selected including Zanjan, Tarom, and Ab-Ali, and quality measurements of alkaloids. Opium alkaloids of two species of Papaveraceae in addition to four species of *Glaucium* Mill were chemically studied using High Performance Liquid Chromatography (HPLC) analysis. Four opium alkaloids, morphine, thebaine, papaverine and noscapine were significantly detected and veriably distributed in the species.

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Paper code: 723

Effect of CH3NH3I Concentration on Efficieny of Mesoporous Methylammonium Lead Iodide Perovskite Solar Cell

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Perovskite solar cells (PSCs) based on organometal halide have emerged as excellent light absorbers in solar cells with a rapid evolution in efficiency from 3.8% in 2009 to 22.1% in 2016 [1,2]. The remarkable achievement in power conversion efficiency (PCE) of perovskite solar cells is attributed to the unique properties of these materials, such as appropriate direct band gap, high absorption coefficient, long charge diffusion lengths, excellent carrier mobility and solution-based fabrication method [3-4].

In this work, we investigated the effects of CH_3NH_3I concentration in mesoporous perovskite solar cells prepared using a two-step solution deposition method. Photovoltaic performance of PSCs is found to strongly depends on the concentration of CH_3NH_3I. Under simulated one-sun illumination, average efficiencies of 6.1% (s.d.±0.31), 9.96% (s.d.±0.67) and 2.4% (s.d.±0. 4) are obtained from solutions of CH_3NH_3I with concentrations of 0.038 M, 0.044 M and 0.063 M, respectively. we achieved the best efficiency of 11.29% with a photocurrent density of 20.22 mA.cm^{-2}, open-circuit photovoltage of 0.814 V and fill factor of 0.66.

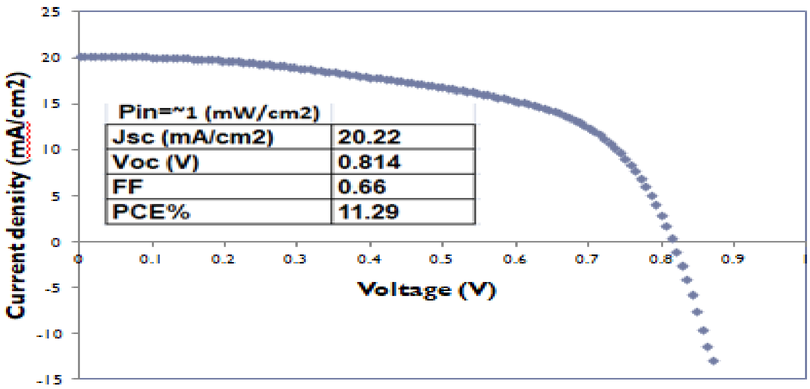

Fig. 1 Current density–voltage curve for the best-performing device.

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Paper code: 724

Experimental Study of the Synthesized Mordenite Zeolite for Simultaneous Reduction of Lead, Zinc and Cadmium ions

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Water contaminates are usually reduced by various adsorbents such as carbon active, fly ash, metal organic frame work (MOF) and zeolites [1,2]. This research was shown the simultaneous absorption of lead, zinc and cadmium ions by mordenite zeolite as an adsorbent. The zeolite absorbent was synthesized under solvothermal conditions (Fig. 1). The initial concentration of heavy metals solution was 50 mg/l that the efficiency of adsorption for lead, zinc and cadmium was 95.780, 35.819 and 47.978, respectively. In order to evaluate the results of the absorption process, Langmuir and Freundlich adsorption isotherms were investigated. The correlation coefficients confirmed that adsorption on mordenite zeolite was more compatible with Langmuir isotherm. Also the first and second order models were studied to determine kinetics of the adsorption metals. The results indicated that the mordenite is a useful absorbent for simultaneous removal of lead, zinc and cadmium ions. Finally, it was found that this compound has the most selectivity for lead ion.

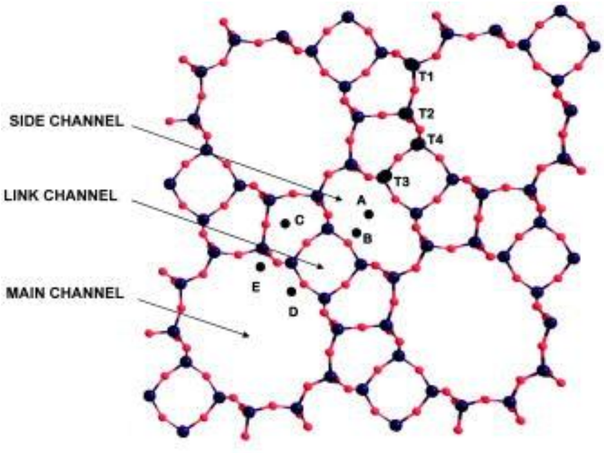

Fig. 1 Structure of mordenite (MOR) viewed along the c -axis showing different channels within the framework. T1, T2, T3, and T4 are the four inequivalent types of framework tetrahedral sites. A (β site), B, C, D, and E (α site) show the extraframework positions.

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Paper code: 729

Synthetic and Thermodynamic Study of Ammonium Absorption on Clinoptilolite Zeolite

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Zeolites are a large family of porous materials that include various groups. clinoptilolite zeolite exhibits a very favorable adsorption isotherm for ammonia removal [1,2]. This paper is evaluated the performance of clinoptilolite zeolite in reducing ammonium ion from aqueous solutions (Fig. 1). The initial concentration of solution used to determine the absorbance was 50 ppm with ammonium ion. The effects of solvent concentration, contact time and adsorbent amount were investigated. These variables were played a significant role in expanding the process of ammonium ion adsorption by using clinoptilolite. In order to determine the types of absorption kinetics, first and second order kinetics models, and also Freundlich and Langmuir models, have been investigated to determine how absorption of ammonium. The results show that clinoptilolite is a proper absorbent to reduce ammonium ions.

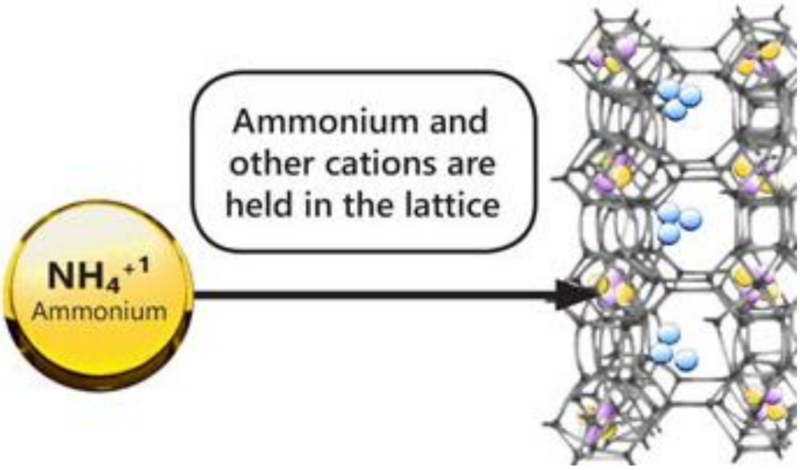

Fig. 1 The Ammonium is held in the negatively charged lattice through cation exchange capacity

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Paper code: 731

A Facile and Low Cost Method for the Synthesis of Magnesium Oxide Nanostructures by Oxidation of Magnesium Metal

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Magnesium oxide is an important semiconductor with a large band-gap having high surface reactivity and adsorption capacity, excellent thermodynamical stability, low dielectric constant, and low refractive index [1]. Magnesium oxide (MgO) is extensively used in catalysis, dye removing agents, defluorination, sensors, and CO_2 storage materials [2].

In this research, a simple sonochemical method for the synthesis of magnesium oxide (MgO) nanostructures is presented. MgO nanostructures are synthesized via oxidation of magnesium metal (ribbons) by sodium hypochlorite under ultrasonic waves. The PEG is used as stabilizer. The structure, morphology and chemical compositions of the synthesized products were characterized by using X-ray diffraction (XRD) analysis, energy dispersive X-ray spectrometry (EDS), and SEM and TEM photography. More information is obtained by FTIR, UV-Vis and PL spectroscopy. The FT-IR spectra of MgO nanostructures shows a peak around 420 nm which is assigned to Mg-O phonon. The XRD pattern of the sample reveals that MgO nanostructures with cubic crystal system are obtained. The average size of MgO nanoparticle is estimated to be about 22 nm according Debye–Scherrer formula. TEM image shows the nanoplates of MgO are formed (Fig. 1).

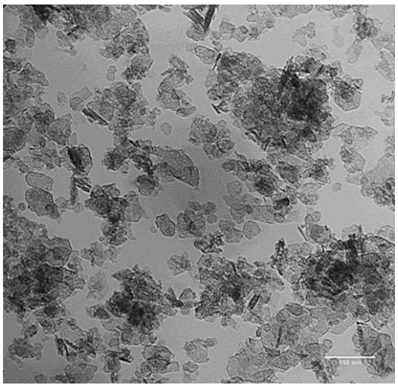

Fig. 1 The TEM image of the synthesized MgO nanoplates.

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Paper code: 734

$LaMnO_3$ High-speed adsorbent to remove methyl orange from aqueous solutions

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Dyes, organic compounds with complex structure, often toxic, carcinogenic, mutagenic, biodegradable and are one of the most common pollutants in the textile and dye industry [1-2]. The purpose of this study was to evaluate the efficiency of methyl orange dye removal from aqueous solutions using nanoparticles of Lanthanum manganite. In this research, the synthesis of Lanthanum manganite nanoparticles was carried out using hydrothermal method [3] and used as adsorbent to remove methyl orange dye. The adsorbent characteristics were made by analyzing XRD, FTIR and pH zero point (pH_{pzc}). In the FTIR analysis, the main adsorbent structure before and after absorption has not changed. The obtained XRD pattern was prepared to study the crystalline structure of the prepared composition. Also, the effects of pH parameters, absorbent dose, initial concentration of dye, contact time were performed. The XRD image shows the presence of nanoparticles of Lanthanum manganite with an approximate size of 52 nm. The results showed that by increasing the contact time for 20 minutes, the amount of adsorbent was 0.0025 g, the initial concentration of 10 mg/L , pH 1.5 and the room temperature increased the removal efficiency of the dye. Studies have shown that experimental data are more consistent with Langmuir isotherm and pseudo -second order kinetic model. Based on the results of this study, it seems that Lanthanum manganite can be used as an appropriate, inexpensive and effective absorbent for methyl orange removal from aqueous solutions.

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Paper code: 738

Preparation of Ag Nano Clusters as a Glucose Fluorescent Sensor

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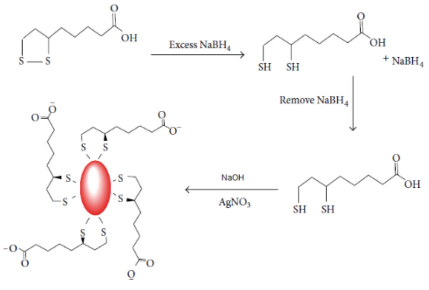
Ultrasmall noble metal nanoclusters (NCs), typically composed of several to a hundred metal atoms, have unraveled new interesting optical and electronic properties, that present unique physical and chemical properties between single atoms and large nanocrystals (42nm). Luminescent Au and Ag NCs are promising optical probes for bioimaging, anti-bacterial and biosensing applications. Two main Ag NCs are reported as Macromoleculeprotected luminescent NCs and Thiol-protected luminescent NCs [1,2]. Here we have demonstrated a new approach for the fabrication of highly sensitive, wider range and stable glucose biosensor. Ag NCs synthesized through green procedure according to Scheme. 1 [2].



SCHEME 1: Synthesis of DHLA and Ag NCs.

The noble-metal clusters offer new fascinating opportunities in the development of fluorescent probes [3]. In this study Ag-DHLA-AgNC glucose sensing probe characterizations are shown in Fig. 1.

The analytical characteristics of the proposed method	
Range of glucose concentration (mM)	**1.03×10^{-1}-$1.05\times10^{+1}$**
Regerassion equation	**A=0.1653+3.4685**
Regression coefficient	**0.980**
LOD (mM)	**0.05**
RSD (Repeatability)	**2.41%**

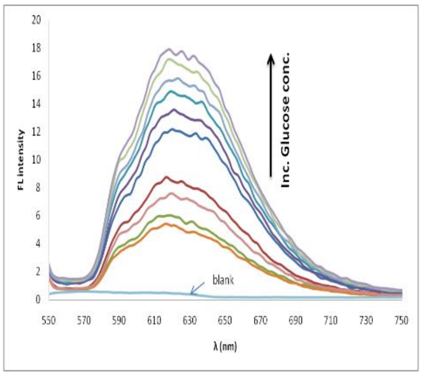


Fig. 1 Ag NCs green synthesis by DHLA-AgN.

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Paper code: 743

A benign route for the production of polymer nanocomposite films based on poly(vinyl alcohol) and SiO_2 nanoparticles modified with folic acid

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The synthesis of high-performance polymer/inorganic nanocomposite (NCs) has attracted much attention. This idea comes from the combination of the advantageous properties of inorganic nanoparticles (NPs) and polymers. Nano-SiO_2 particles are widely used as the inorganic component to prepare polymer/inorganic NCs. the high hydrophilicity originating from the hydroxyl group (−OH) on the silica surface and the high surface energy cause the NPs to easily agglomerate, therefore, it is difficult to disperse the nano-SiO_2 in polymer matrix. Surface modification is the best method for uniform dispersion of NPs [1]. Poly(vinyl alcohol) (PVA) is a water-soluble polymer which has been studied as a host matrix for a large number of nano-fillers, due to its excellent properties. It is biodegradable, biocompatible and nontoxic [2]. In this paper to prevent the agglomeration of SiO_2 NPs, their surface was modified by folic acid (FA) for the first time. Then, modified NPs was placed in the PVA matrix and SiO_2-FA/PVA NC films with 2, 5, and 8 wt% were produced by casting method under ultrasonic radiation as a green and low-cost method. Transmission electron microscopy (TEM) showed that the size of SiO_2-FA NPs in the PVA matrix was between 12-18 nm. Field emission scanning electron microscopy (FE-SEM) showed distribution of homogeneous particles in the PVA matrix.

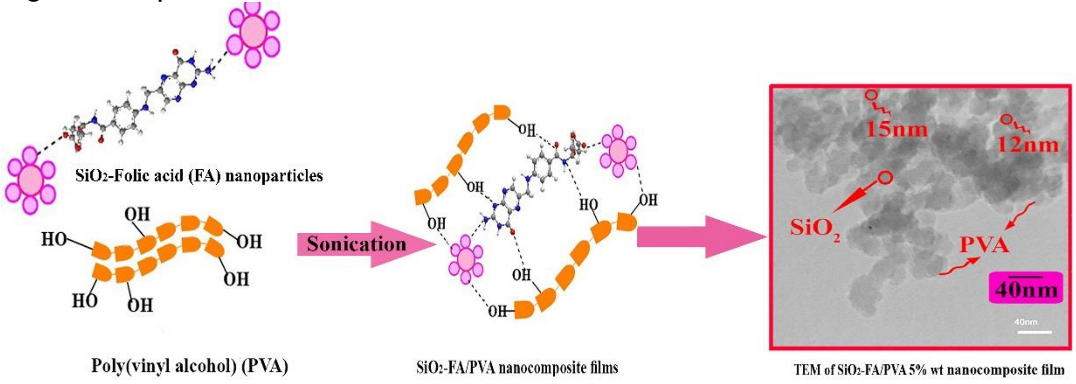

Fig. 1 the schematic preparation of SiO_2-FA/PVA nanocomposite films

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Paper code: 748

In-situ synthesis and characterization of reduced graphene Oxide and sulfonated graphene-polypyrrole nano-composites for use in gas sensor

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Design and development of gas sensors with high sensitivity and selectivity is very important. Among conducting polymers, polypyrrole (PPy) is a promising material having excellent environmental stability, high intrinsic electrical conductivity, low cost and easy synthesis. PPy and its composite with carbon nanotube (CNT) and other metal oxide have shown very attractive gas sensing applications, but graphene is preferred over CNT due to its larger sensing area per unit volume and high electron mobility at room temperature. In this study, graphene oxide (GO) was synthesized from natural graphite powder by a modified Hummers method [1] and was reduced by hydrazine. Graphene derivatives such as reduced graphene oxide (RGO) and sulfonated graphene (SRGO), will be synthesized in nano-sized dimention. The polypyrrole-graphene derivatives hybrid nano-composites were synthesized via in-situ oxidative polymerization of pyrrole. Characterization of graphene-based conducting polymer composites will be done by variety of spectroscopy techniques. According to appropriate solubility of The RGO/PPy and SRGO/PPy composites in organic solvents such as chloroform, the electrospinning technique was used to coate it onto a Cu-IDE surface as chemiresistor gas sensor [2]. In order to evaluate the gas sensing properties of nanocomposites, the electrical resistance and dielectric properties were measured in the presence of different concentration of ammonia and alkyl amines. In the following, the sensing behavior of the SRGO/PPy were compared to RGO/PPy nanocomposite. A typical response of RGO/PPy sensor to ammonia gas at different concentration shown in Fig.1.

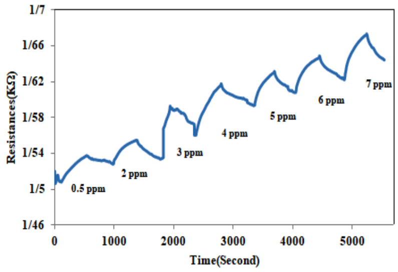

Fig. 1. The ammonia sensing response of RGO/PPy composite at 0.5 ppm to 7 ppm.

The variation in electrical resistance is attributed to the electron charge transfer between ammonia gas and the surface of RGO/PPy composite.

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Paper code: 753

The comparative study of support effect in silver- graphene oxide nano magnetic catalyst

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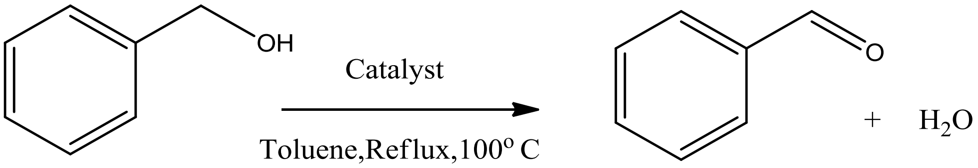
Silver nanoparticles are one of the most interesting material in catalyst synthesis. The large specific surface area causes high catalytic activity, in other hand this property lead to agglomeriation. In addition, nanocatalysts suffer from agglomeration, recovery, temperature instability and sepration. These problems would be solved just by selecting appropriate material as catalyst support[1]. Surface chemistry play a key role in selecting materials as catalyst support and checking catalytic efficiency. among carbon-based materials, graphene oxide (GO) with high specific surface area has the most application in catalysis studies. functional groups such as carbonyl, hydroxyl and epoxy on the GO surface improve selectivity in reactions. According to synergitic effect, combination of different nanomaterials such as metal or metal oxide and GO, enhance their properties . In addition, metal nanoparticles distribute uniformly and functional groups act as nucleation sites by using GO as a support[2].

The amorphous structure and thermally stable mesoporous silica ($mSiO_2$) leads researchers to use it in preparation of different catalysts. This structure of silica provide suitable space for metal NPs with specific size, so aggregation or agglomeration could be avoided[1,3].

In the present study different nanocomposites of silver and graphene oxide, GO-$Fe_3O_4@SiO_2$-Ag and GO-Fe_3O_4-Ag, were synthesized in order to compare their properties. Both catalysts were characterized by different method and their catalytic activity were examined by aerobic oxidation of benzyl alcohol. Using silica in catalyst support increase the yield reaction.



Scheme1. Aerobic oxidation of benzyl alcohol

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Paper code: 761

Fabrication of Pd@gelatin/agarose nanoparticles: a new heterogeneous catalyst for heck reaction

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In last years, stabilized metallic nanoparticles have probably been the most frequently employed in organic synthesis.[1] Heterogeneous catalysis, and supported metal catalysts in particular, play important roles in both industry and academia.It is well known that transition metal nanoparticles (MNPs) such as palladium, are utilized to carry out coupling reactions due to their superiority over traditional metal catalytic systems with respect to controllable size, more degrees of freedom and small surface with active sites accessible to reactants. Also, immobilization of metal NPs in solid supports such as bioorganic beds allowed obtaining recoverable catalysts for cross-coupling reactions. Among the most fundamental reactions in organic chemistry, Mizoroki-Heck cross coupling as a powerful synthetic tool and a major area in multiple organic transformations has received great attention. [2]

In the past 5 years, we have developed an easy synthetic route to preparation palladium nanoparticles by using mixture of natural bioorganic carbohydrate as bed. [3] Based on this former work, we describe here the synthesis of Pd nanoparticles stabilized by mixture of gelatin and agarose, and the use of this system as catalyst in the Mizoroki-Heck reaction, along with its recycling (Figure 1).

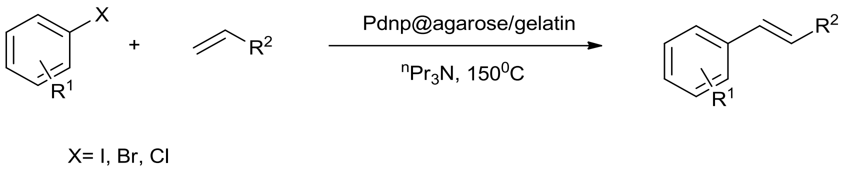

Fig 1. Application of the Pdnp@gelatin/agarose in the Mizoroki-Heck reaction.

The in situ generation of nanoparticles without addition of any external reducing agents, stability toward air and humidity, easy handling and recycle ability are some unique features of the Pdnp@gelatin/agarose catalytic system.

Also the nanocatalyst has been recovered for five runs with some decrease in the catalytic activity of the catalyst.

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Paper code: 763

Photocatalytic degradation of Reactive Black-5 Dye (RB5) from Aqueous Solution by calcium doped lanthanum manganite under visible light irradiation

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calcium doped lanthanum manganite (LCMO) nanostructure was synthesized via the mild hydrothermal method. Properties of materials were characterized by X-ray diffraction, Fourier Transform Infrared Spectroscopy, Field Emission Scanning Electron Microscopy and UV–vis spectroscopy. The results of XRD and FTIR analyses show that the as-prepared material is composed of single-phase structure without impurity and nanorod morphology with a mean diameter of 126.8 nm. The LCMO composition has a band gap of 1.83 eV that indicating its capability as a photocatalyst under visible light irradiation.

The anionic Reactive Black 5 (RB5) dye solution was considersd as a model of wastewater [1, 2] to study the photocatalytic activity of LCMO nanostructure under visible light irradiation. The results of the degradation of RB5 by the heterogeneous photocatalytic reaction show that, over a period of 90 minutes, near to 80% of RB5 is degradated, and the overall reaction rate is first order and is equal to 0.016 min^{-1}.

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Paper code: 766

Plant-based synthesis of ceria nanoparticles and its catalytic activity

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Nanotechnology is a new and emerging technology with the wealth of applications. Green synthesis route is highly relevant as it is nontoxic, decreasing/completely eliminating the use and generation of substances hazardous to human health and the environment. The biological process is a bottom-up method and green route which it uses plant, fungus, biopolymer, bacteria and, algae in the synthesis process. These materials contain some biochemical components acting as capping and/or stabilizing agents in the synthesis process. Cerium oxide is rare in the earth crust and it has wide band gap. CeO_2 nanomaterials have used in a wide range of applications, such as catalyst, gas sensors, polishing materials, solid oxide fuel cells, optical devices, etc. Here, cerium oxide nanoparticles have been synthesized in Falcaria Vulgaris leaf extract by sol-gel method. They were characterized by some physical and chemical methods such as XRD, UV-Vis spectroscopy, FT-IR, and FE-SEM. The XRD pattern confirmed the formation of cerium oxide nanoparticles with average size 19.5 nm estimated by Scherrer equation. The Ce─O vibrational stretching was observed about 410 cm^{-1} and UV-Visible spectrum showed a peak at 313 nm with band gap energy of 3 eV. Due to investigate catalytic properties of synthesized nanoparticles, dye degradation of methylene blue in the presence of sodium borohydride was done. The results showed that the rate of degradation increased when cerium oxide nanoparticles were added to a solution containing a mixture of methylene blue and sodium borohydride; moreover, dye was degraded 90% after 3 hours.

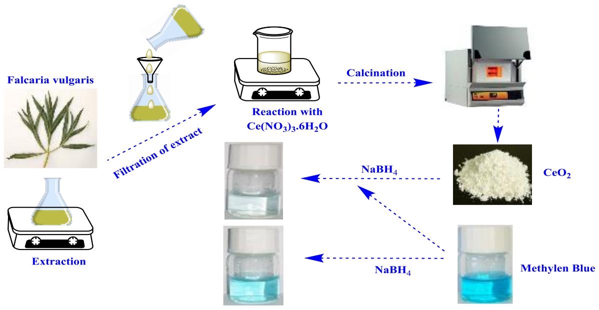

Fig.3. Schematic of CeO_2 nanoparticles synthesis and its catalytic process

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Paper code: 773

Copper supported on citric acid modified magnetite nanoparticles as a novel superparamagnetic nanocatalyst for nitro reduction

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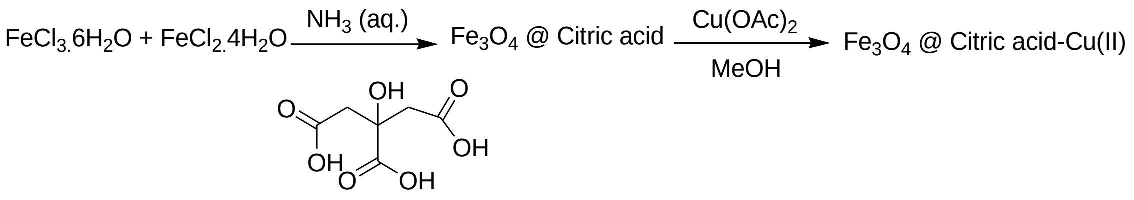
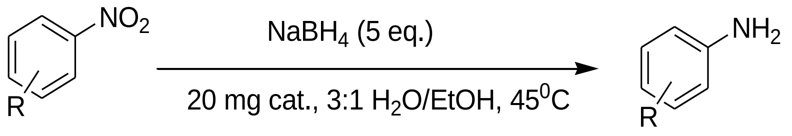
Amines are an important class of organic materials with applications in synthetic chemistry and pharmacology [1]. Reduction of nitro compounds is a way for preparation of amines. Many protocols for reduction of nitro group is reported; however they suffer from problems such as long reaction time, cumbersome work up procedures and poor recyclability of the catalyst [2]. Here we report a novel catalyst with magnetic recyclability for reduction of nitro aromatics. The Fe_3O_4@Cit-Cu(II) is characterized using different methods including FT-IR,XRD, TGA, VSM, ICP, and SEM-EDX.



Scheme 1 Pathway for preparation of Fe_3O_4@Cit-Cu(II).



Scheme 2 Reduction of nitro arenes in presence of Fe_3O_4@Cit-Cu(II).

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Paper code: 780

Synthesis and characterization of novel sulfonated polyimides containing triptycene and xanthene moieties

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Polymer electrolyte fuel cells (PEFCs) have been identified as promising power sources for vehicular transportation and for other applications requiring cleaning, quiet, and portable power [1]. The most important component of a PEFC is polymer electrolyte membrane itself. At present, sulfonated perfluoropolymers such as Nafion have been almost the only advanced membranes that are used in practical systems due to their high proton conductivity, good mechanical strength, and high thermal and chemical stability. Unfortunately, however, there are some demerits which seriously limit their application. These include high cost, low conductivity at low humidity or high temperatures, and high methanol permeability. Thus, the development of alternative materials overcoming these problems is strongly desired. Up to now, a large number of sulfonated polymers such as poly(styrene sulfonic acid) and the analogous polymers, sulfonated polysulfone, sulfonated poly(ether ether ketone), and sulfonated poly(phenylene sulfide) have been developed, and very recently sulfonated polyimides have been reported to be promising materials for PEFC [2,3]. In this paper, a series of novel sulfonated homo- and copolyimides were synthesized from 1,4,5,8-naphthalenetetracarboxylic dianhydride (NTDA), sulfonated diamine, 4,4′-diaminodiphenyl ether-2,2′-disulfonic acid (ODADS) and nonsulfonated diamines containing triptycene and xanthene groups. The sulfonated polymers were obtained in quantitative yields with inherent viscosities of 0.27-0.74 dL g^{-1}. The resulting polymers dissolved in N-methyl-2-pyrrolidinone, *N,N*-dimethylacetamide, *N,N*-dimethylformamide, dimethyl sulfoxide, and pyridine. These polymers were fairly stable up to a temperature >450 °C and lost 10% weight in the range of 477 °C and 575 °C in nitrogen. The UV-V is absorption spectra revealed that most of the polymers had absorption maxima around 310 and 341 nm.

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Paper code: 795

Fabrication of Hollow Silica Structured Organic−Inorganic Hybrid Nanocatalyst for the Oxidation of Alcohols to Aldehydes and Ketones

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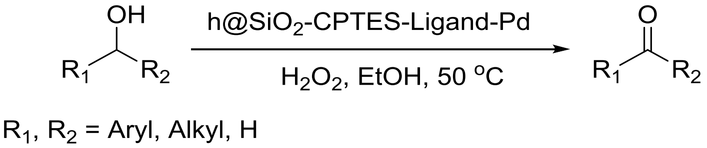
We demonstrate the preparation and characterization of novel organic−inorganic hybrid palladium nanocatalyst fabricated via the covalent grafting of Pyr-ligand on chlorfunctionalized silica-hollow nanoparticles, followed by its metallation with palladium acetate for the selective oxidation of primary and secondary benzylic and aliphatic alcohols to give the corresponding carbonyl products in good yields. The reactions were carried out in ethanol in the presence of hydrogen peroxide as an oxidant at 50°C.

Hollow nanoparticles can be synthesized with various materials such as organic polymer, silicates, carbon, titania, and phosphates [1]. In this work, we report on the synthesis of SiO_2 hollow spheres using magnetic nanospheres as templates. Acting as seeds, magnetic nanospheres were then wrapped with a silica shell by the modified Stöber method [2]. The resulting magnetic silica nanoparticles (MSNPs) were treated with hydrochloric acid and calcinated at high temperature to form a large core cavity. The synthesized substrates are in a spherical morphology and uniform size distribution. The nanostructure and properties of nanocatalyst were studied by TEM, SEM, XRD, BET, TGA, and FT-IR characterizations. The average diameter of nanocatalyst was about 80 nm.



Scheme. 1 Oxidation of alcohols by using H_2O_2 in the presence of ethanol at 50°C.

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Paper code: 796

Synthesis and characterization of Cu(Ⅱ) Schiff base complex immobilized on magnetic graphene oxide sheets as heterogeneous catalyst

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From the view of green chemistry, the design of new and efficient reaction protocols using supported nanocatalysis to synthesize fine chemical and pharmaceutical products has recently gained interest scientists. Carbon materials such as carbon nanofibers, carbon nanotubes and graphene oxide (GO) [1] as promising supports have attracted significant attention as they are inexpensive and readily obtained. Due to the particular properties of GO such as large surface area, high mechanical strength, unique layered structure, excellent physicochemical stability, and high flexibility, they can be applied as support for homogeneous catalysts. Metal transition complexes of Schiff base have been studied extensively due to their potential application in catalytic systems. The Schiff base complexes of transition metals which have been known as homogeneous catalysts can be immobilized on graphene oxide nanosheets performs as efficient catalysts .The incorporation of magnetic components into GO is most favored and will provide high catalytic activity and improve isolation capability [2]. In this work, a Cu(Ⅱ) Schiff base complex supported on magnetic GO and used as efficient nanocatalyst for some of organic reaction. The synthesized nanocatalyst was characterized by various techniques including XRD, FT-IR, TGA, SEM, and ICP-AES analyses. Also, the synthesized nanocatalyst could be separated easily from the reaction mixture using an external magnet and reused for several consecutive times with only minor degradation of its catalytic performance.

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Paper code: 805

Synthesis of 2-amino-4H-chromenes catalyzed by N,N-diethyl-N-sulfoethanaminium hydrogen sulfate

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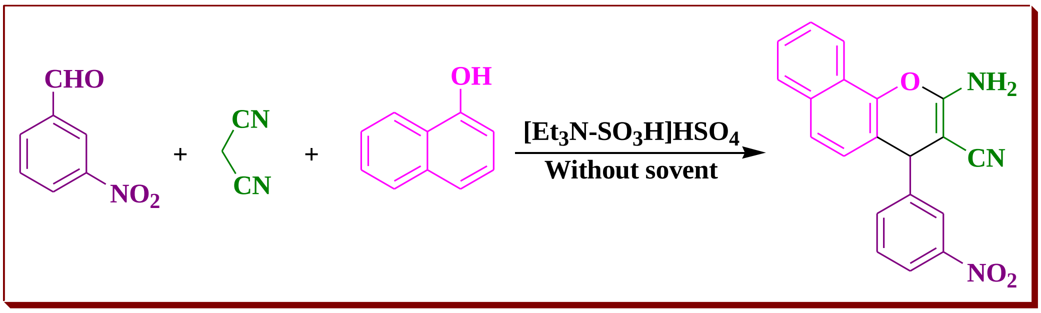
In this research condensation reaction between arylaldehydes, malononitrile and 1-naphthol, in the presence of acidic or basic catalysts, has been used as the best synthetic way toward 2-amino-4H-chromenes as biologically and industrially significant compounds. Some biological activities of this class of chromene derivatives include antimicrobial, antitumor, antiviral, and sex pheromone properties[1].

They have also been employed as potent biodegradable agrochemicals, and as cosmetics as well as pigments .Ionic liquids are of importance because they have been extensively used as solvent, catalyst and reagent in organic synthesis. These attractive compounds have various unique properties including non-flammability, non-volatility, wide liquid-state temperature range, high thermal and chemical stability, large electrochemical window, favorable solvation behavior and enhanced reactivity[2]

In this work, we have introduced Brønsted acidic ionic N,N-diethyl-N-sulfoethanaminium hydrogen sulfateas a highly efficient, general and homogeneous catalyst for the reaction between arylaldehydes, malononitrile and 1- naphthol to afford 2-amino-4H-chromenes in high yields and short reaction times[3]. (Scheme 1).



Scheme 1. The production of 2-amino-4H-chromenes using [Et3N-SO3H]HSO4.

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Paper code: 811

N,N-diethyl-N-sulfoethanaminium hydrogen sulfate as an effective catalyst for the preparation of 14-aryl-14H-dibenzo[a,j]xanthenes

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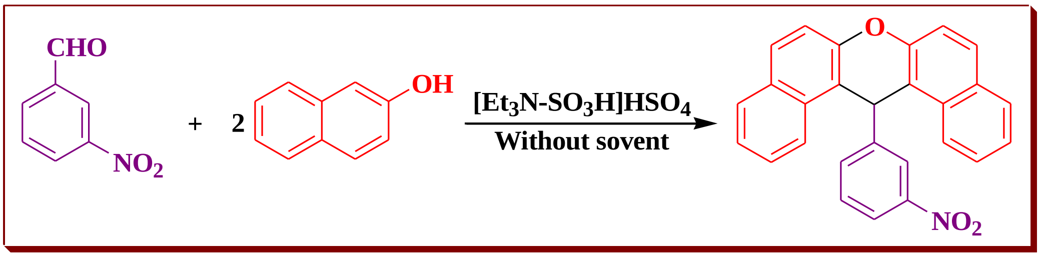
The aim of this study is development of a novel SO_3H-containing Brønsted acidic ionic liquid as catalyst for organic transformations. Therefore, initially, N,N-diethyl-N-sulfoethanaminium hydrogen sulfate {[Et3N-SO3H]HSO4} (as a novel member of this family of ionic liquids) was synthesized, and characterized using ^1H and ^{13}C NMR, FT-IR and mass spectral data[1].

Afterward, its catalytic activity was checked for promotion of one class of useful organic transformations under solvent-free conditions, including the condensation reaction of arylaldehydes with 2-naphthol to give 14-aryl-14H-dibenzo[a,j]xanthenes(Scheme1).The ionic liquid efficiently catalyzed the reaction, and the product were obtained in excellent yields within short reaction times.

Ionic liquids are of importance because they have been extensively used as solvent, catalyst and reagent in organic synthesis. These attractive compounds have various unique properties including non-flammability, non-volatility, wide liquid-state temperature range, high thermal and chemical stability, large electrochemical window, favorable salvation behavior and enhanced reactivity.[2]

Xanthene derivatives, especially benzoxanthenes are of importance since they have various biological activities such as antibacterial, antiviral, and anti-inflammatory, properties. Furthermore, some other benzoxanthenes have found applications in industries, such as fluorescent materials for visualization of biomolecules, and as dyes in laser technology.[3].



Scheme 1 The synthesis of 14-aryl-14H-dibenzo[a,j]xanthenes catalyzed by $[Et_3N\text{-}SO_3H]HSO4$.

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Paper code: 813

Process Variables in Phytosynthesis of Ag@AgCl Nanoparticles by *Syzygium cumini* Fruit Extract

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In recent years, the development of efficient and well-characterized metal nanoparticles synthesis without use of toxic chemicals has become a major focus of researchers. One of the most considered methods is production of metal nanoparticles using organisms. Among organisms, plants seem to be the best candidates because of their advantages such as their availability, rapid single-step method, low-cost, eco-friendly without using high pressure, energy or toxic chemicals, safe for human therapeutic use and they are suitable for large-scale biosynthesis. Moreover, the nanoparticles are more various in shape and size in comparison with those produced by other organisms [1].

At this work, we are reporting the one step phytosynthesis of silver/silver chloride nanoparticles (Ag@AgCl NPs) using aqueous fruit extract of *Syzygium cumini* as a reducing and stabilizing agent without addition of any other external compound. The fruit extract of *Syzygium cumini* is known to possess a variety of flavonoid and other phenolic compounds [2] that could probably mediated the reduction by donating electrons and can act as capping agent [3]. Effective parameters on synthesis of Ag@AgCl NPs such as; pH, the volume of extract, silver ion concentration, temperature and reaction time were optimized to attend control over the particle size and stability. Initially, synthesis of Ag@AgCl was confirmed through UV–Vis spectroscopy which shows the surface plasmonic resonance peak (SPR) at 408 nm and TEM reveals that synthesized Ag@AgCl NPs are spherical in shape with the average size of 16.8 nm. XRD analysis revealed that biosynthesized Ag@AgCl NPs are crystalline in nature. The present investigation may prove to be of great value in synthesizing biomolecule-loaded nanoparticle with well-controlled sizes for a broad spectrum of environmental, biological and industrial applications.

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Paper code: 816

Synthesis of a novel catalyst based on Ag nanoparticles on mesoporous silica for reduction nitro aromatic compounds in aqueous solution

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In the last decade, silver (Ag) nanoparticles have attracted extensive attention due to their catalytic properties for a variety of organic reactions [1]. Several investigations have been reported on preparation and catalytic activity of Ag NPs. However, metal-nanoparticle catalysts always encounter limitations, because of the problems associated with their separation from the products by traditional methods [2].

Nitroaromatic compounds are generally prepared via nitration of simple aromatic compounds and are extensively being used in various industries such as plastics, dyeing, agriculture, etc. As a result, nitroaromatic compounds are usually present in industrial effluents and agricultural waste water [3]. Hereby we report amine functionalized mesoporous magnetite nanoparticles as a robust support for uniform dispersion of Ag nanoparticles. Silver nanoparticles were formed on the surface of mesoporous silica via coordination of Ag^+, followed by chemical reduction. The resulting Fe_3O_4@SiO_2@KIT-Ag nanomaterial was characterized by powder x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), and transmission electron microscopy (TEM). Also, we use it as an effective catalyst in the reduction of a variety of nitroaromatic compounds.

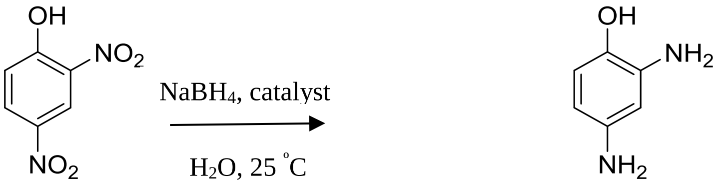

Fig1. Reduction nitro aromatic compound in water at near ambient temperature catalyzed by Fe_3O_4@SiO_2@KIT-Ag

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Paper code: 821

Application of ultrasound waves for extraction of total phenols and flavonoids from Echinacea Purpurea (L.)

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The purple coneflower scientifically called Echinacea Purpurea (L.) Moench is perennial herb that belongs to the asterial family [1]. Due to anti-inflammatory and antioxidant properties of the aerial part (such as flowers), the E. Purpurea was used to cure frostbite and viral infections. In general, the antioxidant property refers to constituent phenolic and flavonoid compounds in this plant [2]. In this study, a central composite design (CCD) was used to evaluate the significant extraction variables to achieving the higher recovery yield of total phenolic and flavonoid content from aerial part of E. Purpurea. Ultrasound-assisted extraction technique was employed as driving force for extraction process. The total phenolic content and total flavonoid content, respectively, were accounted by using Foline-Ciocalteu and aluminum chloride colorimetric method. Effective variables such as plant mass, volume of solvent, sonication time and ultrasound temperature were investigated. The significant variables were optimized by using a CCD combined with desirability function (DF). At optimum conditions values of variables are set as 4 g of plant powder, 17 mL of extraction solvent, 22 min for sonication and 37 °C for ultrasonic bath. Results indicated that there were significant differences ($p \leq 0.05$) among populations for total phenolic and flavonoid contents. Total phenolic content varied from 36.57 to 31.39 (mg gallic acid/100 g dry wt), and total flavonoid content ranged from 58.32 to 307.44 (mg quercetin/100 g dry matters).

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Paper code: 830

An Experimental Study of the Loading and Controlled Release of Salicylic Acid on Zeolite Nanocomposite

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The encapsulation potential of salicylic acid on the zeolite as porous material was studied. The produced composite is working as drug delivery carrier in which the zeolite is a host and the salicylic acid is a guest. Characterization with XRD and FTIR techniques demonstrated the successful loading of salicylic acid into the zeolite nanoparticles. Loading of salicylic acid on the zeolite at 25 °C was 18%. The drug release of salicylic acid in water at pH 7 and 37 °C was achieved to obtain the kinetic data. The kinetic data was modeled to determine the release patterns of the drug delivery system.

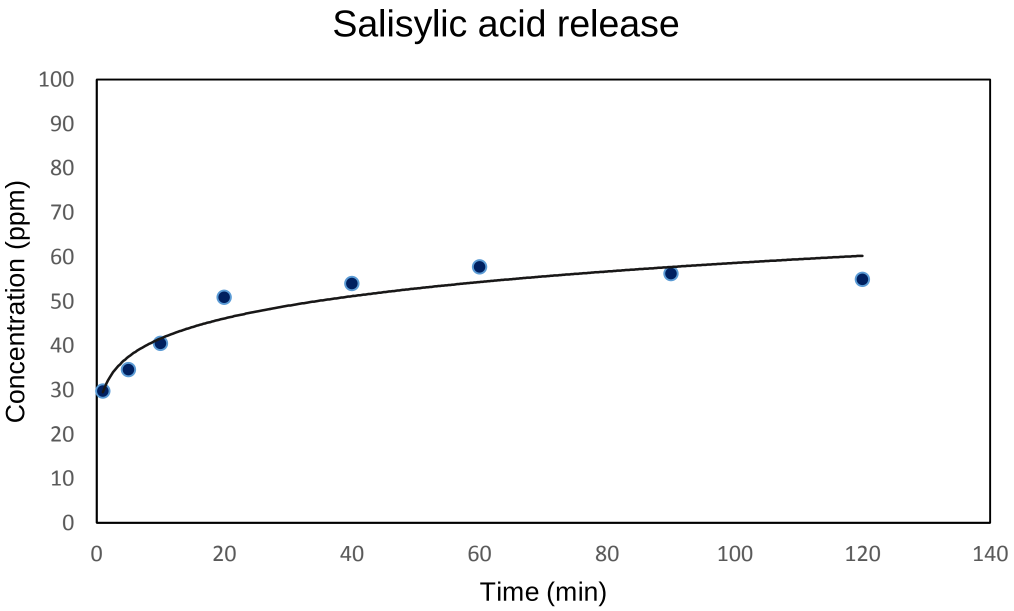

Fig.1 Salicylic acid release from nanocomposite at water pH 7.

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Paper code: 843

Aerobic oxidation of alkenes in the presence of metalloporphyrines without any additives

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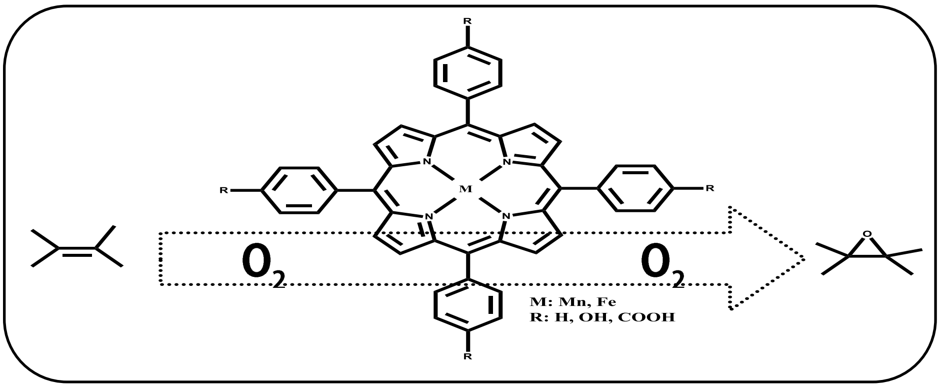
Developing the catalytic procedures for the selective oxidation of organic substrates in the "clean" conditions is environmentally important and many research efforts have been paid to this topic in the last decades [1]. Molecular oxygen as a standard green oxidant can be used for the oxidation processes and great interest have been dedicated to improving new strategies for the activation of O_2 in the green catalytic systems. Unfortunately, using molecular oxygen in the catalytic systems facing some difficulties and the main important problem is because of the spin-forbidden law. However, there are some promising strategies, like using photosensitizers [2] and light aldehydes [3] which can active molecular oxygen in the oxidation systems. Metalloporphyrins as biomimetic catalysts for green oxidation systems, can overcome the problems and activate molecular oxygen to oxidize organic compounds in the mild conditions and various metalloporphyrins have been widely used in the selective aerobic oxidation of hydrocarbons.

In this work, several supported and unsupported metalloporphyrines have been synthesized and characterized by standard methods and used as significant catalysts for the aerobic oxidation of olefins in the absence of any additives in the mild conditions at room temperature.



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Paper code: 853

Effect of solvent, time and method on the amounts phenol, flavonoid and the anitioxidant activity of *Ixiolirion tataricum* (Pall.) Herb extract

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The application of natural and low-risk antioxidants is an unavoidable necessity. Natural antioxidants increase the strength of antioxidants of plasma. Phenol and total flavonoids are derived from secondary metabolites of plants have the potential to eliminate free radicals [1]. Solvent type, physicochemical properties of the solvents, extraction time and method are important parameters on extraction efficiency [2]. In this work, was studied effect of time (60, 90 and 120 min), solvent (H_2O, CH_3OH and n-hexane) and method (soxhlet and ultrasound- assisted) on total phenol content (TPC), total flavonoid content (TFC) and antioxidant activity (according to IC_{50}, FRAP and BCB) for extract of *Ixiolirion tataricum* (Pall.)Herb. The plant (voucher number NP23/2-1) was collected in April of 2017 from Baba Amman Mountains of North khorasan Province in Iran. TPC and TFC were determined using the Folin-Ciocalteu and aluminum chloride methods; respectively. The mounts of TPC, TFC, IC_{50}, FRAP and BCB in the optimum conditions are showed at Table 1. The results show that there is a significant relationship between TPC and the antioxidant activity. The highest amount for TPC, TFC, IC_{50}, FRAP and BCB was found in H_2O and CH_3OH and the lowest value was observed in n- hexane. Also, the amount of TFC in CH_3OH was more than other solvents, which can be related to the better extraction of flavonoid aglycones in CH_3OH in addition to flavonoid glycones in this solvent.

Table1. The results TPC, TFC, IC_{50}, FRAP and BCB in the optimum conditions of extraction

		Time(min)	Solvent	Method
aTPC	221.90±1.25	120	H_2O	soxhlet
bTFC	60.68±1.90	90	CH_3OH	ultrasonic waves
cIC50	0.458±.0.01	120	H2O	soxhlet
dFRAP	993.17±0.05	60	H_2O	soxhlet
BCB	56.35±.10	120	H_2O	soxhlet

[a]mg GAE/g extract; [b] mg quercetin/ g extract; [c] mg/mL; [d]mmol Fe^{2+}/ g extract.

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Paper code: 859

Optimization of extraction process of *Arenaria hispanica* L. using response surface methodology

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The selection of appropriate conditions for increasing the extraction efficiency is important. The response surface method (RSM) is a statistical and mathematical technique which it can be used to examine the dependence between the responses with variables (dependent and interaction terms) in a process and also determination the optimal conditions [1]. In this study, the experimental design of General full factorial (GFF) was used. The variables were time (30, 60 and 90 min), solvent (water, methanol and n-hexane) and method (maceration and ultrasound-assisted extraction). The main effects and also interaction terms were investigated on amounts of total phenolic content (TPC), total flavonoid content (TFC) and the antioxidant activity (according to DPPH, FRAP, IC50 and BCB) of extract of *Arenaria hispanica L.* A multiple regression, first degree model was used to express the responses. An analysis of variance (ANOVA) with 95% confidence level was then carried out for each response (TPC, TFC, IC_{50}, FRAP and BCB) in order to test the model significance and suitability. The significance of independent variables in the form of main effect and interaction terms were analyzed by computing the F-value at probability (p) of 0.001 and 0.05. Water was optimal solvent for TPC, FRAP and BCB, but methanol solvent was obtained for TFC. Also, the extraction time for TPC, TFC, IC50, FRAP and BCB responses was 60, 30, 60, 90 and 30 min; respectively. The maceration was selected for all responses except of TFC. The mounts of TPC, TFC, IC_{50}, FRAP and BCB in the optimum conditions obtained 173.93±0.50(mg GA/g extract), 184.27±4.04(mg QC/g extract), 0.69±0.03 (mg/mL), 734.80±2.02(mmol Fe^{2+}/g exctract) and 21.23±0.22; respectively. Also, the experimental values were in close agreement with values predicated by model.

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Paper code: 873

Synthesis and identification of nano structures of chalcopyrite by $CuFeS_2$ solvothermaite method

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Chalcopyrite $CuFeS_2$ was prepared by solvent process. It is used as an active species to produce cathode lithium ion batteries along with some conductive materials [1]. $CuFeS_2$, a ternary semiconductor belonging to I–III–VI_2 groups, is known as an antiferromagnetic semiconductor with chalcopyrite structure. The structure can be considered as a double sphalerite cell with an ordered arrangement of Cu and Fe ions in the lattice which are in tetrahedral coordination with sulfur. Because of its special structure, $CuFeS_2$ has high conductivity (103 S cm-1 at 100 K) and good electrochemical properties, Therefore it has many potential applications in solar cells, lithium-ion batteries, detectors, optical parametric oscillators, and light-emitting diodes [2]. In this work, firstly, a certain amount of $CuCl_2$, $SC(NH_2)_2$ and $FeSO_4$, was dissolved separately in the distilled water and mixed together. Then, the optimum amount of poly-(PVP) was added to the obtained solution. The solution was then stirred at the room temperature, for 10 min After that, the solution was transferred to the autoclave and heated for 32 h at 190 ^{o}c. Then synthesized black powder was washed wisth distilled water and absolute ethanol and acid to remove any unreacted reagents and was dried in the vacume oven at 60 ^{o}c for 24h.

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Paper code: 886

ZnS@CdS core/shell quantum dots as photokilling agents for pathogenic bacteria

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Recently, research into various kinds of hybrid nanocrystals, such as core/shell quantum dot (QD) nanocomposites, has become an attractive topic in the field of antibacteria and anti-mold technology [1]. These hybrid systems exhibit new properties and functionalities due to the strong interaction between the two different functional components. Several groups have attempted to fabricate the reverse type-I core/shell QDs, where a material with narrower band gap was overgrown onto the core with a wider band gap, and a significant red-shift of the band gap has been observed. In these nanostructures, shell acts as electron and hole sinks and hinder the recombination of photoinduced electrons and holes in the core. Subsequently, the photoinduced electrons can be captured by the adsorbed O_2 and the holes can be trapped by the surface hydroxyl, both resulting in the formation of hydroxyl radical species. It was known that hydroxyl radical species are harmful to microbes due to their high oxidative capacity.

Herein, the ZnS@CdS core/shell QDs, which is conventionally considered as a reverse type-I structure, were prepared and then structural, morphological (shape and size) and optical properties of these nanostructures were characterized by X-ray diffraction (XRD), scanning and transmission electron microscopy (SEM and TEM) and UV-Vis and fluorescence spectroscopy techniques. Detailed investigations of the antibacterial photocatalytic activity of QDs were also carried out using disc diffusion and broth tube dilution methods against *E. coli* and *S. saprophyticus* as model strains of gram-negative and gram-positive bacteria. Compared to ZnS and CdS, the as-formed ZnS@CdS nanohybrid was found to give highly improved bactericidal activity and recyclability toward both gram-positive and -negative cells. Moreover, the minimum inhibitory concentration values of ZnS@CdS nanocomposites were 400.0 μg ml^{-1} for *E. coli* and 300.0 μg ml^{-1} for *S. saprophyticus*, respectively. On the basis of our results, we can conclude that the ZnS@CdS core/shell nanocomposite is a promising candidate for the photocatalytic destruction of bacterial cells.

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Paper code: 887

A fast and green photodegradation approach based on functionalized quantum dots for removal of anthracene from aqueous media

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The impact of pollution is highest due to oil spreads in marine and terrestrial ecosystem, which are a mixture of pollutants like petroleum hydrocarbons (PHCs), polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), heavy metals etc. [1]. In this research, an efficient UV-driven photodegradation approach based on pure zinc sulfide (ZnS) quantum dots (QDs) functionalized with l-cysteine was presented for photodecolorization of anthracene as an industrial pollutant. ZnS QDs were prepared using a water-based chemical precipitation method, at room temperature [2]. Various techniques including X-ray diffraction, transmission electron microscopy, UV–Vis spectrophotometry and fluorescence spectroscopy were performed for characterization of as-prepared QD samples. After characterization, ultra-small (<1 nm) QDs were used as green nanophotocatalysts for the removal of anthracene from aqueous solutions. After optimization the affecting experimental parameters, high efficiency for anthracene removal was achieved using low amount of ZnS QDs (6 mg) at alkaline pH solutions (10) after 15 min ultraviolet irradiation to 50 mL sample solution . Reusability, kinetic model and possible mechanism were also investigated. The results show reasonable reusability after at-least five cycles.

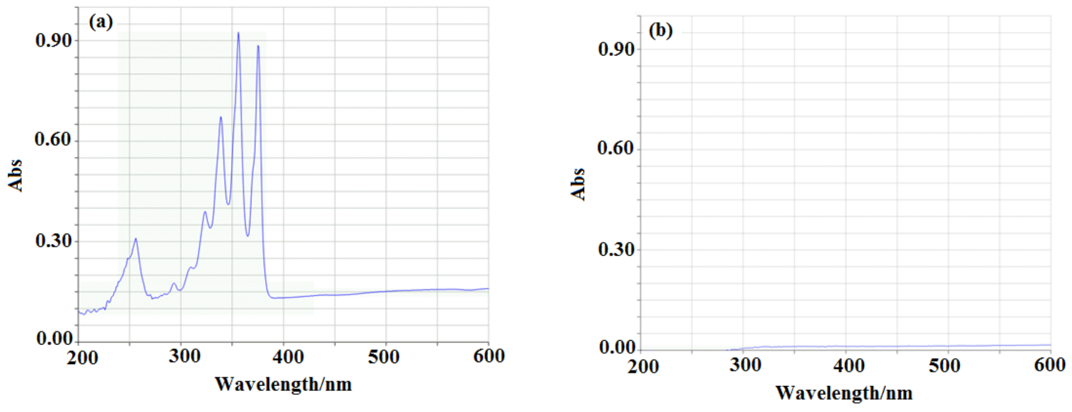

Fig. 1 The change in absorbance spectrum of anthracene (a) before, (b) after addition of ZnS QDs and 15 min UV-irradiation.

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Paper code: 892

Effect of synthesis temperature on the crystal structure of nano-sized CdS spheres synthesized by Ultrasonic assisted Hydrothermal method

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Among the II-VI semiconductors, CdS is one of the most important wide gap semiconductors with a $\Delta E_g \sim 2.5$ eV for the bulk hexagonal wurtzite phase. Many researchers have carried out studies on CdS because it has numerous applications; for example, as a photocatalyst, solar cells and light-emitting diodes [1], piezoelectric[2], optoelectronic [3]. In the present study, nano-sized CdS spheres were synthesized by hydrothermal reactions between $Cd(NO_3)_2.4H_2O$ and CH_4N_2S at a constant stoichiometric 1:2 Cd:S molar ratio. Influence of synthesis temperature (120,150,180˚C) was examined for the synthesis of the target. The synthesized nanomaterials were characterized by PXRD and FESEM techniques. Fig.1 shows the PXRD patterns of the obtained samples when the solvent was water and the reaction time was 48h. The PXRD data indicated that the nanomaterials were crystallized well in a hexagonal crystal system with the space group P63mc. The figure shows that when the reaction temperature was 120˚C, there was an obvious impurity cubic CdS peak position in the mixture. However, with increase the reaction time to 150 and then 180˚C, the impurity peak was disappeared. Fig.2 shows the FESEM images of samples. The images show that when the reaction time was 48h, increasing the reaction temperature has no significant effect on the morphology of the targets. The data show that the material is composed of particle and also sphere structures. It is obvious from the images that the reaction temperature 150 ˚C, produces material with almost particle morphology. However, when the reaction temperature was 120 and 180 ˚C, the morphology of the targets is large size sphere.

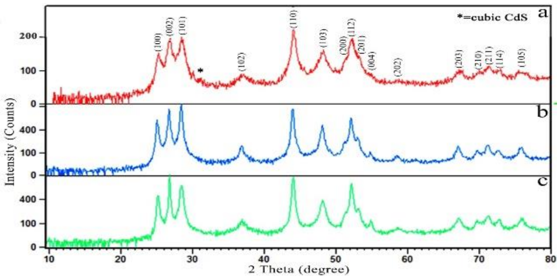

Fig. 1 The PXRD patterns (a)120˚ (b)150˚ (c)180˚

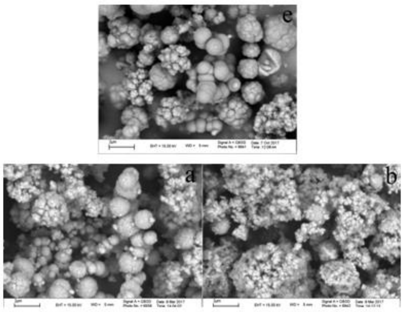

Fig.2 FESEM images (a) 120˚ (b)150˚ (e)180˚

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Paper code: 895

Immobilized Lipase on graphene oxide as Biocatalyst for the Synthesis of Heterocyclic Compounds

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Enzyme as an important group of biocatalyst is superior over chemical catalyst because of its high effectiveness, high specificity and green reaction condition. Among the enzymes from abundant sources, lipase have been widely used including enantioselective hydrolysis, chiral resolution, esterification, synthesis of enantioenriched monomers, and other enzymatic reactions[1].

For this propose, synthesis and chemical functionalization of GO@lipase: In order to prepare GO nanosheet, Functionalization of graphen oxide with APTES. lipase (lipase from Asperjillus Niger) was immobilized on to the GO@NH_2 via covalent binding through GA activation procedure[2]. The synthesized nanobiocatalyst analysed by transmission electron microscopy (TEM), scanning electron microscope (SEM), IR spectroscopy, X-ray diffraction (XRD) and thermogravimetric analysis (TGA). The scanning electron microscope micrographs for the GO nanosheet with bound lipase are shown in Figure 1. According to the SEM pattern, the surface morphology of coated sample (GO@lipas) in shown in Figure 1. This synthesized catalyst could be used in the synthesis of heterocyclic compounds.

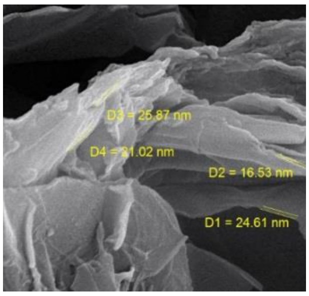
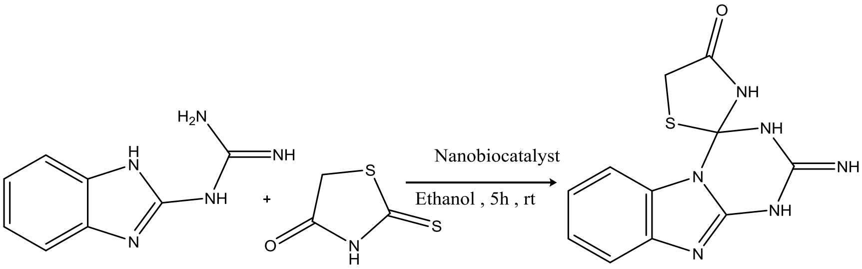


Fig. 1 SEM image of Nano GO@Lipas.



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Paper code: 913

Thermocatalytic activity of $CuCo_2O_4$ nanoparticles prepared by sol-gel method

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Complex oxides with spinel structure are of intense interests in material research because of their remarkable optical, electrical, magnetic, catalytic properties. Ammonium perchlorate (AP) is the main composition in many propellants. The activation energy, reaction rate and pyrolysis temperature of the thermal decomposition of AP are related to the properties of solid propellants, especially the combustion rate [1], [2].

In this research, $CuCo_2O_4$ nanoparticles have been successfully prepared via a simple and facile sol–gel method. Scanning electron microscope (SEM) and transmission electron microscope (TEM) images reveals that the product consisting of spherical nanocrystals of about 25-40nm diameter. X-ray diffraction (XRD) results showed that nanoparticles were in face-centered cubic crystal phase. Chemical composition of the prepared nanoparticles is evaluated by fourier transform infrared (FTIR) spectroscopy. Thermal formation of $CuCo_2O_4$ nanoparticles and its thermocatalytic activity towards thermal decomposition of ammonium perchlorate (AP) were investigated using differential scanning calorimetry (DSC) technique and results showed that the thermal decomposition temperature of AP shift downward about 103 °C, (Figure 1). Two mechanisms based on proton and electron transfer processes have also been proposed for AP decomposition in the presence of nano-sized $CuCo_2O_4$.

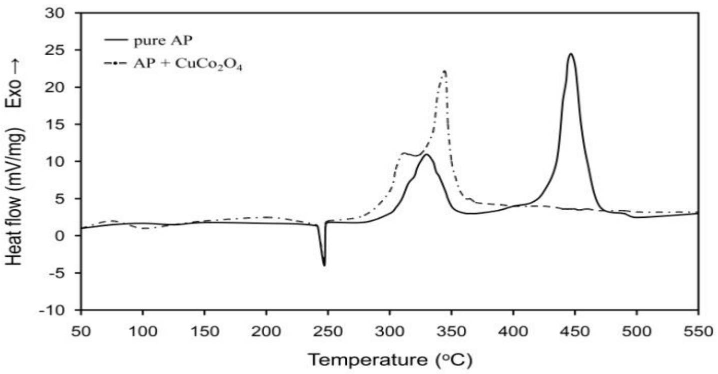

Fig. 1 DSC curves of pure AP and AP with synthesized $CuCo_2O_4$ nanoparticles.

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Paper code: 916

Design of headspace paper sensor for determination of Arsenic (III) in drinking waters using smart mobile phone based on chemical hydride generation

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Arsenic is one of the most environmental drinking water pollutants. [1]. A large number of analytical methods have been reported for the analysis of arsenic. But this methods need complex and expensive tools with high operating costs. In the present study, a simple and portable paper sensor was designed for trace colorimetric analysis of arsenic in drinking waters using mobile smart phone. This paper sensor don’t need any laboratory equipment and skilled workers. For the fabrication of the paper sensor, filter paper, sticker templates with circle patterns and a waterproof eye pencil were used [2]. The proposed method involves in situ arsine generation, transfer of the volatile to the headspace and its reaction with mercury (II) bromide at the detection zone of a paper sensor. The chemical reaction between mercury (II) bromide and arsenic results in the formation of a yellow-brown product which can be analyzed by a smartphone that connected with the image processing application (Image J). Experimental parameters, namely composition of the paper sensor and hydride generation factors were optimized. Under optimal conditions, the limit of detection and the relative standard deviation were 10 ngmL^{-1} and 5.6%, respectively. The obtained calibration curve has two linear ranges of 20–100 ngmL^{-1} and 100–500 ngmL^{-1}. Remarkably, the limit of detection of the method reported herein was as same as the maximum contaminant levels set by the World Health Organization in drinking water. As the result, the paper sensor could be used to determine arsenic concentration in water samples.

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Paper code: 917

Synthesis, characterization and antimicrobial activity of zinc oxide nanoparticles prepared by a green approach based on extract of *Seidlitzia rosmarinus* after microwave and maceration extraction method

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Microwave-assisted extraction (MAE) has been accepted as a potential and powerful alternative for the extraction of organic compounds from plant materials. This extraction technique with shortened extraction time, reduced solvent consumption, increased pollution prevention, and with special care for the constituents has gained attention [1].*Seidlitzia rosmarinus* is a perennial woody plant grown mostly along the banks of salt marshes and in soils with high saline water tables [2]. In this research, the aqueous extract of *Seidlitzia rosmarinus* plant was obtained in the various frequencies of microwave irradiation (90 and 270W) as well as maceration methods. The obtained extracts were used as a natural stabilizer and capping reagent for green synthesis of zinc oxide nanoparticles. Characterization of as-prepared ZnO NPs was carried out by various techniques such as SEM, XRD, UV-Vis absorption and fluorescence spectroscopics (Fig.1). In addition, antimicrobial activities of the samples were investigated with well diffusion (WD) technique; minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) methods. The antibacterial testing showed that the sample has acceptable antibacterial activity. Anti-bacterial properties of the samples prepared by MAE were more than maceration method.

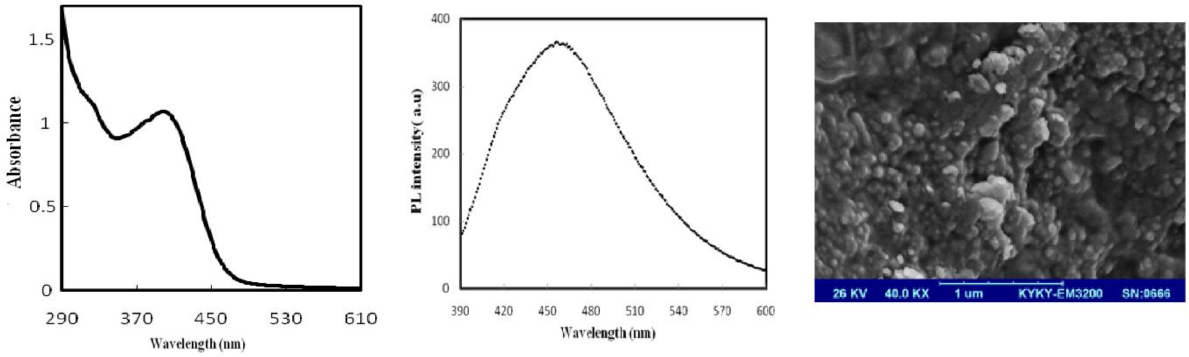

Fig.1. Typical results of absorption, fluorescence and SEM image of ZnO NPs.

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Paper code: 928

Heteroatom-doped porous carbon nanospheres for selective oxidation of alcohols

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The oxidation of alcohols to carbonyl compounds is a fundamentally important organic transformation, and thus, extensive effort has been devoted to verifying the catalytic activity and, in particular, to achieving a selectivity of heterogeneous catalysts in the oxidation of alcohols [1, 2]. Recently, Au, Pd, Mn_2O_3, Fe_3O_4, TiO_2-based hybrid nanoparticles were found to Show high efficiency as a catalyst for the oxidation of alcohols. Herein, we report the synthesis of Pd@P-doped Carbon spheres and their high catalytic activity resulting from entirely exposed Pd particles and highly porous Carbon support. This hybrid Pd@P-doped Carbon spheres efficiently catalyze the oxidation of benzyl alcohol as well as that of various substituted benzyl alcohols. Combined high catalytic activity and thermal stability were achieved with a well-structured nanoparticles which were synthesized by a hydrothermal method for carbonization of glucose in presence of phosphine as phosphor precursor. Pd nanoparticles were then produced on phosphorous doped porous carbon spheres.

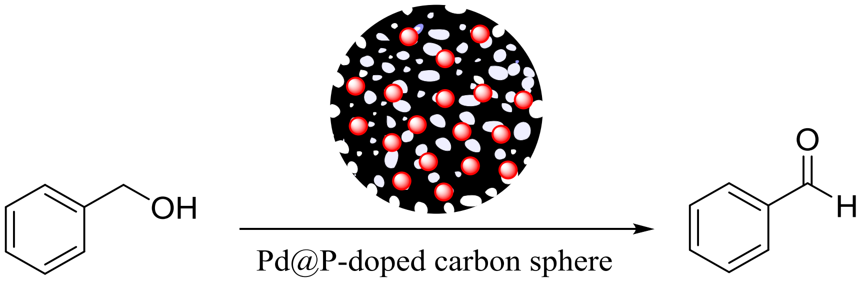

Fig. 1 Schematic pathway of reaction.

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Paper code: 929

Synthesis of nanoparticles within the modified pores of SBA-15: An efficient catalyst for reduction reaction

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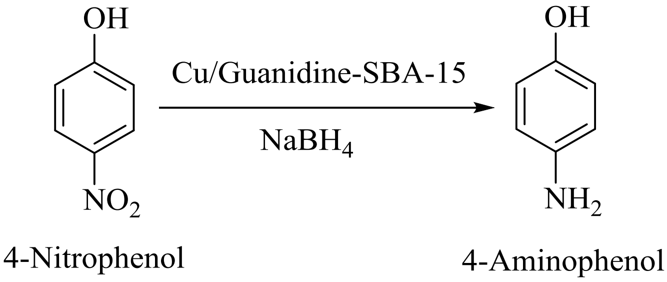
We have developed Cu NP dispersed on mesoporous silica (SBA-15) catalyst for the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP). This catalyst can offer several advantages, such as (i) due to high surface area and porous structure of the silica support, the reactants get easy access to the active catalytic site, i.e. CuNP, (ii) growth of CuNP within the pores of SBA-15 helps to prevent agglomeration and leaching of CuNP, (iii) this supported catalyst can easily be separated from the reaction mixture at the end of the reaction by simple filtration or centrifugation. In this paper, we report the synthesis of CuNP-dispersed on aminoguanidine modified SBA-15. Initially Cu^{2+} ions were adsorbed on the modified pore surface of SBA-15 followed by their reduction by trisodiumcitrate. Citrate ions help to control and stabilize the size of CuNP by complexing with it. Reduction reaction of 4-nitrophenol to 4-aminophenol is important because nitrophenols and their derivatives are formed during the production of pesticides, herbicides, insecticides, synthetic dyes etc. To investigate the catalytic property of the synthesized CuNP containing SBA-15 catalysts, we have studied the reduction reaction of 4-nitrophenol to 4-aminophenol in the presence of excess sodium borohydride. The reaction was monitored by using a UV–Vis spectroscopy.



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Paper code: 935

Cu nano particles supported on graphene oxide nano sheets (CuNPs@GO) for novel synthesis of N-(phenyl(4-phenyl-1H- 1,2,3-triazol—yl) methyl) benzamine

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Graphene oxide supported nanometals such as Cu, Ag, Pd , … has been used as a heterogeneous catalyst for the synthesis of 1, 2, 3- triazoles[1,2]. In this work we hope to use CuNPs@GO as an efficient catalyst in the synthesis of N-(phenyl(4-phenyl-1H-1,2,3-triazol—yl) methyl)benzamine from the the reaction of sodium azide, terminal alkynes, and different imines in H_2O as a green solvent at room temperature. The CuNPs@GO were characterized by FT-IR, CHN, TGA, ICP, XRD, SEM,TEM techniques, successfully.The activity of the prepared catalyst was tested for the synthesis of N-(phenyl(4-phenyl-1H-1,2,3-triazol—yl) methyl) benzamine via click chemistry reactions which lead to the desired products in high yields and short reaction time.

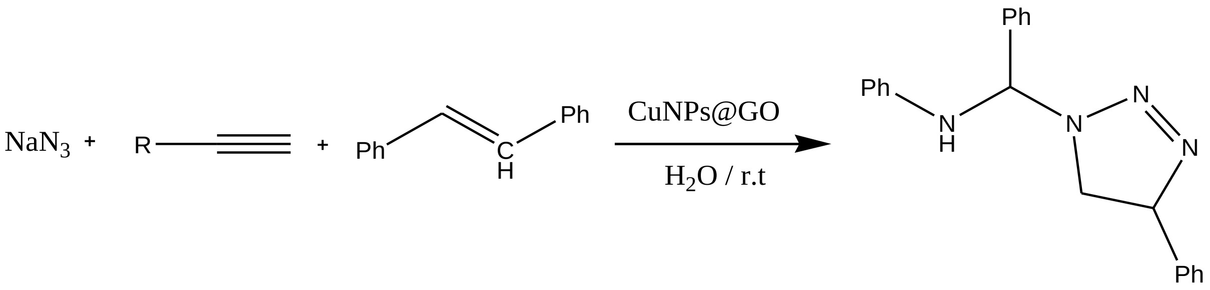

Fig. 1 Schematic pathway of reaction

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Paper code: 937

Investigation of physically treated recycled cross-linked polyethylene foam waste for automotive insulator

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Nowadays recycle of thermoset polymers has attracted for reducing environmental pollution and preserving natural resources. The main purpose of this article is to investigated possible use of recycled commercial cross-linked polyethylene (XLPE) foam waste [1,2]. Structure of the foam was confirmed by using FT-IR technique. The most XLPE structural polyethylene foams are closed cells. Their application is in certain cases, including automotive and building section because of these industries require low weight, high damping of sound and thermal insulting. Physically treated (using two type of milling) recycled of the waste foam obtained from the AKT plant product examined. The recycled foam was added to the original formula of insulating for 55 to 75 min of compounding. Their effect was study in both laboratory (3.5 kg) and industrial (700 kg) scales. Addition of the XLPE waste was not affected on the main characters of the final product in laboratory (tensile strain, elongation at break (Figure 1), shear strain and density). On the other hand, properties such as loss factor slightly change (from 0.060% to 0.056%) and shrinkage (from 1.0% to 2.5%). Although the recycle waste was added to the compound their mechanical properties were not change so much in both laboratory and industrial scales which in using now.

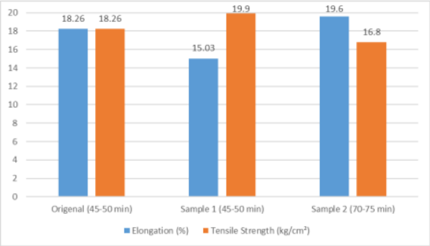

Fig. 1 Schematic of tensile strength results obtained from laboratory sample.

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Paper code: 946

Fatty acid composition and antioxidant activity of *Ferula persica* Boiss

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The human body has several antioxidant defense systems to protect healthy cell membranes from free radicals and active oxygen species. The innate defense systems may be supported by antioxidative compounds taken as foods, cosmetics and medicine. There is an increasing interest in natural antioxidants, e.g., poly-phenols, flavonoids, present in medicinal and dietary plants, which might help prevent oxidative damage [1].

Ferula Persica (Apiaceae) is the well-known species of the genus Ferula that is traditionally used as laxative, carminative, anti-hysteric, and for the treatment of diabetes, rheumatism and backache. *Ferula persica* Boiss. was collected from Shahmirzad (Semnan province). The aerial parts of the plant were dried at room temperature and protected from light and fine powdered. The gas chromatography analysis of the oily mixture, which prepared after soxhlet in hexane and trans-esterification process, was performed with a HP 5890 series II gas chromatograph.

The methanol, methanol/water and aqueous extracts of *Ferula persica* were prepared by maceration method in room temperature and the amounts of total phenolics and flavonoids were estimated [2]. Antioxidant activities of all extracts were evaluated by DPPH radical scavenging and total antioxidant assays [3].

The results of this study have shown that the aerial parts of the plant contain the unsaturated fatty acids: α- linoleic acid (40.6%) and linoleic acid (22.7%) as major components. The aqueous/methanol extract of the Ferula was assigned highest amount of total phenolic (4.39±0.22 mg GAE/gram of dried plant) and highest amount of total flavonoids (18.90±0.44 mg QE/gram of dried plant). The methanol and methanol/water extracts were shown the high DPPH radical activity ($IC_{50} = 40 \pm 0.5$ µg/ml). The methanol/water extract has shown the most effective in the total antioxidant assay against the other extracts. The antiradical and antioxidant activities of the methanol/water extract of *Ferula persica* were correlated with the amounts of total phenolic and flavonoids. It can be concluded that, this plant have the potential that can be used as an accessible source of natural antioxidants with consequent health benefits.

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Paper code: 948

Investigations of Flame-Retarded Poly(Imide−Urethane)s Containing Phosphorus Units

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An attractive synthetic method to improve the properties, especially the flame retardant characteristics, is the utilization of monomers containing phosphorus, such as 9,10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide (DOPO) which possess a polar P=O group and a bulky structure. The introduction of DOPO groups into the macromolecular chains leads to polymers having improved flame retardancy, thermal oxidative stability, and solubility in organic solvents, good adhesion and low birefringence. The use of DOPO and its derivatives as flame retardants for polymers has been widely investigated due to its high thermal stability, good oxidation and hydrolysis resistance [1,2].

In the research, we would like to report a new method for the synthesis of flame retarded poly(urethane-imide) (PUI). Thermal, and flame retardant properties of nanocomposites was determined using suitable techniques such as thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and limiting oxygen index (LOI).

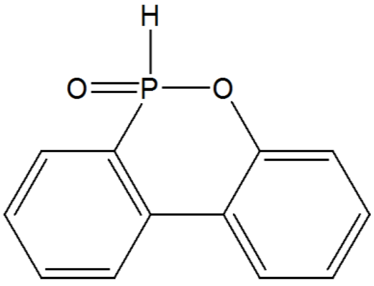

Fig. 1 Structure of DOPO.

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Paper code: 957

Efficient visible light photocatalytic activity based on magnetic graphene oxide decorated ZnO/ZrO_2

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In the present study, ZnO/ZrO_2/MGO nanocomposite were successfully prepared by an hydrothermal process. The obtained sample were characterized by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), Raman spectroscopy, PL spectrum. The observation of diffuse reflectance spoctroscopy (DRS) showed that the energy gap of ZnO/ZrO_2 nanoparticles were supported on Graphene oxide, are lower than that of ZrO_2. The results show that, the addition of ZrO_2 to ZnO decreased the electron-hole recombination and increased the rate of radicals formation [1,2]. The photocatalytic activity of all samples is evaluated by degradation of RhB under visible light irradiation [3]. The nanocomposite ZnZrMGO exhibited the superior activity relative to the pure nanoparticles. In addition, influence of pH, quantity of catalyst, dosage of ZrO_2 and ZnO on the degradation activity was investigated in detail and the results were discussed.

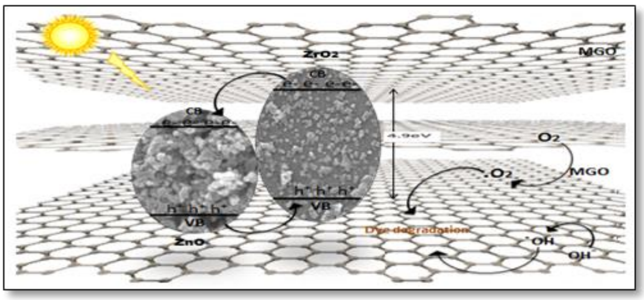

Fig.1 Proposed mechanism for photocatalytic degradation

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Paper code: 960

Proposition of Activated Carbon Use in Structure of BCT Absorbent and Catalyst

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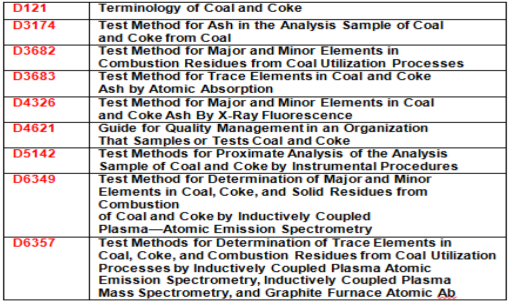
Petroleum coke, or "petcoke" for short, is no longer a left-over by product of the “bottom-of the-barrel" refinery processes whose chief purpose is the production of other products. "Petcoke" can be produced from virgin crude residues by precipitation reactions of high molecular weight compounds, asphaltenes, and resins or from highly aromatic tar or decanted oil stokes by condensation and polymerization of aromatic compounds. The Sulfur content of the "petcoke" strongly depends on the nature of the coking feedstock (crude oil) and its Sulfur content [1]. Standard test method for total Sulfur in coal and coke combustion residues using a high-temperature tube furnace combustion method with infrared absorption has been introduced which is mentioned in the bellow table [2].

Table: The standard method of desulfurization "petcoke"



D121	Terminology of Coal and Coke
D3174	Test Method for Ash in the Analysis Sample of Coal and Coke from Coal
D3682	Test Method for Major and Minor Elements in Combustion Residues from Coal Utilization Processes
D3683	Test Method for Trace Elements in Coal and Coke Ash by Atomic Absorption
D4326	Test Method for Major and Minor Elements in Coal and Coke Ash By X-Ray Fluorescence
D4621	Guide for Quality Management in an Organization That Samples or Tests Coal and Coke
D5142	Test Methods for Proximate Analysis of the Analysis Sample of Coal and Coke by Instrumental Procedures
D6349	Test Method for Determination of Major and Minor Elements in Coal, Coke, and Solid Residues from Combustion of Coal and Coke by Inductively Coupled Plasma—Atomic Emission Spectrometry
D6357	Test Methods for Determination of Trace Elements in Coal, Coke, and Combustion Residues from Coal Utilization Processes by Inductively Coupled Plasma Atomic Emission Spectrometry, Inductively Coupled Plasma Mass Spectrometry, and Graphite Furnace Atomic Ab

Carbon is used in the Aluminum industry, preparation of nanostructures, Carbon fibers, and electrodes. The activated Carbon derived from the desulphurization of "petcoke" in the structure of BCT catalyst and absorber has used by Yousofvand[3]. This patent will be used by the State Environmental Protection Agency of the Islamic Republic of Iran in order to control the quality of urban pollution which has been caused by the Sulfates.

Desulphurization of "petcoke" is done by using Hydrogen at the temperature of 800 °C. Our proposed method in this paper in order to produce the "petcoke" is the production of Sulfur lasers in the plasma environment.

Adding the produced activated Carbon to the BCT catalyst and absorber, causes it's instability and increases the rate of Sulfate pollutant absorption.

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Paper code: 962

The effect of neutron radiation on the activity of urease enzyme

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The urease enzyme belongs to a large family of amidohydrolases and phosphorescens [1]. The enzyme is used as a catalyst for the hydrolysis of urea to carbon dioxide and ammonia. Specifically, urea accelerates urea hydrolysis to produce ammonia and carbamates. Carbamates that are produced during hydrolysis are degraded to ammonia and carbonic acid [2]. The activity of urease, due to the production of ammonia, increases pH of the medium .Neutron radiations have a range of energy-related collisions with matter, including collisions such as elastic, non-elastic, neutron absorption, nuclear fission. In this study, pH changes during the hydrolysis by urease were measured under Neutron radiation at different times, 24, 48 and 72 hours. The solutions of enzyme ($0.5 mg.ml^{-1}$) were prepared in phosphate buffer, pH 7. The enzyme was exposed under neutron radiation. After the desired time, the enzymatic reaction was started by adding the enzyme solution to the urea solution. The pH changes represent the activity of the enzyme. The maximum activity of the enzyme was observed in the presence of radiation and increasing the radiation time caused an increase in enzymatic activity. The effect of irradiation time is such that with increasing time, the pH changes also increase enzymatic activity which is probably due to the structural changes applied by the beam to the structure of the enzyme urease.

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Paper code: 970

Plant-mediated green synthesis of Ag, Cu, Pd and Au metallic nanoparticles for environmental and catalytic applications

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In recent years, nanotechnology converts to an attractive research field which increasingly progressed in the field of materials technology. Up to now, different physical, chemical and biological methods for preparation of nanoparticles have been reported [1, 2]. However, chemists generally work on designation and performance of eco-friendly chemical processes to produce safer products, thus nanobiotechnology numbered among the most promising areas of nanoscience [3]. Biological methods of nanostructure synthesis using bacteria, fungi, yeast and plants benefits to many aspects such as no requirement to the usage of hazardous chemicals, large amounts of energy, high temperature or pressure and do not producing the toxic products [2,3]. In green synthesis process using plant extracts, nanoparticles are generated through biological reductions undergo plant biomolecules as stabilizing, capping and reducing agents [2,3]. Different characterization methods such as UV-Vis, FT-IR, XRD, FESEM, EDS, VSM, BET and TEM techniques can be used to identification of nanoparticles. Due to their large surface area, nanomaterials can be used as catalyst in organic transformations. However, to prevent the agglomeration of small NPs, employing the solid supports is of great importance. Some of the advantages of nano catalysts are improving the efficiency and selectivity of chemical processes, energy saving and increasing the purity of the products.

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Paper code: 972

Effects of Palmitic Acid@SiO$_2$ on the Synthesis of Microcellular Polyurethane foam

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Polyurethane microcellular foams with the high cell density and small cell size are a new class of polymers. These foams provide many excellent thermal and mechanical properties such as higher impact strength, increased fatigue life, higher thoughness and enhanced thermal stability compared with ordinary foams. Microcellular PU foams are used in many applications such as automobiles, electronics, sporting goods, footwears, coatings and foam industries [1]. The use of functional materials such as phase change materials (PCMs) can greatly improve the energy storage properties of the foams.

PCMs are important materials in subject of thermal energy storage which have high latent heat values and can absorb or release a large amount of energy while the temperature of the materials are kept constant during a phase change process. There are three type of PCM: organic (paraffin and fatty acids), inorganic (salts, metals and etc) and eutectic PCM. The combination of PU foams and PCMs was developed the thermal insulation and thermal energy storage. PCM can be incorporated into PU foams by encapsulation. Nanoencapsulation PCM consists of a PCM as core and a polymer or inorganic as shell. In this study, we aimed to incorporate different percentage of Nanoencapsulated PA@SiO$_2$, which contain palmitic acid (PA) as the core and SiO$_2$ as the shell, into the microcellular PU foam. Structure and surface morphology were characterized using IR and SEM. DSC and TGA were used to investigate thermal properties, stability and conductivity [2].

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Paper code: 974

Immobilization of dioxomolybdenum(VI) complex on the Schiff base coated magnetic nanoparticles: A highly active, selective and reusable catalyst in oxidation of sulfides to sulfoxides

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A molybdenum complex was immobilized on amino propyl and Schiff base modified magnetic $Fe_3O_4@SiO_2$ nanoparticles by covalent linkage. The obtained nanoparticles were characterized with various characterization methods and employed as catalysts for the selective oxidation of sulfdes to corresponding sulfoxides using ureahydrogen peroxide as the oxidant. The catalysts showed the similar catalytic activity but different stability and recyclability. Immobilization of Mo(VI) complex on the MNPs trough the Schiff base ligand resulted in the formation of nanocatalyst that could be recycle more than four times. In contrary, the immobilization through the amino propyl linkage did not lead to the formation of a highly stable and fully recyclable nanocatalyst.
The EDX survey of nanocatalyst (Fig. 1) confirmed the presence of molybdenum in the nanoparticles structure.

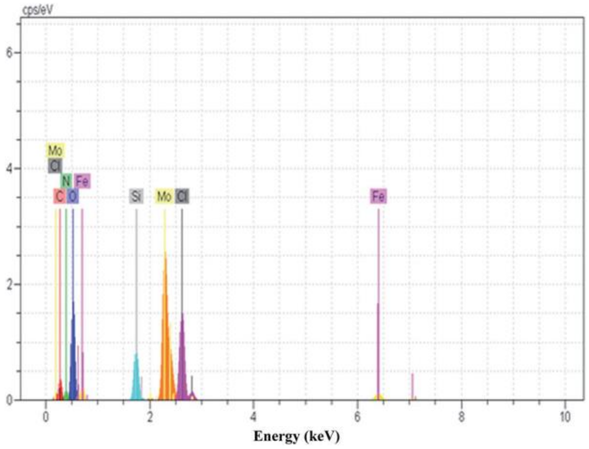

Fig. 1 The energy-dispersive X-ray spectroscopy (EDX) of the nanocatalyst

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Paper code: 984

Green synthesis of graft copolymer of psyllium musilage with acrylamide/acrylic acid and investigation of properties of its hydrogel

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Graft copolymer is a branched polymer having sidechains composed of different monomers to that of the main chain. Graft coplymerization can be used to modify natural polymer such as starch, cellulose , chitosan, guar-gum and psyllium. The modified polymers can be used for removal, separation metal ions from aqueous solutions and can play an important role for environmental remediation of municipal and industrial wastewater[1]psyllium is a medicinal plant, uses against various diseases like constipation, diarrhea and diabetes[2].Its mucilage is composed of arabinose, xylose and traces of other sugars[3].In this study,graft Copolymer of psyllium musilage with acrylamide/acrylic acid was synthesized and converted to hydrogel by using Cross Linker and the amount of absorption was measured by a tea bag To method. To get the highest percentage of water absorption (Ps) in the hydrogel, various parameters, including weight ratio of monomers, type and amount of initiator, type and amount and cross linker, pH, reaction temperature and reaction time might be investigated.Maximum *P*s 4000.194gr/gr was observed at0.05gr of APS in the aqueous solution. FTIR spectrum natural psyllium and grafted psyllium are shown below.

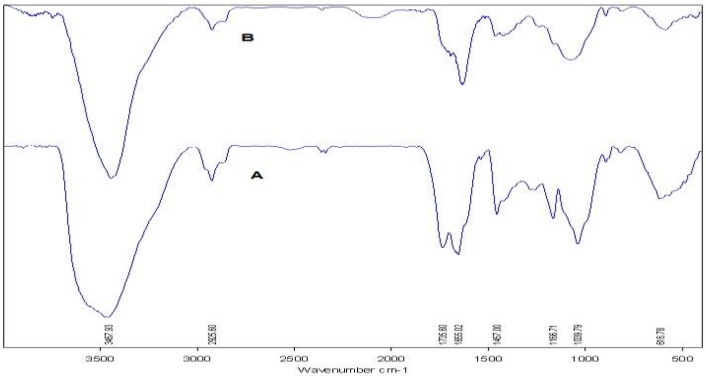

Figure1. FT-IR spectrum a) grafted psyllium b) natural psyllium

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Paper code: 985

The green synthesis of gold nanoparticles using extract of *Dracocephalum kotschyi* Boiss

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The development of green processes for the synthesis of nanoparticles is evolving in to an important branch of nanotechnology [1] gold nanoparticles (Au-NPs) hare many applications in biology such as biosensors and DNA labeling [2]. In this study, Au-NPs were synthesized by extract of *Dracocephalum kotschyi* Boiss. The synthesized gold nanoparticles were characterized by UV- visible spectroscopy, X –ray diffraction (XRD), Fourier transform infrared (FT-IR) and scanning electron microscopy (SEM). The selection of optimum conditions for synthesis of Au-NPs was applied a central composite design (CCD) using Minitab 17software. An analysis of variance (ANOVA) with 95% confidence level was then carried out for each response in order to test the model significance and suitability. The variables were volume of extract, concentration of $HAuCl_4$, pH, temperature and time of extraction. The appearance of a absorption peak at 530 nm of UV- visible spectroscopy and peaks of absorption at 3432, 1631, 1599 and 1384 cm^{-1} for FT-IR spectroscopy and also, the peaks at $2\theta = 38.48$, 44.69, 64.05 and 77.50 degree in XRD confirmed the synthesis of nanoparticles of gold. The average of Au-NPs obtained 37.87 nm (Fig. 1). Also, the optimum conditions synthesis of Au-NPs for the studied variables was 1mL, 0.001 mM, pH 8, 60 min and 90°C.

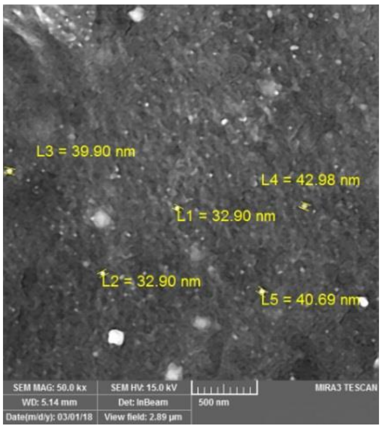

Fig. 1 SEM of gold nanoparticles (Au-NPs)

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Paper code: 986

Synthesis of magnetically separable copper nanocatalyst and their application as an efficient catalyst for C(sp2)–C(sp) and C(sp2)–C(sp2) cross-coupling reactions

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A copper complex was immobilized on Schiff base modified magnetic Fe_3O_4@SiO_2 nanoparticles by covalent linkage. The obtained nanoparticles were identified with various characterization methods. The nanocatalyst shows good activity toward Sonogashira and Suzuki cross-coupling reaction in environmentally friendly solvent (H_2O/DMF) under mild conditions. The catalyst shows not only high catalytic activity, but also offers many practical advantages such recyclability and air stability. Expectedly, the nanocatalyst can be applied in large-scale industrial synthesis.

The SEM micrographs of the products Fe_3O_4 and nanocatalyst are given in Fig. 1(a) and Fig. 1(b) respectively. It was found that the nanoparticles were present as uniform particles with spherical morphology. SEM images reveal that Fe_3O_4 particles are aggregated particles having rough external surfaces (Fig. 1(a)). Silica coating makes the particles exhibit smooth and spongy surfaces (Fig. 1(b)) which indicatives the successful coating of silica over the magnetic nanoparticles. However, the nanocatalyst particles still fall in the nano-size range.

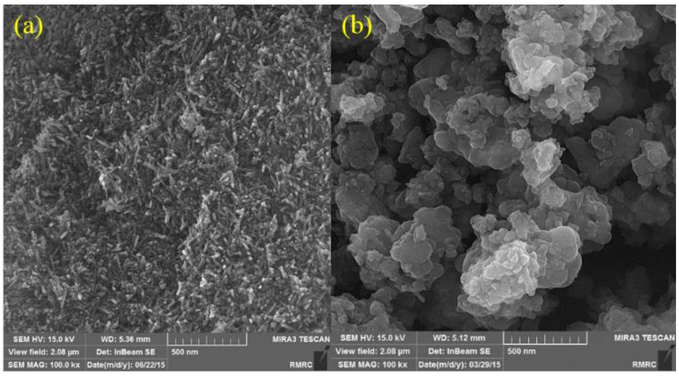

Fig. 1(a) SEM images of Fe_3O_4 and (b) nanocatalyst

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Paper code: 988

Antibacterial properties of polyethylene containing thymol and silver nanoparticles against *Aeromonas hydrophila*

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Recently, there has been a tremendous research work on the development of food packaging films that can be employed for controlling the microbiological decay of perishable food products [1]. One option is to use packaging to provide an increased margin of safety and quality. The next generation of food packaging may include materials with antimicrobial properties. These packaging technologies could play a role in extending shelf-life of foods and reduce the risk from pathogens. Antimicrobial polymers may find use in other food contact applications as well [2].

Thus, the antibacterial properties of polyethylene samples containing silver nanoparticles and thymol were evaluated by disk diffusion method against Aquaculture pathogenic bacteria, *Aeromonas hydrophila* and the diameter of the zone inhibition of bacteria for polyethylene containing Ag nanoparticles was 7.92 mm and polyethylene with 0.5 wt% of thymol, was 7.45 mm, and polyethylene with 1.5 wt% and 5 wt% of thymol had no antimicrobial properties.

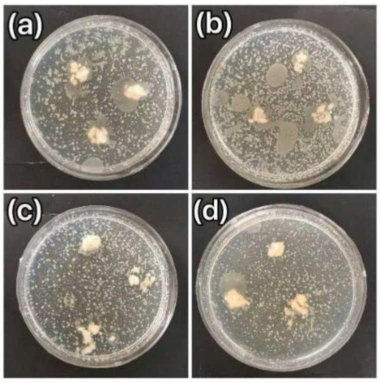

Fig 1. Representative photographs of the antibacterial activity against *Aeromonas hydrophila*: (a) PE/Ag nanoparticles, (b) PE with 0.5 wt% of thymol, (c) PE with 1.5 wt% of thymol, (d) PE with 5 wt% of thymol

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Paper code: 989

Chitosan/bentonite/ZnO nanoparticles composites: From synthesis to antibacterial properties

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In recent years, designing of environmentally friendly and high performance materials based on biodegradable polymeric systems have much interest in scientific researches. The benefit of using biodegradable polymers is their potential of decomposing naturally over short periods of time in nature [1]. Nowadays, attention is great to Chitosan due to the wide range of applications, especially in the aquaculture hatcheries systems, because of its ease of moulding into gel, sponge, nanocomposite, scaffolds, powder, beads, and films [2]. The antibacterial activity of the composites were evaluated against *Streptococcus iniae* and the diameter of the zone inhibition of bacteria for the composite containing CS (4 g), BN (2 g) and ZnO (20 mg), was 20.2 mm, the composite containing CS (4 g), BN (4 g) and ZnO (20 mg), was 11.54 mm, the composite containing CS (4 g), BN (2 g) and ZnO (60 mg), was 11.62 mm, and the composite containing CS (4 g), BN (4 g) and ZnO (60 mg) had no antimicrobial properties (fig. 1). The antibacterial activity of these composites provides the possibility of further clinical investigations leading to its application in aquaculture industry.

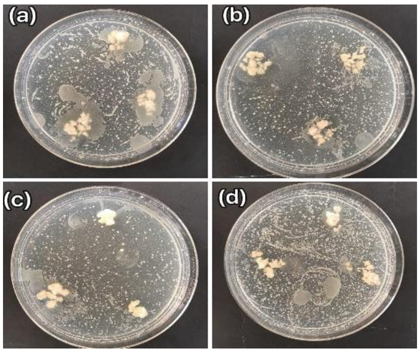

Fig 1. Representative photographs of the antibacterial activity CS/BN/ZnO nanoparticles composites against *Streptococcus iniae*: (a) CS (4 g), BN (2 g) and ZnO (20 mg), (b) CS (4 g), BN (4 g) and ZnO (20 mg), (c) CS (4 g), BN (2 g) and ZnO (60 mg), (d) CS (4 g), BN (4 g) and ZnO (60 mg).

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Paper code: 995

synthesis of graft copolymer of itaconic acid/acrylamide on starch and investigation of water absorption behavior of its hydrogel

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Hydrogels are a group of polymeric materials have swelling and water absorption properties due to their hydrophilic structure. We can use natural polymer such as a starch, and their derivatives in the synthesis of hydrogel due to low cost and biodegradable [1,2].

The aim of the present research was synthesize the graft copolymer of itaconic acid / acrylamide onto starch and investigation of water absorption behavior of its hydrogel. For this purpose ammonium persulfate (APS) was used as initiator and 1,4-buthylene bis methacrylate (BGDMA) as cross linker.The effect of various parameters such as monomer concentration, crosslinking agent and initiator concentration, time and tempreture reaction, and pH might be investigated on grafting efficiency and adsorption capacity of the starch hydrogels. Percentage of water swelling (PS) of hydrogel was investigated by tea bag method. Maximum Ps1848.7 was obtained using 1 g starch, 1g acrylamide, 1 g itaconic acid, 0.01 mL BGDMA, and 0.1g ammonium persulphate (APS) in the aqueous solution. FTIR spectrum natural starch and its grafted copolymer are shown below.

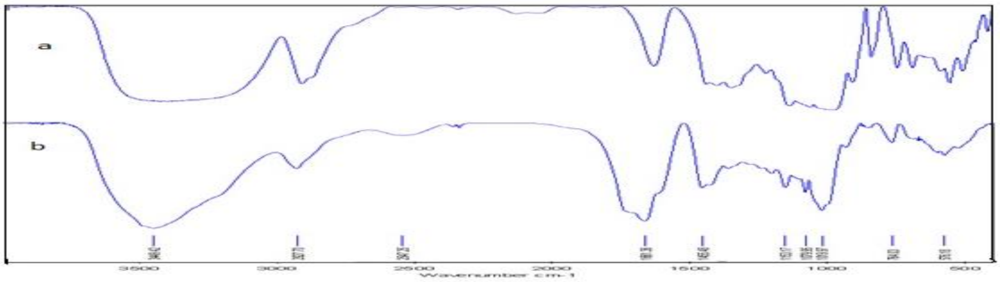

Fig. 1. FT-IR spectrum a) natural starch b) grafted starch

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Paper code: 1000

Surfactant modified clinoptilolite as novel antifungal agents against *Saprolegnia sp.*

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Fungal diseases cause much damage to the aquaculture industry annually. Saprolegnia fungus, in particular, causes mortality in hatchery systems. The control of Saprolegnia on trout eggs is a problem encountered in aquaculture industry. Several methods have been used to control the fungal disease in the past, including the use of Malachite green and formalin. The banning of chemicals increased the demand for finding effective alternative treatments to control the disease [1]. At this study, by using a cationic surfactant, Hexadecyletrimethye ammonium chloride (HDMA), Surface and Layer structure of clinoptilolite and bentonite were modified, respectively. X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, field emission scanning electron microscopy (FESEM), Energy Dispersive X-Ray (EDX) analyses were used to characterize the modified materials. The antifungal activity of HDMA clinoptilolite and bentonite were investigated against Saprolegnia sp. at different amounts of materials and time of exposure. All of the synthesized materials were found to have antifungal activity. These results showed that modified clinoptilolite and bentonite can be used as effective growth inhibitors in different biological systems, making them applicable to applications in aquaculture.

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Paper code: 1002

Polyurethane nanocomposite for removal of Lead from water

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The rapid growth of the human population as well as the released waste waters from various industries, demand for developing an adequate water purification method is necessary. In the past decades there are several methods had been reported in this area which all of them has their own merits and drawbacks namely additives additions into the water wastes and etc. which need some additional recovery and separation methods.

In the recent years a well-known method has been developed for water purification based on using solid polymeric supports enable to capture heavy metals from water wastes.
Among the tested variables, pH was found to be the most critical parameter for the adsorption of metals on nano composite. To evaluate the effect of pH on the retention efficiency, the pH of 10 mL of sample solution containing 5 mg L−1 of lead ions was adjusted to fit in the range of 4-7.

In the current communication the performance of graphene oxide functionalized polyurethane rigid foam is evaluated for removing of heavy metals from drinking water through a cation exchange process is reported. In addition,Fourier transform infrared spectroscopy (FTIR), thermo gravimetric analysis (TGA), were used to characterize the foam and UV technique is done on the untreated and treated samples in order to evaluation of the foam performance.

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Paper code: 1005

Synthesis of nanofibrous composite PAN/Schiff-base as sorbent for adsorption phosphorus-containing as a nerve agents simulant

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Nerve agents are considered the most nefarious of synthetic chemical derivatives. They are potent acetylcholinesterase (AChE) active agents, clearly differentiated from other chemical warfare (CW) type agents (blister, blood, choking, incapacitating, tear and vomit agents) because of their phosphorylating mode of action, derived from their organophosphonate structure. Specifically, this unique structure is the key to its danger expressed by mammalian toxicity nerve agents compared with similar related species (vide infra)[1].

The purpose of this study is to understand and to evaluate the adsorption abilities of electrospun composite nanofibrous against nerve gas simulant dimethyl methylphosphonate (DMMP) along with trimethyl phosphate (TMP), methyl dichlorophosphate (MDCP), and trichlorophosphate (TCP) and assess the possibility of using the electrospun nanofibers as protective membranes in face masks and warfare clothing [2]. Adsorption of stimulants of organophosphonate, was investigated on the surface of PAN nanofibrous embedded with Schiff-base. The result showed the role of modified PAN nanofibrous with schiff-base on the effective adsorption of organophosphonate, as a stimulant of nerve agents, and possesses a suitable candidate for protecting cloth. The surface morphology and other properties of the PAN/Schiff-base composite nanofibrous are characterized by various techniques, including SEM, TEM, FT-IR, TGA and UV-vis spectroscopy.

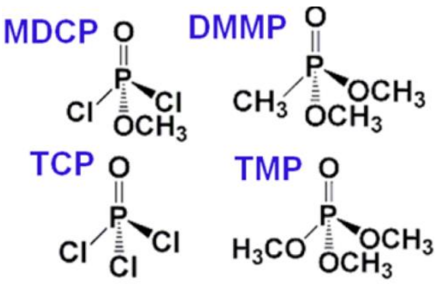

Fig. 1 Structures of Nerve gas simulant

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Paper code: **1007**

Sonochemical Synthesis and Structural Characterization of a New Nanostructured Sm(III) Porous Coordination Polymer

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A novel three dimensional (3D) micro and nano-structure coordination polymers based on $Sm(NO_3)_3.6H_2O$ prepared by the solvothermal and sonochemical methods. Micro size was prepared by reacting the ligands and metal ions at high temperature in autoclave [1,2]. Nanoparticles of this new coordination polymer were synthesized by ultrasonic assistance at different concentrations. The parameters which were affected on micro to nano-structure conversion such as time and power of irradiation, and concentration of initial reagents were optimized. The effect of these parameters was evaluated on size and morphology of nano-porous structures. The results indicated that by increasing the time of ultrasonic radiation, smaller nano-structure was formed and morphology was changed [3].

This porous lanthanide coordination polymer which is shown in Fig.1 was characterized by elemental analysis, FT-IR, scanning electron microscopy (SEM), and single crystal X-ray diffraction analysis. Single-crystal X–ray data show this compound is three-dimensional coordination polymer, and iso-structural which the Ln^{3+} ion is eight-coordinated and linked by two ligands.

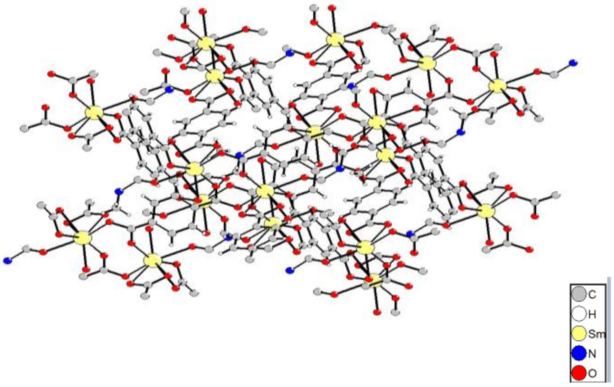

Fig.1 Nano-pore structure of the coordination polymers

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Paper code: 1008

Synthesis of high yield gold nanosheets with electrocatalytic activity toward NADH and investigation of their self-assembly at toluene/water interface

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Two-dimensional (2D) gold nanosheets (AuNSs) are very attractive nanostructures owing to their unique surface features. They have interesting structure due to their micrometer size and nanometer thickness and show surface plasmon resonance (SPR) in the near infrared (NIR) region .[1, 2] These interesting characteristics make these nanostructures as efficient tools for applications in many fields including new nanodevices, electrochemistry, plasmonics, gas sensors, electronics, biosensors and etc.[3] Herein, a simple, in-situ and cost effective method is introduced for high-yield synthesis of thin and large gold nanosheets at room-temperature. In this procedure, carbon nanodendrite structures and Gum Arabic (GA) were used as low-cost, green reducing and shape controlling agents, respectively. Several shapes including triangular, truncated triangular, hexagonal gold nanosheets were prepared. Morphology and structure of the as-synthesized products were characterized using different techniques such as UV-Vis spectroscopy, field emission scanning electron microscopy (FESEM), transition electron microscopy (TEM), X-ray diffraction (XRD) analysis and atomic force microscopy (AFM). Moreover, the self-assembly of gold nanosheets was studied at the toluene/water interface. The synthesized thin gold nanosheets with their sharp edges and corners, exhibited electrocatalytic effects toward NADH oxidation.

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Paper code: 1010

Elaeagnus angustifolia extract-Hydroxyapatite incorporated PCL based nanofibers for bone tissue engineering

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The bone defects due to trauma, inflammation and tumor are very common in clinical practice. A tissue engineering strategy involving the combination of cells, scaffolds and other bioactive agents has emerged as a new approach in bone regeneration. The scaffold serves as an initial structure to retain the cells in the defects and to support the cell growth and phenotype maintenance [1, 2]. Electrospun biocomposite nanofibers mimic the composite nature of bone as well as the nanoscale features of extracellular matrix (ECM). Elaeagnus angustifolia (E.A) is one of the medicinal herbs with antinociceptive, anti-inflammatory, antibacterial and antioxidant properties widely used in the treatment of patients with rheumatoid arthritis and osteoarthritis symptoms. For the first time, E.A-Hydroxyapatite (E.A-HA) was loaded on PCL nanofibers and studied their potential application in bone tissue engineering. Physiochemical and biological properties of these nanofibers were detected. SEM photographs showed that nanofibers had free-bead morphologies. The cell response to the E.A extract-HA loaded PCL based nanofibers was evaluated by human dental pulp stem cells (hDPSCs). hDPSCs showed improved adhesion and proliferation capacity on the E.A-HA loaded nanofibers compare to pristine nanofiber. Alkaline phosphatase activity (ALP) confirmed the nanofibrous scaffolds could induce the osteoblastic performance of hDPSCs ($p<0.01$). The results suggested that E.A-HA loaded with PCL based nanofibers might have potential application for bone tissue engineering.

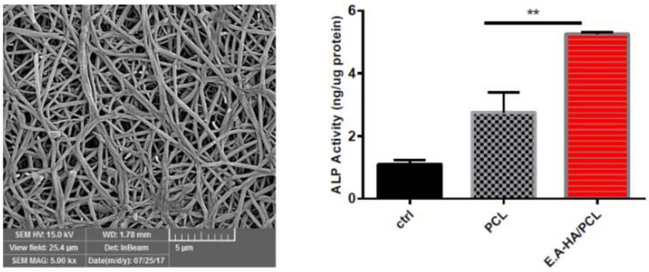

Fig. 1 SEM image and ALP activity of E.A-HA loaded PCL nanofibers

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Paper code: 1012

Synthesis and characterization of Walnut shell/diopside nanocomposite for removal of Congo red dye: Experimental design and optimization

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Recently, removal of different dyes from industrial effluents has got a judgmental subject [1]. Congo red (CR) is pretty toxic agent in terms of its resistance to heat, chemical reagent, and capability of producing cancer and mutagens owing to existence of different reactive center and charge nature [2].

In this research, Walnut shell/diopside nanocomposite were made and used for removal of CR from aqueous solution. The nanocomposites were characterized by FTIR, XRD, and FE-SEM. Also, the surface area, the pore volume and the pore size distribution of the Walnut shell/diopside nanocomposite were calculated by BET technique. Effects of adsorbent dose, initial pH, contact time and the initial dye concentration on CR removal were studied by central composite design (CCD) and the optimized condition obtained at adsorbent dose=0.00875, pH= 4.5, Contact time= 15 min, and initial dye concentration= 65 ppm.

The maximum adsorption capacities (Q_m) calculated by best fitting model (Langmuir) were 333.33 mg/g at 313 K. Also, the adsorption kinetic was well confirmed with pseudo-second-order equation.

Removal of CR by Walnut shell/diopside nanocomposite is shown in Fig. 1.

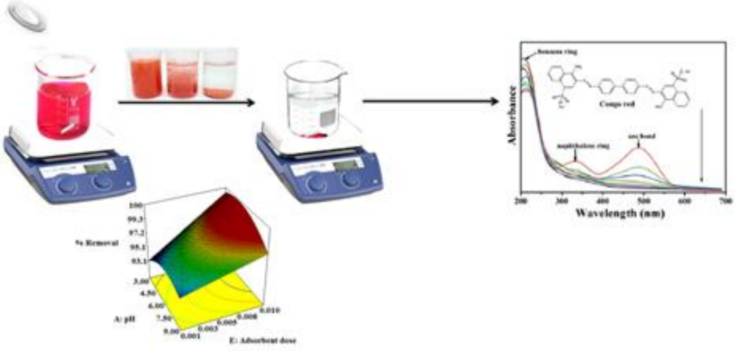

Fig. 1 Optimization of removal of CR from aqueous solutions by Walnut shell/diopside.

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Paper code: 1015

Synthesis of pressure-sensitive adhesives based on butyl acrylate, effect of cross-linking agent

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Pressure-sensitive adhesives (PSAs) are viscoelastic materials which can adhere strongly to solid surfaces upon applying of slight contact pressure with a short time [1]. Synthesis of acrylate PSAs latex is accomplished through out a semi-continuous emulsion polymerization using butyl acrylate and acrylic acid monomers [1,2]. Urea formaldehyde resin (UF) was used as crosslinking agent to controlling the adhesive properties. In this work, effect of prepared urea formaldehyde resin on the latex of copolymer of butyl acrylate and acrylic acid properties such as shear strength, tack and peel strength was investigated. As the amount of urea formaldehyde was increased (up to 3.09%) in the resin, shear strength was increased from 230 kPa to a limited value of about 513 kPa (Figure 1), peel strength were increased from 0.23 N/mm to 0.31 N/mm, however, the amount of tack of the latex was reduced (from 2.9 cm to 5.5 cm).

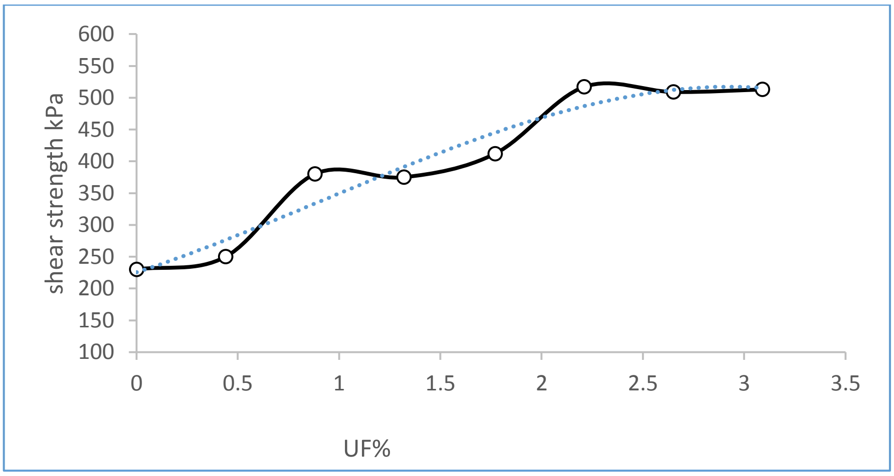

Fig. 1 Effect of urea formaldehyde concentration on shear of the latex.

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Paper code: 1019

s-Triazinium-based ionic liquid immobilized on silica-coated Fe_3O_4 magnetic nanoparticles: an efficient and magnetically separable heterogeneous catalyst for synthesis of dihydropyrano[3,2-*b*]pyran-3-carbonitrile derivatives and evaluation of their antioxidant and antifungal properties

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A new method for heterogenization of s-triazine catalyst has been explored by readily preparation of ionic liquid based s-triazine-immobilized silica-coated Fe_3O_4 magnetic nanoparticles [Fe_3O_4@SiO_2-*s*-triazine]. The structure of newly prepared nanoparticles was characterized by Fourier transform infrared (FT-IR), X-ray powder diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive X-ray (EDX) method, vibrating sample magnetometry (VSM) and thermo gravimetric analysis (TGA).These nanoparticles were identified as an efficient catalyst for the one-pot three-component synthesis of 4,8-dihydro [3,2-*b*] pyran derivatives in excellent yields.The catalyst was easily separated by magnetic decantation and the recovered nanoparticles were reused for four cycles without any significant loss of catalytic activity.The synthesized dihydropyrano[3,2-*b*]pyrans were evaluated for their antioxidant and antifungal activities and found to be relatively active.

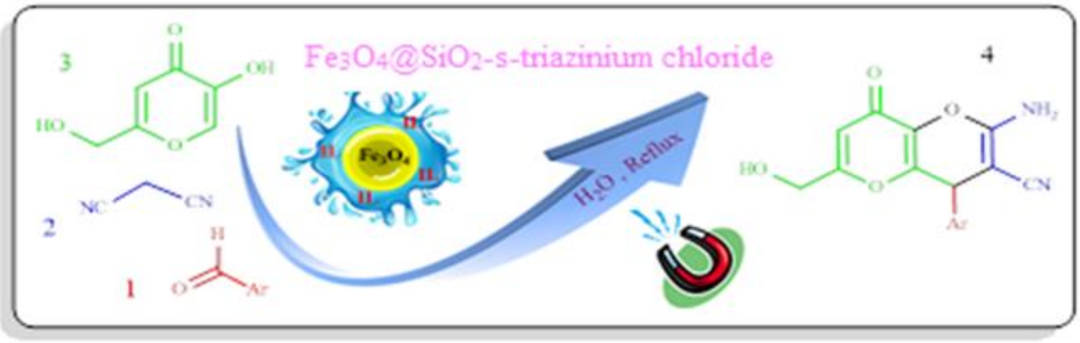

Fig. 1 Synthesis of 4H-pyrano[3,2-b]pyran-carbonitriles catalyzed by Fe3O4@SiO2-s-Triazinium

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Paper code: 1025

Synthesis and characterization of a novel colloidal ceramic nanocomposite coated by Ag nanoparticles

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Today, the synthesis of new nanocomposites is very common due to their importance in various applications such as medical, drug delivery, catalysts, etc. [1]. In this research, ceramic based nanocomposite [2] coated by silver nanoparticles was synthesized using chemical precipitation under the argon gas and was stabilized using two biopolymers stabilizer. The final composite is so stable and colloidal which could be used for different fields such as drug and gene delivery applications. The structure and chemical composition of the synthesized nanocomposite were characterized using FTIR spectroscopy, FESEM and TEM microscopy, DLS, Zeta potential and XRD. Figure 1 shows a schematic structure of the synthesized nanocomposite.

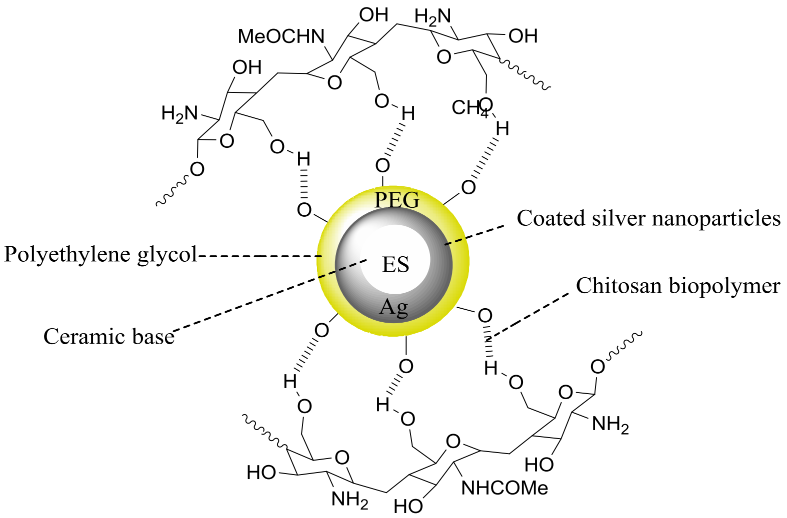

Fig. 1. Schematic structure of the synthesized nanocomposite.

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Paper code: 1052

Functionalized graphene oxide decorated with Au nanoparticles as a designed catalyst for reduction of organic dyes

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The accumulation of organic dyes in the water bodies causes eutrophication, reduces the reoxygenation capacity and makes severe damage to the aquatic organisms by hindering the infiltration of sunlight [1]. The superiority of photocatalytic degradation by nanocatalyts in wastewater treatment is due to its advantages over the conventional methods, such as quick oxidation, no formation of polycyclic products and oxidation of pollutants. It is an effective and rapid technique in the removal of pollutants from wastewater. In this research, Graphene oxide (GO) was first synthesized from natural graphite flakes by a modified Hummers method [1]. In the following, the surface of GO functionalized during several steps. First, carboxilation of GO via reaction with bromoacetic acid and formed GO-COOH. In the other step, the GO-COOH converted to GO-COOCl in the presence of thionylchlorid. The obtained GO from previous step reacted with 4-aminothiophenol which nucleic reaction easily done and SH functional group coordinated with Au (III) ions. Finally Au NPs synthesized by reduction with sodium citrate as a mild and green reducing agent. The synthesized catalyst have been used for the rapid reduction of 4-nitrophenol (4-NP), methyl orange (MO) and methylene blue (MB) in the presence of $NaBH_4$ and shown high catalytic activity.

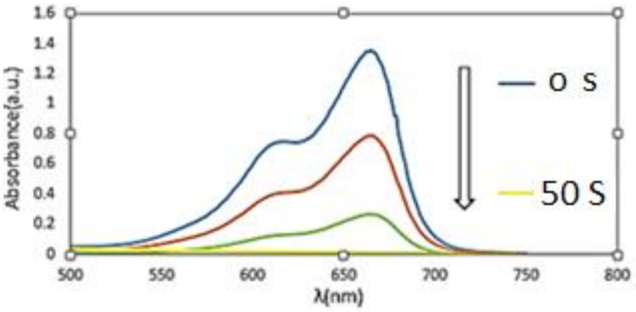

Figure Time dependent UV–Vis absorption spectra for the reduction of MB.

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Paper code: 1055

Aerobic oxidation of organic compounds in the presence of the free base porphyrins and porphyrins supported onto nanostructure solid as **photosensitizer**

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Photosensitizer generation is a simple and controllable method for the production of $^1O_2$ oxygen, requiring light at specific wavelengths, and a photosensitizer capable of absorbing and using that energy to excite oxygen to its singlet state. The types of photosensitizers are: (1) the organic dyes and aromatics; (2) the porphyrins, phthalocyanines, and related macrocycles; (3) semiconductors; and (4) transition metal complexes. The porphyrins and their derivatives have the ability to absorb several wavelengths in the UV-vis range used as photosensitizer in synthetic chemistry and have high photostability compare to other photosensitizers [1].

In recent years, immobilized photosensitizers have been used for generation of singlet oxygen [1-2]. In present study, *meso*-tetrakis(4-hydroxyphenyl)porphyrin (H_2THPP) and *meso*-tetrakis(4-carboxyphenyl)porphyrin (H_2TCPP) immobilized on the functionalized multi-walled carbon nanotubes (MWCNTs) were utilized as highly efficient, stable and reusable heterogeneous photocatalysts for the aerobic oxidation of olefins under green conditions. The influence of different parameters including the photosensitizer to olefin molar ratio, solvent, type of light source has been investigated. The use of 1,4-benzoquinone and 1,3-diphenylisobenzofuran as the quencher of superoxide anion radical and singlet oxygen species revealed that oxidation reaction mainly proceeds with a singlet oxygen mechanism.

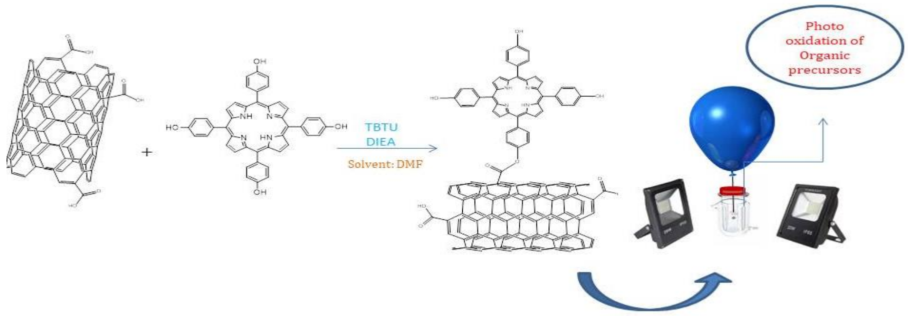

Fig. 1 The synthesis of H_2THPP supported on MWCNTs and photooxidation reaction used in this study.

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Paper code: 1056

Green Synthesis of Silver Nanoparticles from *Berberis Integerrima* Extract and Their Antihyperglycemic Properties

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This study investigates a comparison between antidiabetic effect of *Berberis Integerrima (B. Integerrima)* aqueous extract and its green synthesized silver nanoparticles in Streptozotocin-induced diabetic rats compared to diabetic rats that have been treated with chemical medicine Glibenclamide and we consider changes in their blood glucose and weights during treatment.

Aqueous Extract of *B. Integerrima* were synthesized and it has been used for producing silver nano particles [1], [2]. The freeze-dried extract and green synthesized silver nanoparticles were characterized by SEM and uv-vis spectroscopy.

25 Rats weigh 200 - 250 grams divided into 5 groups:

Normal group, Non-treated diabetic group, Diabetic group treated with *B. Integerrima* extract, Diabetic group treated with Silver Nanoparticles that are synthesized by B. Integerrima extract, and Diabetic group treated with Glibenclamide.

Diabetes was induced by a single dose of Intraperitoneal injection of 50 mg/kg streptozocin dissolved in saline serum, in diabetic groups.

It has been seen that B. integerrima extract and Glibenclamide had approximately same effect on reducing blood glucose of diabetic rats, and the diabetic group of the rats that has been treated with silver nano particles synthsised with B. integerrima extract showed the most weight gaining during treatment.

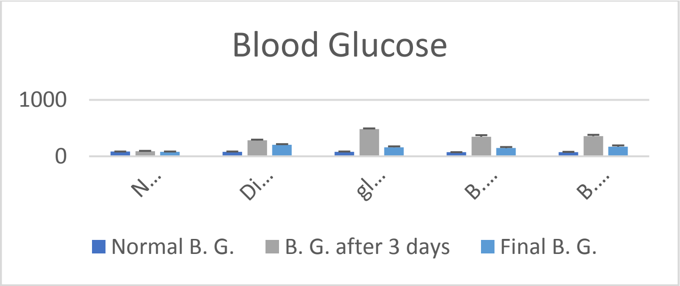

Fig. 1. Blood glucose changes of all groups during treatment

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Paper code: 1061

Valuation of Syringe Pump’s Performance for Reproducible Synthesis of Gold Nanoparticles using Sodium Borohydride as-Reducer

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Gold nanoparticles (Au NPs) have paid much attention due to their exceptional properties which make them suitable for a wide range of applications [1]. Moreover, gold nanoparticles have a broad Surface Plasmon Resonance (SPR) band in the visible region of the electromagnetic spectrum, which is suitable for designing new (bio) sensing devices. However, these properties directly depend on the dimensions and size distribution of the NPs and so, a strict control of the synthesis parameters is required to obtain well-defined nanomaterials. Nanoparticles are usually prepared by means of batch processes, which have limited reproducibility due to the difficult control of some steps such us the addition of reagents and injection volume being difficult to obtain a colloidal suspension with the same characteristics in different batches [2].

In the present work, Au NPs have been synthesized by a simple one-phase reaction in which gold (III) chloride solution was reduced by sodium borohydride. The volume of sodium borohydride was added by syringe pump. Synthesis repeatability was characterized using the SPR band intensity and shift, as the specification parameters. The obtained results indicated that the approach with the use of a syringe pump was superior because it has higher repeatability than the original method (Fig. 1).

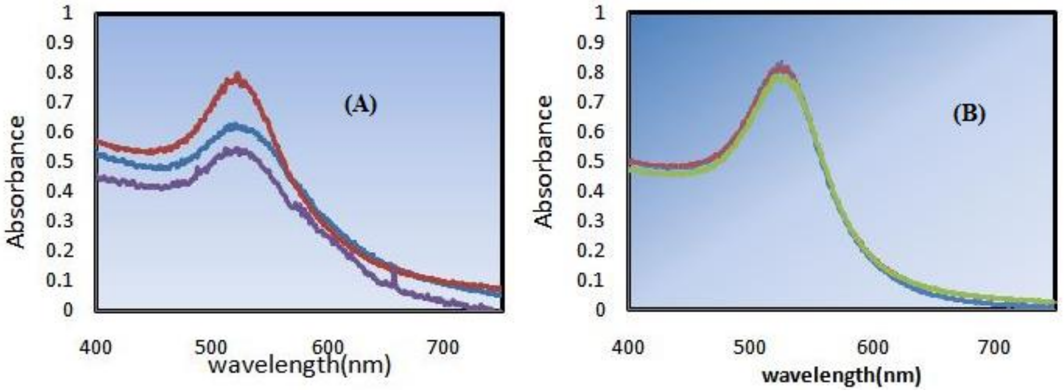

Fig. 1 UV-Vis spectra of synthesized gold nanoparticles by sodium borohydride in constant conditions (A) without using of syringe pump (B) using of syringe pump.

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Paper code: 1064

Comparison of different pretreatment on the recovery of gold and silver from Sarcheshmeh copper anode slime

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The anode slime produced in the refining of copper by electrolysis contains that part of the anode which is insoluble in electrolyte and contains varying quantities of copper,nickel,silver,gold,selenium,tellurium,arsenic,lead,etc.depending on the anode. The main object in treating anode slimes has been to separate the valuable metals with high recovery[1]. In the treatment of anode slime selenium is usually removed . In this paper we compare influence of different methods to removal of selenium on the recovery of gold and silver. Sulfating roasting, soda roasting and oxidative leaching were tested then cyanidation of gold and silver was carried out[2]. results showed Se removal by oxidative leaching pretreatment, remarkably improved the extraction of silver from levels of less than 87% to 99% and gold from less than 90% to 99.2% during subsequent cyanidation. On the other the consumption of cyanide and the time of reaction decreased significantly.

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Paper code: 1068

Effect of cyclic electrodeposition on performances of Lead Flow Battery

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The lead-acid battery is the most global energy storage device and its extensive list of applications includes electrical power supply for automobiles, communications, and railways. But this type of battery conventionally has a low specific capacity because of its heavy weight [1-2]. Unlike the conventional lead-acid battery lead flow battery has high specific capacity and the simplicity in its design, leading to quite inexpensive architectures [3].

Here in we report an electrochemical deposition method of lead dioxide for application in lead flow batteries. Lead dioxide was deposited by cyclic voltammetry (CV) method in 10% methane sulfonic acid solution with different cycles on the graphite substrate. The morphology and crystal structure of electrodeposited $PbO2$ samples have been characterized using by powder X-ray diffraction (XRD) and scanning electron microscopy (SEM) methods. The pore structures of the prepared samples were tested by $N2$ adsorption-desorption measurements. Study of the electrochemical characteristics of the samples was done by CV, galvanostatic charge/discharge (GCD) and electrochemical impedance spectroscopy (EIS).

The XRD patterns revealed that highly crystalline $PbO2$ particles were obtained, also the samples were found to be α-$PbO2$. The SEM images showed that the uniform nanostructure of $PbO2$ was composed. The results of cells galvanostatic discharge shown that the capacity density of lead flow batteries were 207.89 mAh/g. While cell efficiency of the samples was changed from 98 to 96%.

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Paper code: 1069

Synthesis of PE/MgO nanocomposites via in-situ polymerization using Ziegler-Natta catalyst

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Nanocomposites, based on their matrix materials, are divided into several classes, particle-reinforced polymer are one of these classes that are used by organic polymers such as polyolefins which have been of interest in industry because of their lightness, good processing ability and low cost [1]. One of the methods for preparation of nanocomposites is the use of polymerization with olefins such as ethylene and propylene in the presence of nanoparticles [2].

In order to prepare a nanocomposite of PE/MgO, in-situ polymerization was carried out using a Ziegler-Natta catalyst ($TiCl_4/MgCl_2$) in the presence of different content of magnesium oxide (0.1 and 0.42 weight percent) nano-particles (~20 nm) at the same polymerization condition. The result showed that activity of the catalyst slightly enhanced by increasing of the MgO during polymerization (from 427 to 688 g PE. mmol cat^{-1}. hr^{-1}), however, further increacing of the chemical (up to 0.42%), a slightly decrease activity of the catalyst (500 g PE. mmol cat^{-1}. hr^{-1}). The structural properties of the results products were studied using FT-IR technique (Fig.1). The result showed that branching density and vinyl content of product was increased with increasing of MgO-particle to the reaction mixture.

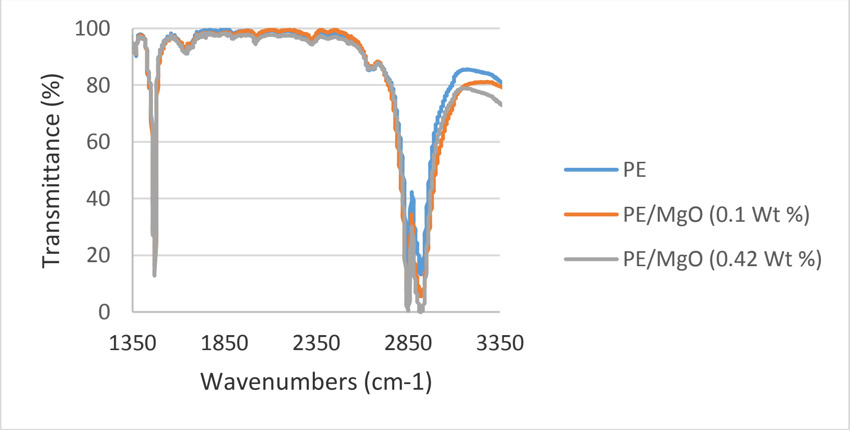

Fig. 1 FT-IR spectrums of the PE and PE/MgO nanocomposites.

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Paper code: 1074

Leaching of low grade sulfide copper ore by ferric sulfate

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In this study, low grade sulfide copper leaching by ferric sulfate is investigated. The main copper containing mineral was chalcopyrite. Leaching of this mineral is so hard and a little amount of copper can be dissolved by conventional reagent. Ferric ion as an oxidant can be increased the copper dissolution. First, the sample was grinded and particle sizes reach to -300 micron. Then, the effects of reagent concentration and leaching time in the room temperature were optimized. Solid/liquid ratio was 1:10.

XRD analysis and microscopic studies showed that qurtz, pyrite and clay minerals are the main minerals in the ore and a small amount of copper is accumulated in chalcopyrite and covelite. Atomic Absorption Spectroscopy (AAS) was used for copper and iron content of ore and final solution.

According to the obtained results, optimum ferric sulfate was 0.01 M during the optimum leaching time of 2 h. Under the optimum conditions, about 30% of copper was extracted.

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Paper code: 1076

Measurement of pressure drop due to connections in the flow path of water flow in a multipurpose device

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Pressure drop is defined as the difference in total pressure between two points of a fluid carrying network. Pressure drop occurs by the resistance to flow on the path of fluid flow, act on a fluid as it flows through the tube. The main determinants of resistance to fluid flow are fluid velocity through the pipe and fluid viscosity. Pressure drop increases proportional to the frictional shear forces within the piping network [1,2]. Many factors cause a loss of pressure in the flow path of the fluid, Change height in fluid flow path, friction lost, valve, Changed in the cross-section of fluid, fluid flow measurement equipment such as: orifice plate and venturi meter. All of these parameters cause a pressure drop in the flow network and in different fluid flow; the effect of each factors has been measured and compared with each other. In fig 1. the laboratory apparatus used for measurements is observed. A digital manometer is used to measure the pressure drop between two points of pipelines. The required pressure is supplied by a centrifuge pump with a power of 0.37 Kw. Fluid flow measured depending on the amount of fluid passed from pipeline over time. It should be noted, however, that for experimental testing, two devices with different tube diameters and pipe lengths and different orifice and venture meter diameter have been used to the effect of the different diameter and length of the pipeline is also observed in the results. These two devices complement each other and they can be used to measure different parameters of the system pressure drop and compared with each other.

Fig. 1 one of Pressure drop measuring device by Different channels of fluid flow.

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Paper code: 1078

Synthesis of PE/graphene nanocomposite via *in-situ* polymerization using a multinuclear catalyst of late transition metals based on cobalt

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During the last few decades, polyethylene composites are properly used instead of PE in numerous applications. Various types of additives in different size of particles can be used to preparing these composites [1]. Graphene is a two-dimensional, single-layer hybrid of sp_2 carbon atom with a macroscopic dimension but with atomic thickness. The properties of graphene-based polymer composites depend heavily on the dispersion of the graphene plates in a polymer matrix. In-situ polymerization is one of the most effective method to synthesis nanocomposites in presence of nano-materialis [2].
Polymerization of ethylene with PE/nanocomposites were carried out using (1E, 1'E)-N,N'-(2,3,5,6-tetramethyl-1,4-phenylene)bis(1-(6-((E)-1-((2,6-diisopropylphenyl)imino)pyridine-2-yl)ethan-1- imine) cobalt(II) chloride prepared catalyst, while methylaluminoxane (MMAO) was used as cocatalyst. The optimum polymerization condition was attained at 50 °C, for 30 minutes, with [Al]:[Co] molar ratio of 1000:1. The PE/graphene nanocomposites (1.7-2 nm with 10-12 layers) were synthesized through *in-situ* polymerization using the catalyst. The result showed that activity of the catalyst slightly enhanced (from 210 to 350 g PE. mmol $(Co)^{-1}$. hr^{-1}) with increasing of the graphene (0.22 weight percent) during the polymerization. The obtained polyethylene samples were analyzed with FT-IR technique (Fig. 1). As expected, the resultant products distinguished as high density polyethylene (HDPE), and as indicated, the sample prepared in presence of graphene showed higher vinyl content and lower branching density than the neat PE (Fig. 1).

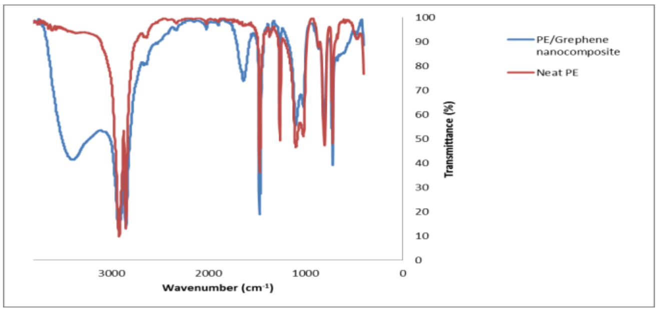

Fig. 1 FT-IR spectrums of the neat PE and PE/grephane nanocomposites.

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Paper code: 1083

A systematic study on the effects of Ni^{2+} and OH^- ions on performance of direct ethanol fuel cell

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At present, concerns about global warming, population growth, as well as the rapid decline of world oil supplies, caused the use of new energy sources is considered. As a result, in the last few decades numerous studies has been focused on the direct alcohol fuel cells (DAFCs). Electro-oxidation of ethanol on the nickel modified graphite electrode and effective parameters on its efficiency are investigated. Nickel modified graphite electrode is prepared by cycling at two cathodic and anodic potential ranges in nickel chloride and alkaline solutions, respectively. Nickel oxyhydroxide is formed by repetitive potential cycling in alkaline solution. The effect of nickel and hydroxide ions concentration on electro-oxidation of ethanol are studied. The results show that at a certain concentration of nickel deposited on graphite electrode, increasing the concentration of hydroxyl ion leads to an increase in the current density of ethanol oxidation as the result increase the kinetic of reaction of oxidation and the cell performance. On the other hand, the concentration of NiCl2 can affect the peak current density of ethanol electrooxidation. At a constant concentration of hydroxide, increasing the concentration of nickel ions up to a certain amount, can also increase the oxidation of ethanol. To find the optimum concentration of NiCl2 solution for preparing the modified electrode, in separate experiments, the graphite electrode modified by different concentrations of NiCl2. The concentration of 0.7 M NiCl2 is suitable enough for saturating the surface of the electrode by nickel ion and enhancement of ethanol oxidation.

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Paper code: 1085

Synthesis of $CuFe_2O_4$ hollow sphere and their application in the preparation of 4,4′-(aryl methylene)bis(3-methyl-1H-perazol-5-ol)s derivatives as catalyst

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Hollow micro-/nanostructured materials possess attractive properties such as high specific surface area, low density and high loading capacity, which endow them with potential applications in dye-sensitized solar cells, lithium ion batteries, super capacitors, catalysis, drug delivery, sensors, water treatment, nano-reactors, and fuel cells[1].

Bis pyrazoles have a wide range of biological activities. These compounds are used as anti-inflammatory drugs, anti-anxiety, antibiotics, antivirus, anti-tumor, and gastric secretion stimulant [2].

In this study, recyclable magnetic $CuFe_2O_4$ hollow sphere has been prepared and effectively has been used in the synthesis of 4,4-(aryl methylene)bis(3-methyl-1H-perazol-5-ol)derivatives under solvent-free conditions.

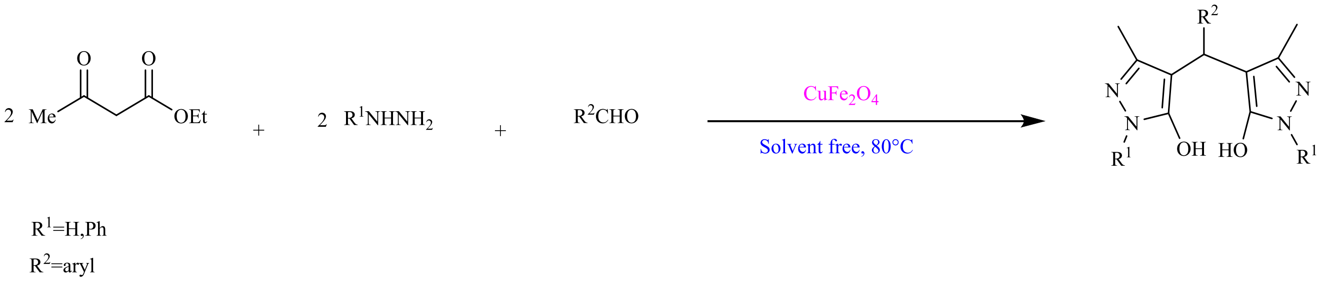

Fig. 1 Scheme of reaction.

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Paper code: 1087

Synthesizing porous anti-reflection and self-cleaning coatings as a cover for the glass of solar cells

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Nowadays the use of photovoltaic systems has been increasingly common. These systems can be installed everywhere such as rooftops, deserts and outdoors in which different particles such as dust can deposit on their surface glass. These particles will limit the photons of the incident light to reach the inner layers of the solar cells which are responsible for energy conversion and as a result the efficiency of these panels will be reduced [1]. Also, the surface of the solar cells, without a cover layer, reflects back a considerable portion of the incident light which reduces the output of these devices (~30%). The idea of using a coating over the glass arises from this loss [2]. For solving these problems the application of self-cleaning antireflection coatings (ARC) on the cover glass of the solar panel is proposed and developed during the recent years. These coatings may be hydrophile or hydrophobe. Both of these coatings bring about the self-cleaning property which eliminates the need for cleaning the glass cover of the solar panels [3].

In this study TiO_2-based, TiO_2-free and SiO_2-based photocatalysts were synthesized and applied to solve the above-mentioned problems simultaneously. The aim was to trap the light by using the antireflection materials and imposing the self-cleaning effect with applying compounds with photocatalytic activity. The catalysts were prepared through sol-gel synthesis method and were coated on the glass slides using the dip coating method at different withdrawal speeds. The thickness of the deposited layer varied at different withdrawal rates. The catalysts were deposited on the slides in µm-thickness. Then the transmittance of the coatings was checked using WPA Spectrawave S1200 and S1200T Visible Spectrophotometer, also their self-cleaning capability was tested and compared to find the best ARC.

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Paper code: 1088

Synthesis and Characterization of a New man-sized Magnetic Core/shell of (Fe3O4@CuO)

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In this study, we reported the synthesis and characterization of a new super paramagnetic Fe_3O_4@CuO core/shell nanostructure by a fast method. The Fe3O4@CuO has spherical shape with average 30-40 nm. Various techniques were employed to thoroughly characterize of the nano structure, such as field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD) and energy-dispersive spectra (EDS). Also we check the synthesized structure with Fourier-transform infrared FT-IR spectroscopy and TEM image.

The elemental analysis results of the CuFe3O4 nano materials are tabulated in Figure 1. The EDX results confirm the presence of O, Cu, and Fe on the man-sized core/shell samples (Figure 2).

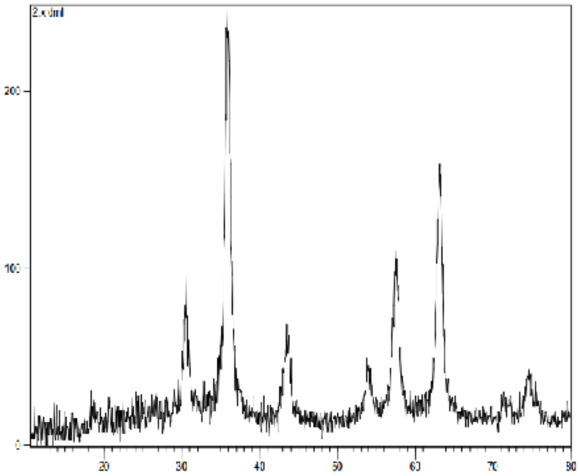

Fig. 1. The XRD pattern of Fe_3O_4@CuO

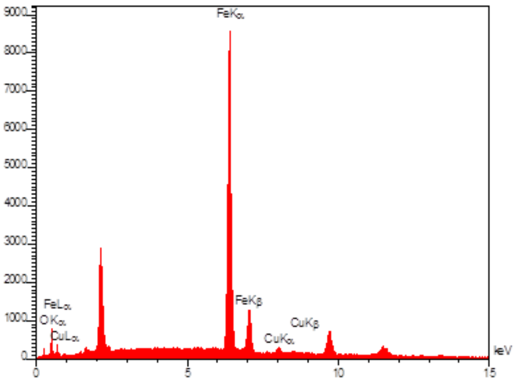

Fig. 2. The EDX spectra of Fe_3O_4@CuO

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Paper code: 1101

Study of the self-cleaning effect of silver nanoparticles and silver / zinc oxide on the basis of graphene

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Recently, some nanoparticles, such as silver, have attracted increasing attention due to antimicrobial activity. In this study, the antimicrobial activity of silver and silver / zinc oxide nanoparticles was studied in graphene-based synthesized self-cleaning coatings Antibacterial properties of the synthesized coatings were investigated in weight percentages (5%, 3%, 2%) of silver nanoparticles / graphene and silver - zinc oxide / graphene. By performing bacterial tests, nanoparticles of silver and silver-zinc oxide were synthesized in all of the weight percentages of all bacteria present in the environment, but the zinc oxidizing properties of zinc were only lower than those of nanoparticles, By reducing the weight of zinc oxide in the environment its bactericidal property also decreases

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Paper code: 1104

Sequential one-pot synthesis of high-quality magnetite@CdS type-II core/shell nanocrystals with improved photocatalytic activity

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High-efficiency photocatalytic materials entail the generation and preservation of high-energy charge carriers with suitable solvent access to initiate redox chemistry. This further requires the prohibition of competing mechanisms (i.e., electron/hole recombination, photo-corrosion and charge trapping) that decrease catalytic activity. One approach to reducing the impact of these competing mechanisms is to design and develop new multicomponent core/shell systems consisting of two (or more) semiconductors [1]. In this regard, the core/shell type composites can be classified into three categories, namely “type-I” (both electron and hole wave functions are localized in the core), “inverted type-I” (both electron and hole wave functions are localized in the shell), “quasi-type-II” (one charge carrier is confined to the core or shell while the other is delocalized over the whole heteronanocrystal), and “true type-II” (spatially separated photocarriers, i.e., electron and hole wave functions reside mainly on different sides of the heterojunction). The separation of charges in the lowest excited states of type-II heterojunctions should make these nanohybrid composites more suitable for photovoltaic or photocatalytic applications.

Herein, the magnetite@CdS core/shell nanocrystals, which are considered as type-II structure, were prepared and then structural, morphological (shape and size) and optical properties of these nanostructures were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and UV-Vis and fluorescence spectroscopy techniques. We thereafter investigated the interfacial photoinduced electron transfer and related secondary photochemical behavior in the system via time-resolved fluorescence spectroscopy. The increased lifetime of magnetite@CdS nanohybrid compared with single CdS QD suggested the charge transfer process between the magnetite core and CdS nanoshell. Finally, the hybrid photocatalytic performance was successfully demonstrated towards photodecomposition of xylenol orange under sunlight irradiation.

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Paper code: 1118

Synthesis and characterization of a manganese(II) coordination complex based on highly pre-organized ligand of 1,10-phenanthroline-2,9-dicarboxylic acid

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The continuity of the searches for new materials with the higher performance than those used currently are necessary in order to satisfy daily improving technology. For this purpose, the sensible choice of suitable ligands with fixed geometry and flexible coordination capability plays a vital role for the design and synthesis of functional materials with interesting geometric configurations. In this respect, 1,10–phenanthroline as chelating nitrogen donor ligand has a rigid framework, and exhibits an excellent coordination ability with transition metal ions.[1-3] Additionally, pre-organized ligands have proven to be important in inorganic chemistry, biomedical, environmental, and industrial fields.[4] In this work, we have synthesized a Mn(II) coordination compound by employing 1,10-phenanthroline-2,9-dicarboxylic acid (PDA) ligand, $[Mn(PDA)(Cl)(H_2O)]\cdot H2O\cdot EtOH$ (**1**) (Fig. 1). This complex has been characterized by melting point, elemental analysis and infrared spectroscopy. Finally, further experiments involving different pre-organized ligands and metal ions with complementary characterizations such as TGA and SXRD as well as high level DFT are in progress in our laboratory to obtain different supramolecular assemblies in order to have further insight into this type of coordination compounds. Continued efforts to explore the construction of novel functional hybrids base on POMs incorporating other new pyridinedicarboxylic acid and azide ligands are also underway.

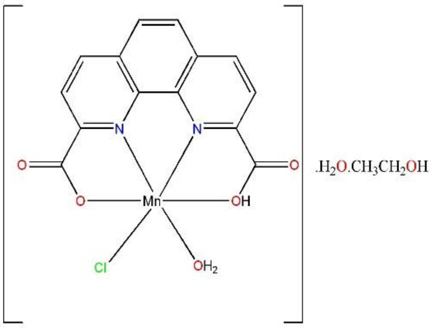

Fig. 1 The molecular structure of **1**.

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Paper code: 1119

Metal-organic framework composite membrane for fuel cell applications at high temperature and low humidity

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Advancement of new proton exchange membranes (PEMs) that work under anhydrous condition is one of the most critical requirements for proton exchange membrane fuel cells (PEMFCs) technology [1]. PEMFCs which can work under anhydrous conditions and temperature higher than 100 °C resolve substantially certain problems such as water and heat management, CO poisoning and amended electrode kinetics [2]. For this reason, many attempts have been made for developing new high-temperature polymeric electrolytes with high thermal and mechanical properties, high oxidative resistance and high proton exchange properties when doped with a strong acid [3]. So in this work a proton-conducting sulfonated poly(ether sulfone)-MOF membrane (SPES-MOF membrane) with high proton conductivity at high temperature and anhydrous conditions was synthesized by anchoring the Cr-MIL-101-NH_2 to the aromatic polymer backbone via a Hinsberg reaction. The effect of MOFs as the pendant porous aminated moieties on membrane features such as water uptake; swelling ratio; mechanical, oxidative and thermal stabilities; morphology; acid retention capacity; ion exchange capacity; long-term durability; hydrogen crossover; proton conductivity and fuel cell performance was methodically studied. The presence of holes and -NH_2 groups in MOFs structure enhanced the acid retention capacity of the SPES-MOF membrane. This resulted in satisfactory performance of the membrane at high temperatures and low humidity (the proton conductivity of membrane reached 0.041 $S.cm^{-1}$ (compared to Nafion = 0.0029 $S.cm^{-1}$) at 160 °C). Moreover, the crosslinking produced by MOFs increased the dimensional stability (the swelling ratio was reduced from 57% to 4%), oxidative resistance, tensile strength, and also improved water uptake and hydrogen crossover of the polymer.

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Paper code: 1120

Synthesis of magnetic Pd nano composite and its application as recoverable catalyst for the C-C cross coupling Suzuki reaction

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So far, various substrates for the stabilization of palladium nanoparticles have been used, including polymers which are very useful due to these functional groups [1]. In this work, two polymers with difference base were used for immobilization of Pd nanoparticles. Snake skin polymer as a natural polymer (Keratin base) and polyaniline as a synthesized polymer with Fe_3O_4 nanoparticles were used for preparation Nano composite with different combine percentages. For this purpose polyaniline was synthesized in mild condition that possesses high environmental stability. Also Fe_3O_4 nanoparticles were prepared by the conventional co- precipitation method separately [2,3] and snake skin was ready for made a Nano composite. Finally, palladium nanoparticles were immobilized on prepared Nano composite. The reason why iron nanoparticles are used as substrates: 1- low toxicity 2- high-volume ratio 3- easy separation and high dispersion. This heterogeneous catalytic system was investigated for the C-C cross coupling Suzuki reaction in Ethanol/water as a green solvent at room temperature which shown high catalytic activity and reusability.

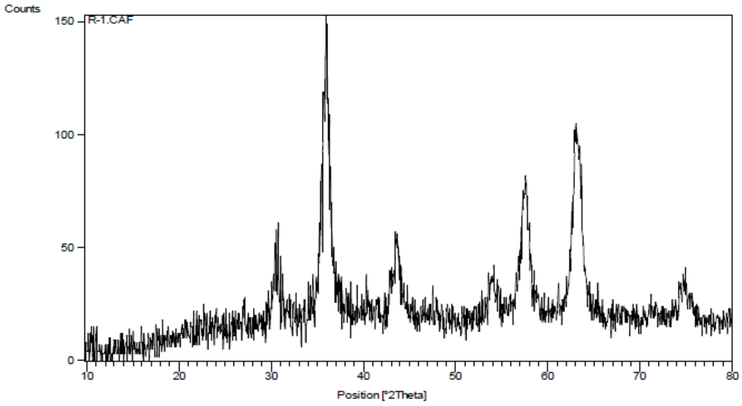

Fig. 1 XRD of magnetic Pd nano composite

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Paper code: 1133

Cytotoxic evalution of chenopodium botrys essential oil on the cancer cell category of the tumor cervix(Hela)

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Carcinoma of the uterine cervix is the second most common female tumor worldwide, surpassed only by breast cancer. Its incidence is disproportionately high (>80%) in the developing world and its treatment of disease is usually palliative, amied only at symptom control [1]. *Chenopodium botrys* is a fragrant herb. In this research ,the toxicity of *chenopodium botrys* on cervical cancer (HeLa) essential oil was investigated.

The seeds of *chenopodium botrys* was collected from sabzevar city ,and then essential oil was extracted by hydrodistilation. The cytotoxic effect of essential oil on the HeLa cell line was evaluated by MTT assay . the cultivated cells were exposed to various dilutions of (5, 10, 30, 50, 75, 100, 130, 170, 200) for 24 hours.The results were analyzed by Graphpad prism 6 software. The results showed that the essential oil of the *chenopodium botrys* has cytotoxic effects on the HeLa cell line in 24 hours (Fig . 1). The essential oil showed the highest cytotoxicity at a concentration of 200 µg/ml. The IC_{50} of *chenopodium botrys* essential oil was and 79.44 µg/ml.

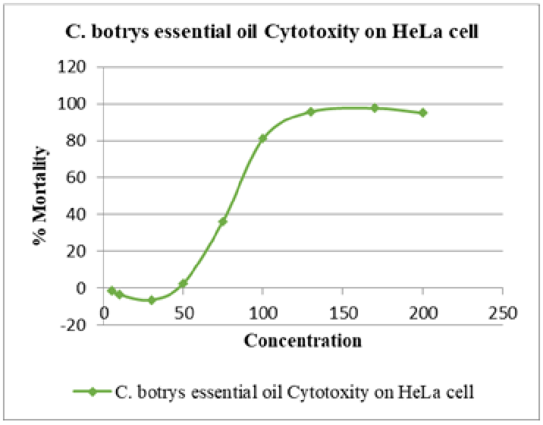

Fig . 1 Cytotoxicity of *C. botrys* essential oil on HeLa cell at the 24 hours.

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Paper code: 1163

PEG/HEMA: pH Responsive Nanohydrogel for Controlled Released of Methotrexate

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Reversible addition-fragmentation chain transfer (RAFT) polymerization is a facile means for the controlled synthesis of various functional polymers with predetermined molecular weights, narrow molecular-weight distributions, and controlled architectures. Many synthetic polymers are smart carrier candidates for their potent application in medicine, especially in controlled drug delivery. These materials can be loaded with specific drugs for therapeutic applications, releasing treatment in response to a stimulus. In this era of new technologies, there is an ongoing interest in enhancing the efficiency of polymer-based drug delivery systems, in particular cross-linked hydrogel systems [1].

In this work, novel modified nanohydrogel carrier is introduced as efficient host for methotrexate conjugation using 2-hydroxyethyl methylacrylate (HEMA) based RAFT polymerization. The chemical structure and the topography characterization were carried out by FT-IR, ^{1}HNMR, DLS, SEM, TEM, and AFM. To illustrate the efficiency of the modified particles, the anti-cancer drug methotrexate was conjugated to hydroxyl groups through estric bond formation. The controlled release activity of established nanoparticles was evaluated in simulated cellular fluid. Later, the anti-cancer behavior of drug conjugated nanoparticles was evaluated in vitro in MCF-7 cell line which showed enhanced toxicity after 48 h.

^{1}H-NMR spectroscopy showed detailed information about poly (HEMA-*co*-PEG) and made the facility of the molecular weight's determination. DLS studies of the diluted HEMA-PEG dispersions confirmed successful particle formation. The gel permeation chromatography (GPC) profiles of the poly (HEMA-*co*-PEG) show Molecular weight and molecular weight distribution. It is very obvious that the molecular weights increase with the increasing conversions in the experimental condition, suggesting the propagation of living chain with time.

Conclusively, the modified nanoparticles have remarked as powerful carrier to be applied as an anti-cancer agent.

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Paper code: 1164

Synthesis, characterization, DFT calculation and antibacterial activities of new cupper complexes containing novel thiourea derivatives

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On the basis of the pharmacological studies of the compounds containing carbonyl and thiocarbonyl groups such as urea, thiourea and their related analogues, it is proposed that the thiourea derivatives and their transition metal complexes represent a wide diversity of biological functions including antibacterial, antifungal, anti-diabetic, antitubercular, anti-human immunodeficiency virus (anti-HIV), anti-Hepatitis C virus (anti-HCV), antitumor, antithyroid, anthelmintic, rodenticidal, insecticidal, herbicidal, and plant-growth regulator properties [1].

In this study, three new thiourea ligands derived from the condensation of aroyl- and aryl-isothiocyanate derivatives with 2,6-diaminopyridine, named 1,1'-(pyridine-2,6-diyl)bis(3-(benzoyl)thiourea), 1,1'-(pyridine-2,6-diyl)bis(3-(2-chlorobenzoyl)thiourea) and 1,1'-(pyridine-2,6-diyl)bis(3-(4-chlorophenyl)thiourea) and their cupper complexes were synthesized and characterized by elemental analysis, FTIR and ^{1}H NMR and UV-visible spectroscopies. Proposed structures for free thiourea ligands and their cupper complexes were corroborated by applying geometry optimization and conformational analysis. These compounds were studied in vitro in terms of antibacterial properties against Staphylococcus aureus and Enterococcus faecalis and Escherichia coli and Pseudomonas aeruginosa as 2 standard gram-positive and 2 standard gram-negative bacterial strains, respectively, through minimum Inhibitory Concentration by using the broth macrodilution procedure and inhibition zone via the disk diffusion method. The infrared spectra of these samples exhibit all the expected frequency regions of the (N–H), (C=S), (C=O) and (C–N). Electronic excitation study of these samples in DMSO solution displays several absorption bands in the UV and visible regions. All compounds inhibited the growth of bacteria with MIC values ranging between 64 and 1024 µg/ml. On precise examination of the theoretical results, it can be found that antibacterial activities have some relationship with the LUMO energies and the difference between LUMO and HOMO energies. We find that the thickness of inhibition zones for abovenamed standard bacterial strains is linear with these features in some samples. The experiments showed that cupper complexes had the superior antibacterial activities than novel thiourea derivatives against all Gram-positive and Gram-negative bacterial strains.

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Paper code: 1165

Synthesis of graphene oxide/ metal oxide/amalgam nanocomposite and its effectiveness as a dental filler

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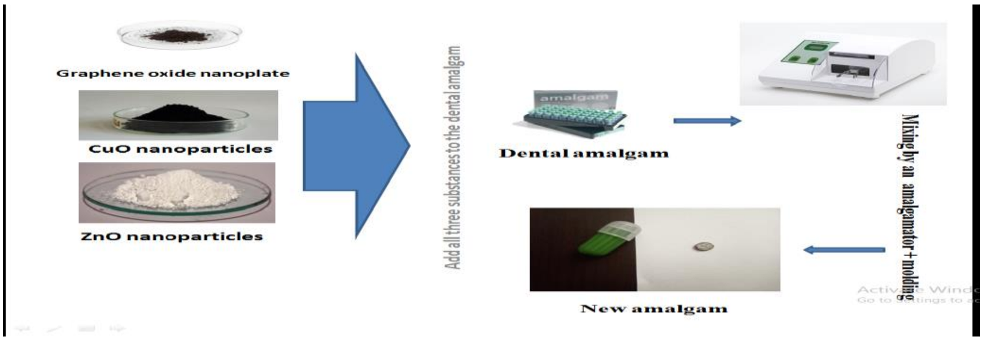
Teeth munch a few million times a year which made them vulnerable and they need to be restored or refilled. Most teeth are filled with metal materials (amalgam) which are not too tight and subject to destruction. Dental amalgam restorations often corrode and change color in the mouth [1, 2]. The purpose of this study is application of the novel nanostructures to improve the performance of amalgam. In the first stage of the research, graphene oxide nanoplates (modified by Hummer method) and metallic oxide nanoparticles (zinc oxide-copper oxide) synthesized using metal salt were applied. The synthesized products were investigated by XRD and SEM analyses. The crystallite sizes of 10, 8.5 and 17.8 nm were obtained for graphene oxide, zinc oxide and copper oxide, respectively. In the second stage, nanoparticles were added to the amalgam capsule (dental filler) and combined with an amalgamator. Nanocomposites were produced each time by combining different percentages of nanoparticles and mechanical properties including molded hardness were measured by the microhardness gauge. As a conclusion, improvement of the mechanical properties including hardness according to the comparison of the statistics done between the results and controlled amalgam was acquired.



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Paper code: 1174

Synthesis of Molybdenum Sulfide Nanocomposite and Investigation of Its Catalytic Application

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The increasing worldwide energy demand and environment concerns lead to extensive research to develop sustainable and environment-friendly alternative energies to replace exhaustible fossil fuels. Hydrogen, as a renewable and clean energy resource, has been proposed as a potential candidate for future fuel owing to its high energy density and environmental friendliness [1]. Pt- based materials are the effective catalysts in hydrogen evolution reaction, but they are expensive and difficult to recycle, so that their application is impeded in the development of economical hydrogen energy [2]. Recently, transition metal disulfides (TMDs) have received tremendous attention as hydrogen evolution reaction (HER) catalysts due to their favorable chemical and catalytic properties [3].

In this research, the MoS_2 and BCN nanostructures were synthesized through sulfurization of MoO_3 powder and milling methods. Carbon-based nanocomposite containing MoS_2 and BCN nanostructures in appropriate ratio were prepared under optimum condition. The synthesized nanostructures were characterized by FTIR, XRD and FESEM-EDX to determine functional groups, crystalline structures, morphology and elemental analysis. The performance of synthesized nanocomposite was investigated as a nanocatalyst for hydrogen production. The effective parameters on process efficiency were investigated and optimized. The obtained results showed that this nanocatalyst improves the process of hydrogen production. Also this catalyst exhibits high stability, suggesting that this nanocomposite is a good candidate for the hydrogen evolution reactions.

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Paper code: 1264

Comparison of thermal and mechanical properties of epoxy networks cured with α,ω-diamino polyoxytetramethylene and isophorone diamine

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Epoxy–amine networks based on diglycidyl ether of biphenyl A (DGEBA) and aliphatic/aromatic diamines are widely used in different industrial applications such as coatings, adhesives and composite materials, due to their outstanding chemical and mechanical properties [1,2].

In this work, we compared thermal and mechanical properties of epoxy networks cured with α,ω-diamino polyoxytetramethylene (APOTM) and isophorone diamine. Wide range of properties were developed via the embodiment of APOTM into epoxy resin formulations. Low shrinkage, good color, flexibility and tough, high gloss are characteristics of epoxy resins cured with APOTM. Improvement of the segment flexibility reduces the Tg of the epoxy network. The resulting DGEBA/APOTM and DGEBA/IPD epoxy networks are thoroughly characterized by field emission scanning electron microscope (FE-SEM) techniques, thermogravimetric analysis (TG/DTG), and dynamic mechanical thermal analysis (DMTA) measurements. According to the tan δ-T plots in Fig. 1 epoxy network cured with APOTM shows T_g value lower than epoxy network cured with IPD.

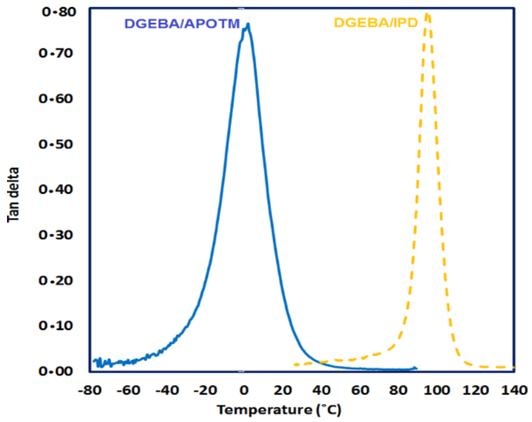

Fig 1. Loss factors of DGEBA/APOTM compared to DGEBA/IPD.

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Paper code: 1265

Effects of surface- modified SiO_2 and Fe_3O_4 nanoparticles on improving thermal and mechanical properties of DGEBA/IPD epoxy networks

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Epoxy resins are widely applied as adhesives [1], coatings and matrix in polymer composites due to its low viscosity, good insulating properties even at high temperatures and good chemical and thermal resistance. However, most of the epoxy systems are brittle [2]. A variety of approaches have been proposed to enhance the epoxy systems mechanical and thermal properties. In this regard incorporation of nanofillers in to the epoxy systems has drawn a special attraction [3].

In this article , we studied effect of surface- modified SiO_2 nanoparticles and surface-modified magnetic iron oxide nanoparticles on improving thermal and mechanical properties of DGEBA/IPD epoxy networks.The resulting epoxy/ SiO_2 nanocomposites and epoxy/Fe_3O_4 nanocomposites are thoroughly characterized by Fourier transform infrared (FTIR), X-ray diffraction (XRD), field emission scanning electron microscope (FE-SEM) techniques, thermogravimetric analysis (TG/DTG), differential thermal analysis (DTA) and dynamic mechanical thermal analysis (DMTA) measurements. Fig. 1 shows FE-SEM of epoxy/Fe_3O_4 compared to epoxy/ SiO_2 nanocomposites.

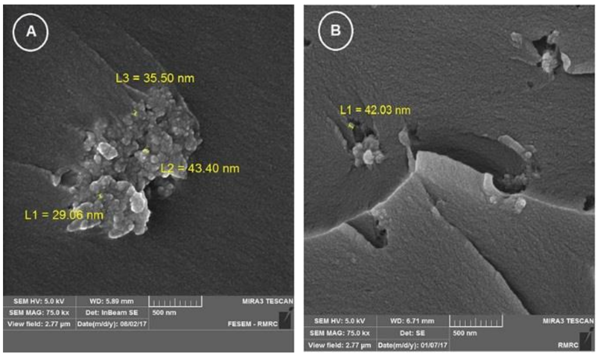

Fig 1. (A) FE-SEM micrograph of epoxy/Fe_3O_4 compared to (B) epoxy/ Sio_2 nanocomposites

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Organic Chemistry

Paper code: 5

Multicomponent Solvent-free Synthesis of Novel 2-((Benzylthio)((alkyl or arylamino)thio)methylene)malononitriles as Antimicrobial Agents

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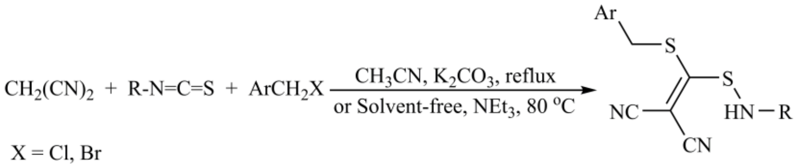
Organic compounds containing C-S-C bonds are known as sulfides or thioethers. These functional groups exist alone or alongside others in various pharmaceutical and biologically active molecules [1]. New methods and procedures were proposed to synthesize organic sulfides [2]. In this study, multicomponent reaction of malononitrile, alkyl or arylisothiocyanates and various benzyl halides was developed as an efficient strategy for the synthesis of novel 2-((benzylthio)((alkyl or arylamino)thio)methylene)malononitrile derivatives *via* two different procedures: (a) in the presence of K_2CO_3 as a base in acetonitrile and (b) under solvent-free conditions in the presence of thriethyamine (Fig. 1). Higher yields with shorter reaction times were obtained from later procedure. Chemical structure of all molecules were determined according to their spectral data and elemental analyses. *In vitro* inhibitory activity of all derivatives was evaluated against some Gram-negative and Gram-positive bacteria as well as some pathogenic fungi according to the CLSI guidelines [3]. The results as inhibition zone diameter (IZD), the minimum inhibitory concentration (MIC) and the minimum bactericidal concentration (MBC) and the minimum fungicidal concentration (MFC) values were compared with those of antibiotics and antifungal drugs. These thioethers can be introduced as potential antimicrobial agents based on their broad-spectrum inhibitory properties.



X = Cl, Br

R = C_6H_5, 4-O_2N-C_6H_4, 4-H_3C-C_6H_4, C_2H_5

Ar = C_6H_5, 2-O_2N-C_6H_4, 2-Cl-C_6H_4, C_6F_5, 2,4-$(O_2N)_2$-C_6H_3, 2,4-$(Cl)_2$-C_6H_3

Fig. 1 Multicomponent synthesis of 2-((benzylthio)((alkyl or arylamino)thio)methylene)malononitriles

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Paper code: 6

Green Multicomponent Synthesis, Antimicrobial and Antioxidant Evaluation of Novel 5-Amino-isoxazole-4-carbonitriles

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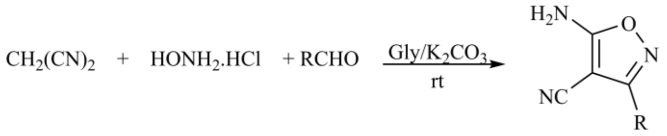
Isoxazoles are five-membered aromatic heterocycles containing adjacent oxygen and nitrogen atoms. The Isoxazole ring system is found in variety of naturally occurring compounds and biologically active molecules. They are especially useful in medicine, since many antifungal drugs belong to the isoxazole class [1]. Various methods were developed for synthesizing isoxazole derivatives [2,3]. In this study, 5-amino-isoxazole-4-carbonitriles were prepared *via* a green and efficient multicomponent procedure. Malononitrile, hydroxylamine hydrochloride and different aryl aldehydes were simultaneously reacted in K_2CO_3/glycerol deep eutectic solvent (1:4) (Fig. 1). Polysubstituted isixazoles were obtained in excellent yields and short times. Chemical structure of all molecules were characterized by spectral data and elemental analyses. *In vitro* inhibitory activity of all derivatives was evaluated against some pathogenic bacteria including both Gram-negative and Gram-positive strains as well as some fungi. Broad-spectrum antimicrobial activities were observed with isoxazoles. In addition, assessment of free radical scavenging activity of all the synthesized heterocycles against DPPH proved their antioxidant potentials.



R= 4-H_3C-C_6H_4; 4-HO-C_6H_4; 4-O_2N-C_6H_4; 2,4-$(Cl)_2$-C_6H_3; 2,6-$(Cl)_2$-C_6H_3;
2-HO-3-H_3CO-C_6H_3; furan-2-yl; thiophen-2-yl; pyridin-4-yl

Fig. 1 Multicomponent synthesis of 5-amino-isoxazole-4-carbonitriles in deep eutectic solvent

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Paper code: 7

Synthesis of an Organic Dye for Dye-sensitized Solar Cells

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The organic molecules with D–π–A structures have attracted increasing attention since they can serve as electro active and photoactive materials in molecular electronics [1]. Recently, more and more attention has been directed to the application of metal-free organic dyes in DSSCs [2]. In this work, new metal free dye is reported and its optical, electrochemical, photovoltaic properties and structural relationships are investigated in detail. The general procedure for preparing metal free organic dye is given in Figure 1. The absorption spectrum of dye in CH_3CN has three distinct absorption bands at around 288, 320 and 395 nm, respectively. The absorption peaks at around 320 nm correspond to the π→π* electron transition of the conjugated molecule; and the absorption peaks at around 385 nm can be assigned to an intramolecular charge transfer between the phenothiazine-based donor and the cyanoacrylic acid [2], providing efficient charge-separation at the excited state. The λ_{max} of dye adsorbed on a TiO_2 film is 419.5 nm. Upon dye adsorption on to a TiO_2 surface, the wavelength of maximum absorption is bathochromically shifted by 24.5 as compared to the corresponding spectra in solution, implying that dye adsorbed on to TiO_2 surface contain partial J-type aggregates. The DSSCs were prepared and compared to investigate the relationships between the sensitizing behavior of dye molecule and its structures. The solar-energy-to-electricity conversion efficiency (η) of the DSSCs is 5.32 %.

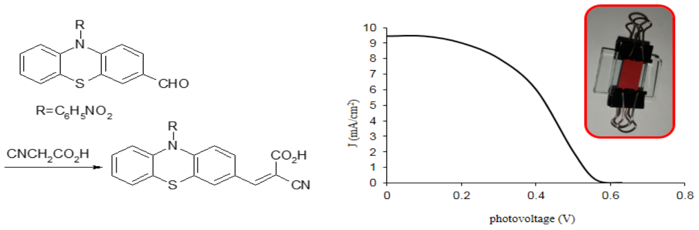

Fig. 1 Synthesis route for the prepared dye and J-V curve of solar cell.

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Paper code: 8

Preparation of Dye-sensitized Solar Cells Based on New Organic Dye

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Dye-sensitized solar cells (DSSCs) are current topic of research in the field of green chemistry and renewable energy resources. Organic dye molecules have considerable importance in comparison with inorganic dye molecules by their applicability to green chemistry in DSSCs [1]. Several types of organic dyes have been reported including near IR dyes for DSSCs applications [2]. In this work, new metal free dye based on Indigo is reported and its optical, electrochemical, photovoltaic properties and structural relationships are investigated in detail. The general procedure for preparing metal free organic dyes is given in Figure 1. The absorption spectrum of dye in THF has two distinct absorption bands at around 320 nm and 545.5 nm. The absorption peaks at around 545.5 nm can be assigned to an intramolecular charge transfer between the donor group and the cyanoacrylic acid [2], providing efficient charge-separation at the excited state. The λ_{max} of dye adsorbed on a TiO_2 film is 568 nm. Upon dye adsorption on to a TiO_2 surface, the wavelength of maximum absorption is bathochromically shifted by 22.5 as compared to the corresponding spectra in solution, implying that dye adsorbed on to TiO_2 surface contain partial J-type aggregates. The DSSCs were prepared and compared to investigate the relationships between the sensitizing behavior of dye molecule and its structures. The solar-energy-to-electricity conversion efficiency (η) of the DSSCs is 4.73 %.

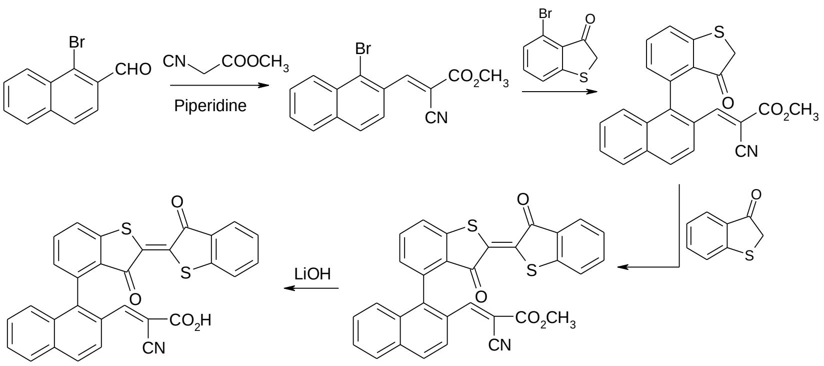

Fig. 1 Synthesis route for the prepared dye.

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Paper code: 18

Nano γ- Alumina supported boron trifluoride as a novel solid acid catalyst for the synthesis of pyrroles at room temperature under solvent-free condition

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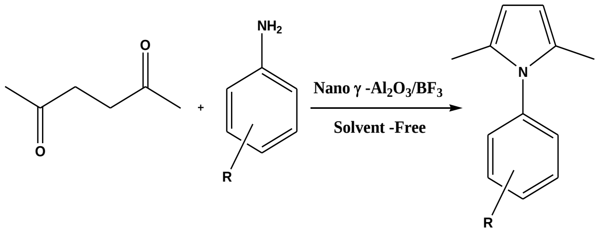
Pyrroles are a significant category of heterocyclic compounds and are structural units contained in an immense array of natural products, synthetic material, and bioactive molecules, like heme, vitamin B12, and cytochromes[1]. Because of these properties, synthesis of pyrrole derivatives has an important role in heterocycle chemistry and there is increasing interest in the synthesis of this kind of compounds[2]. There are several methods for the synthesis of pyrrole derivatives. Generally, these methods are based on the cyclocondensation reactions. Classical procedures for the synthesis of pyrroles include the Knorr, Hantzsch, and Paal-Knorr condensation reactions. In the Paal-Knorr reaction, 2,5-dicarbonyl compounds are converted to pyrroles in the presence of ammonia or primary amines [3]. Recently, many catalysts have been used for this conversion such as montmorillonite KSF, $Bi(NO3)_3$-$5H_2O$, $Sc(OTf)_3$, layered zirconium phosphate, zirconium sulfophenyl phosphonate, silica sulfuric acid (SSA) [4]. However, some of these methods suffer from certain drawbacks such as prolonged reactions times, use of volatile or hazardous organic solvents, tedious conditions, use of extra energy source, and toxic metals. Herein, We wish to report a simple, clean, practical and efficient method for the synthesis of pyrrole derivatives by nano γ-Al_2O_3/BF_3 as heterogenous catalyst under solvent-free condition at room temperature (Scheme1). This synthetic procedure has several advantages, including the availability, safety, and reusability of the catalyst, high yields, short reaction times and also has an environmentally benign nature in agreement with the concepts of green chemistry.



Scheme1

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Paper code: 35

Solvent-free esterification of alcohols, silyl and tetrahydropyranyl ethers with carboxylic anhydrides using hexachloroacetone as a catalyst

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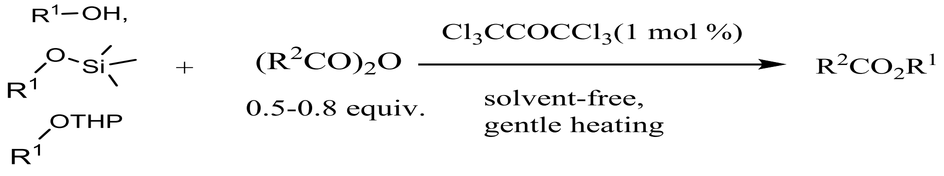
Esterification reaction is one of the most important strategies in organic synthesis due to its various applications in different fields such as drug synthesis (e.g. aspirin) and agricultural chemistry. Some important compounds such as oils, flavoring agents and fragrances and synthetic polymers contain the carboxylic ester moiety in their structures [1]. In addition, this reaction can be used for protection of hydroxyl group in some multi-step synthesis. In order to increase the efficiency of this reaction and access to better results, carboxylic esters have been obtained from the reaction of alcohols with activated carboxylic acid derivatives such as carboxylic anhydrides instead of carboxylic acids [2].

Now in the present abstract, in continuation of our previous work on the esterification of aromatic aldehydes with alcohols (1:1) using air as the simplest available oxidant and KCN [3], we report an efficient method for the conversion of alcohols, silyl and tetrahydropyranyl ethers to carboxylic esters using carboxylic anhydrides (0.5-0.8 equiv.) in the presence of hexachloroacetone (1 mol%) as a catalyst under solvent-free conditions with gentle heating. Different types of starting materials such as benzylic and phenolic containing electron withdrawing or donating groups in various positions of phenyl ring, cyclic, allylic and primary, secondary and tertiary aliphatic can be easily esterified in excellent yields *via* the present method (Scheme 1).



R^1= cyclic, allylic, benzylic, primary, secondary and tertiary aliphatic and aryl

R^2= CH_3CH_2,C_6H_5

Scheme 1. Solvent-free esterification of alcohols and ethers with carboxylic anhydrides using hexachloroacetone as an efficient catalyst.

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Paper code: 36

Immobilized ionic liquid on γ-Fe_2O_3 as an efficient and reusable nano-catalyst for the synthesis of pyrano[2,3-*d*] pyrimidinone derivatives

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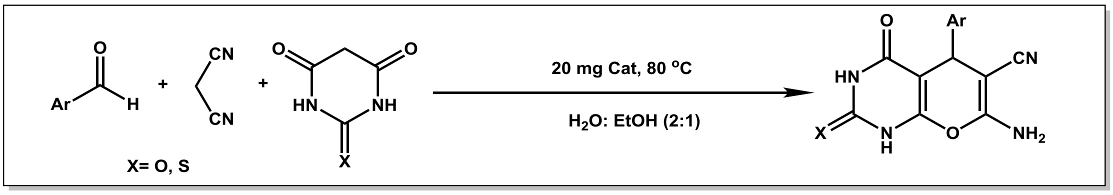
In recent years, γ-Fe_2O_3 magnetic nanoparticles (MNPs) have been appeared as a new kind of efficient catalyst support due to low toxicity, ease of surface modification, unique physical properties including the high surface area and superparamagnetism. In order to prevent the aggregation of γ-Fe_2O_3 MNPs, its surface is usually modified with a silica layer, taking advantage of being biocompatible, hydrophilic and, also, because the surface of silanol groups can easily react with various organic and inorganic materials to achieve the certain purposes especially in the field of catalysis [1].

NPs, especially MNPs have appeared as a bridge between homogeneous and heterogeneous catalysts. The magnetic nature of these particles allows for easy recovery and recycling of the catalysts by an external magnetic field. To improve the chemical stability as well as to achieve some advantages as the versatility in surface modification, MNPs commonly coat with different organic or inorganic compounds and precious metals [2,3].

In this work, γ-Fe_2O_3@SiO_2@IL is prepared, characterized and used to synthesis of pyrano[2,3-*d*]-pyrimidinediones(thione) derivatives *via* a three-component reaction of different aromatic aldehydes, (thio)barbituric acid and malononitrile in a solution of water/ethanol. The structures of the products were characterized using FT-IR, ^1H NMR and ^{13}C NMR spectroscopy. The present methodology suggests several advantages such as easy catalyst separation and high reusability for several consecutive runs without significant loss of its catalytic efficiency, high yields of obtained products, simple procedures, low cost and short reaction times (Scheme 1).



Scheme 1. Synthesis of pyrano[2,3-*d*]pyrimidinone derivatives catalyzed by γ-Fe_2O_3@SiO_2@IL

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Paper code: 38

One-Pot Synthesis of Functionalized 1,4-Dihydropyridines Catalyzed by Deep Eutectic Solvent

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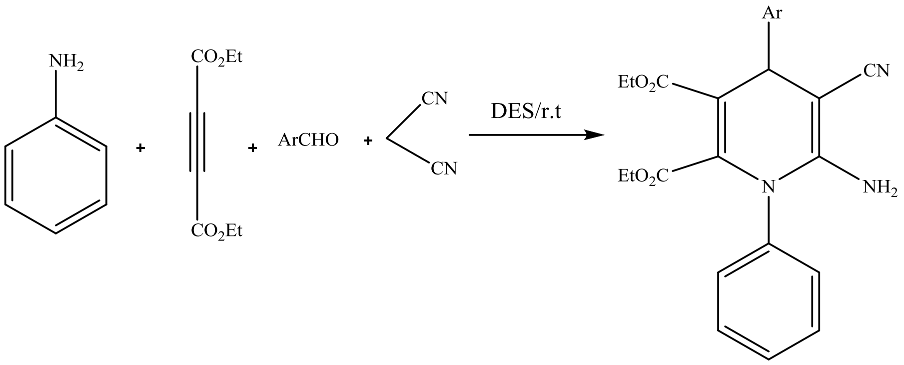
1,4-Dihydropyridines (1,4-DHPs) are one of the most wellknown heterocyclic framework, since a large number of these molecular buldingblock show interesting pharmacological properties such as, antiangin [1], antiviral [2], and anticancer activities [3]. In this research, deep eutectic solvent (DES) catalyzed for the one-pot four-component synthesis of functionalized 1,4-dihydropyridine derivatives by a condensation of various aldehydes, malononitrile, diethylacetylenedicarboxylate and aniline at room temperature (Scheme 1). This method developed by using an environmentally benign synthetic method along with the use of cost effective catalyst.



Scheme 1. One-pot four-component synthesis of functionalized 1,4-dihydropyridine derivatives

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Paper code: 42

An Efficient Method for the Synthesis of Neuroprotective Drug Riluzole

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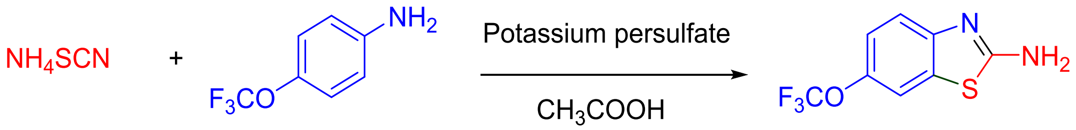
Benzothiazole nucleus structures, are main classes of organic compounds in the pharmaceutical industry. The benzimidazole moieties are found in several synthetic drugs, exhibiting an extensive spectrum of biological activities, including anti-cancer, anti-tumour and anti-fungal [1]. Riluzole with benzothiazole core is used to treat a certain type of nerve disease called amyotrophic lateral sclerosis [2].

General synthetic procedures for the synthesis of Riluzole include the reaction of 4-(trifluoromethoxy)aniline derivatives with ammoniumthiocyanat [3] or potassiumthiocyanate [4] in the presence of oxidant for cyclization.

In this research, 4-(trifluoromethoxy)aniline reacted with ammoniumthiocyanat in acetic acid in the presence of a Potassium persulfate at a low temperature for appropriate time to afford the 6-(trifluoromethoxy)benzo[d]thiazol-2-amine,after completing the reaction the mixture are basified with ammonia and the crude recrystallize in toluene and cyclohexane. This method can be used and generalized in pharmaceutical industry.



Scheme 1. reaction between 4-(trifluoromethoxy)aniline and ammoniumthiocyanat.

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Paper code: 43

Pd nanoparticles decorated on chitosan functionalized graphene oxide as an efficient catalyst for reduction of nitroarenes in water

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In this work, graphene oxide [1] was functionalized with chitosan (GO-Chit) [2] followed by a simple approach for immobilization of palladium nanoparticles onto a chitosan grafted graphene oxide surface. The Pd-nanocomposite (GO-Chit-Pd) was characterized using Transmission Electron Microscopy (TEM), Fourier transforms infrared spectroscopy (FT-IR), and X-ray diffraction (XRD) measurements. GO-Chit-Pd was used as an efficient catalyst for the reduction of aromatic nitro compounds using sodium borohydride in water (Fig. 1). To achieve the best catalytic efficacy, various parameters such as temperature, solvent, mole ratio of hydrogen sources and the amount of catalyst, were optimized. The method has been applied to reduction of a broad range of nitroarenes with different properties. The easy purification, convenient operation, environmental friendliness, and high product yields render this method viable for use. The nano-catalyst can be easily separated and efficiently recovered and reused for multiple cycles without appreciable loss in its catalytic activity.

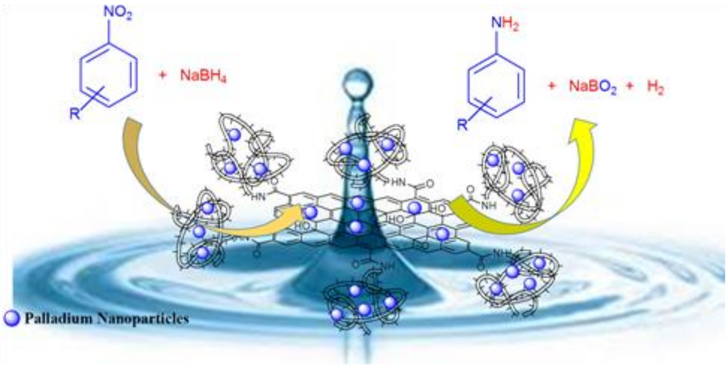

Fig. 1 Reduction of nitroarenes using GO-Chit-Pd

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Paper code: 45

The Synthesis of Formylated-Triarylmethanes and Their Use in the Preparation of Hydrazone and Azine Derivatives

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Hydrazones and azines have attracted great interests in organic synthesis due to their versatile applications as synthons in the preparation of heterocyclic compounds as well as medical agents [1], [2]. Several methods are available for the synthesis of triarylmethanes (TRAMs), however their synthetic applications has gained less attention until now. In continuation of our work on TRAMs, herein we report controlled catalytic procedures for the synthesis of azine and hydrazine derivatives bearing triarylmethane unit(s) [3]. First, formylated-triarylmethanes were synthesized *via* the Friedel-Crafts reaction of arenes with dialdehydes catalyzed by silicasulfuric acid (SSA) under solvent-free conditions. Then, the aldehydes were reacted with hydrazine hydrate (1:2 molar ratio) in the presence of *L*-proline, as an organocatalyst, and under N_2 atmosphere to afford the corresponding hydrazones, quantitatively (Figure 1). It was perceived that this reaction can be also used for the synthesis of azine products by changing the molar ratios of substrates and choosing an appropriate catalyst. Accordingly, the reaction of formylated-triarylmethanes with hydrazine hydrate in 2:1 molar ratio, catalyzed by either AcOH or SSA, gave the corresponding azines. The structures of the synthesized compounds were characterized by elemental analyses, and FT-IR, ^{1}H-NMR, and ^{13}C-NMR spectral data.

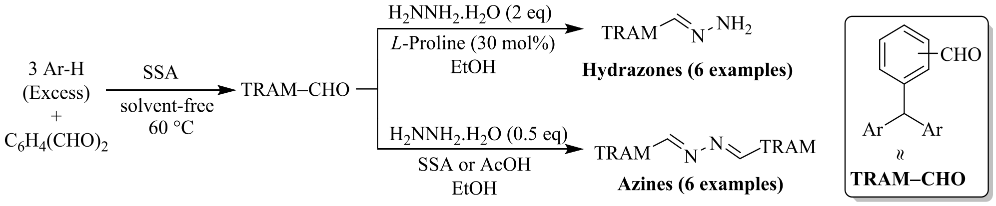

Fig. 1 Synthesis of formylated-triarylmethanes, and their conversion into hydrazone, and azine derivatives.

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Paper code: 50

An efficient method for the one-pot synthesis of 4-phenyl-hydrazineyl thiazole derivatives using nano-SiO_2

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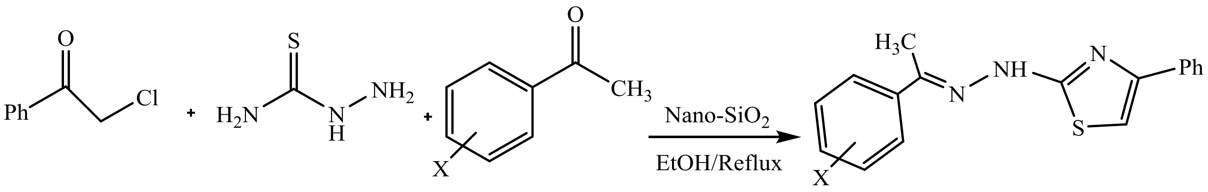
Thiazoles are widely found in bioorganic and medicinal chemistry with application in drug discovery. Thiazoles exhibit diverse biological activities such as antimicrobial [1], and anti-diabetic [2] activities. Also, various thiazoles such as 2-arylthiazole received much attention due to unique structure and its usage as anticancer agents [3]. In this research, one-pot three-component synthesis of 4-phenyl-hydrazineyl thiazole derivatives was developed by a condensation of various acetophenones, phenacyl chloride, and thiosemicarbazid in the presence of nano-SiO_2 in ethanol at reflux conditions (Scheme 1). The products formed in excellent yields over short reaction times under an environmentally friendly conditions.



Scheme 1. One-pot synthesis of 4-phenyl-hydrazineyl thiazole derivatives

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Paper code: 52

Facile synthesis of *N,N'*-diarylformamidines by Acidic ionic liquid immobilized on nanoporous TiO_2

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Formamidines are one of the noteworthy classes of compounds because they have a wide range of biological and pharmacological properties, for example they have been used as pesticides and antimalarial reagents [1-2]. The general procedure for the preparation of formamidines involves the reaction between two moles of aniline derivatives with one mole of ethyl orthoformate in the presence of an organic or mineral acid catalyst [3] Various methods have been proposed for this reaction, but provided methods have disadvantages, including the use of homogeneous catalysts that have several serious problems.

In this work, a green and efficient procedure is reported for the preparation of *N,N'*-diarylformamidines using acidic ionic liquid immobilized on nanoporous TiO_2. The procedure gave the products in excellent yields in very short reaction times under solvent-free conditions. The reusability of the catalyst is the other important feature of the reported method [fig. 1].

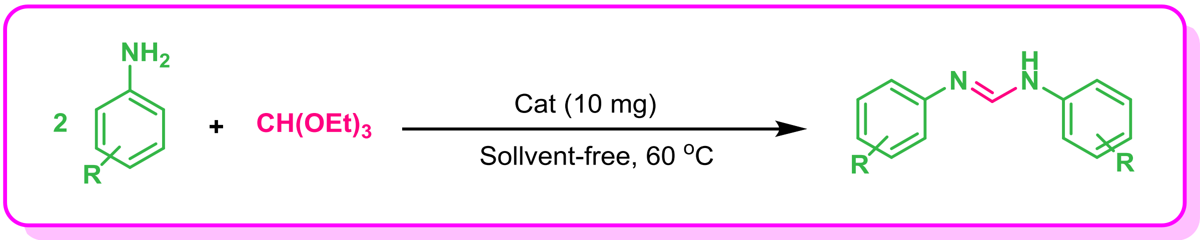

Fig. 1 Synthesis of *N,N'*- diarylformamidines derivatives catalyzed by acidic ionic liquid immobilized on nanoporous TiO_2.

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Paper code: 56

TiO_2 nanoparticles supported on the Fe_3O_4/GO nanocomposite: a novel magnetic nanocatalyst for the synthesis of 2- Aminothiazoles

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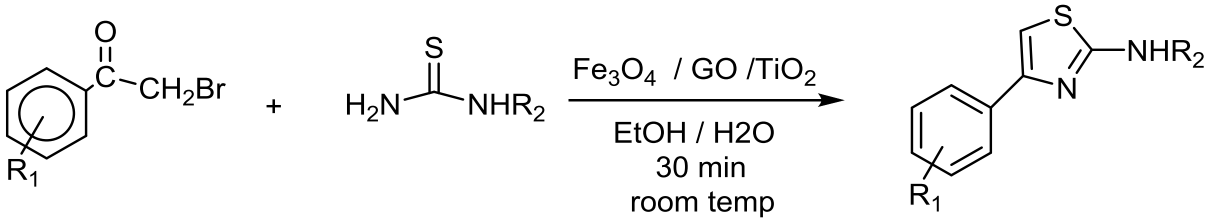
2-aminothiazoles are very important heterocyclic compounds in medicinal chemistry and applied as a ligand in estrogen receptor [1]. In the recent years, application of modified magnetic nanoparticle (Fe_3O_4) as a reusable and highly stable magnetic nanoparticle has attracted much attention in 2-aminothiazole synthesis [2]. Among many materials, graphene and its derivatives are considered potential materials for the immobilization of nanoparticles. In the present study, Fe_3O_4/GO/TiO_2 nanocomposite was prepared by a sol-gel method for titania coating on Fe_3O_4/GO. The Fe_3O_4/GO/TiO_2 composite particles were characterized by FT-IR and TEM. In this reaction thiourea was reacted with various α-bromo Acetophenones in the presence of (Fe_3O_4/GO/TiO_2) catalyst affording the desired 2-aminothiazoles in high yields. In conclusion, we have successfully demonstrate for the first time that Fe_3O_4/GO/TiO_2 composite could be used as an efficient solid recyclable magnetic nanocatalyst for convenient synthesis of 2-aminothiazole derivatives under mild conditions. The novelty and synthetic volubility of this method developed the mild reaction conditions, easy experimental procedure, avoiding the use of organic solvents and recovery of the magnetic nanocatalyst.



$R_1 = CH_3$, Cl ,Br ,H R_2 = H, Ph , 4-ClPh

fig.synthesis of 2-aminothiazoles catalysed Fe_3O_4 / GO / TiO_2 Nanocomposite

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Paper code: 73

Efficient synthesis of bis-coumarins using Isatin-*N*-sulfonic acid under solvent-free conditions

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Coumarin derivatives are an important class of compounds in medicinal chemistry. These compounds possess several pharmacological properties such as anticancer, anti-HIV, anticoagulant, spasmolytic, antibacterial and anti-inflammatory activities. These compounds have been also used as fluorescent molecules, and laser dyes for the blue-green region (400–520 nm) [1]. Bis-coumarins, as an important member of coumarin derivatives, are prepared by the reaction of 4-hydroxycoumarin with arylaldehydes [2]. Although some catalysts have been introduced for the production of bis-coumarins; many of them are associated with at least one of these disadvantages: relatively long reaction times, moderate yields, utilization of volatile organic solvents as reaction media and poor compliance with the green chemistry protocols.

Multicomponent reactions (MCRs) are powerful, versatile, and popular tools for the synthesis of novel and complex molecular structures that have advantages over a conventional multistep synthesis such as energy saving, lower cost, shorter reaction time, high atom economy and expensive purification [3].

In this research, we have introduced Isatin-*N*-sulfonic acid as a highly efficient and general solid-acid catalyst for the synthesis of bis-coumarins in high yields and short reaction times by the pseudo multicomponent reaction of 4-hydroxycoumarin with arylaldehydes (Scheme 1).

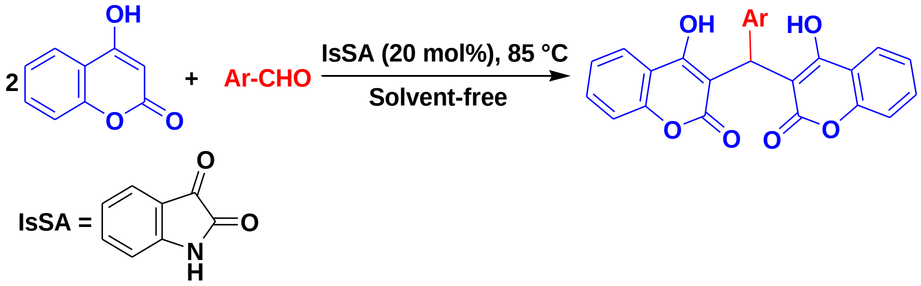

Fig. 1 The production of bis-coumarins using IsSA.

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Paper code: 74

Pyridinium-*N*-sulfonic acid hydrogen sulfate as a highly effective and dual-functional catalyst for the synthesis of 1-carbamatoalkyl-2-naphthols

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Carbamate skeleton is significant moiety of several natural products and versatile precursors for synthesis of pharmaceutics such as saxitoxin, mitomycin and bleomycin. Compounds which have both carbamate and a hydroxyl group such as 1-carbamatoalkyl-2-naphthols are of considerable interest, because hydrolysis of carbamates can produce a variety of amino alcohols; these compounds are the main sub-structure of a variety of biologically important natural products and potent drugs including a number of nucleoside antibiotics and HIV protease inhibitors, such as ritonavir and lipinavir [1, 2].

Ionic liquids have various (ILs) unique properties, including non-flammability, non-volatility, high thermal and chemical stability and enhanced reactivity. Brønsted acidic ILs are an important class of these compounds, which have been widely applied as efficient catalysts for organic transformations [3].

In this work protic acidic ionic liquid pyridinium *N*-sulfonic acid hydrogen sulfate {[Py-SO_3H][HSO_4]} has been used as a highly effective and homogeneous catalyst for the one-pot multi-component reaction of arylaldehydes, 2-naphthol and alkyl carbamates under solvent-free conditions to synthesize 1-carbamatoalkyl-2-naphthols (Scheme 1). Excellent yields, short reaction times, easy work-up and purification of the products, easy production of the catalyst and relatively mild conditions are some advantages of this procedure. High effectuality of [Py-SO_3H][HSO_4] can be attributed to its dual-functionality.

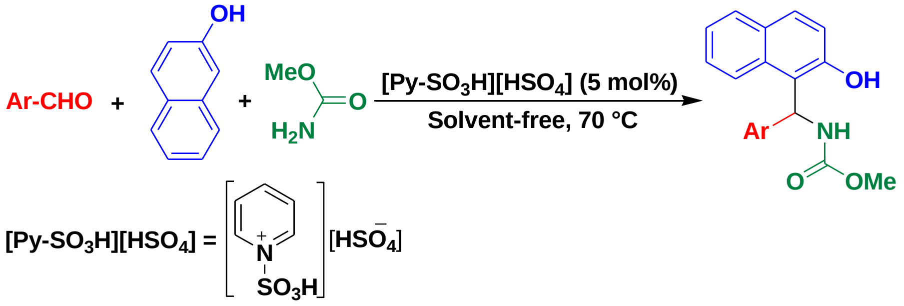

Fig. 1 The production of 1-carbamatoalkyl-2-naphthols using [Py-SO_3H][HSO_4].

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Paper code: 79

One-pot procedure for the synthesis of diverse derivatives of novel heterocyclic system benzo[e]pyrazolo[5',1':2,3]pyrimido[5,4-b][1,4]diazepine

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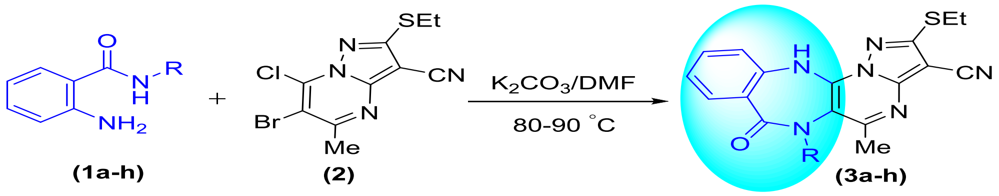
The 1,4-diazepine and 1,4-benzodiazepine structures have been found in the naturally occurring products and are significant biomolecules in medicinal chemistry with a wide range of biological and pharmacological activities such as antibiotic, [1] antimalarial, [2] anti-HIV, [3] and anticancer.[4] The benzodiazepines are also the most widely prescribed minor tranquilizers in current use, and they are known to act on the central nervous system. Therefore, benzodiazepines are an important class of psychotherapeutic compounds. [5]

Due to the widespread biological activities of fused heterocyclic systems, in this study, we synthesized various derivatives of benzo[*e*]pyrazolo[5',1':2,3]pyrimido[5,4-*b*][1,4]diazepine as a novel heterocyclic system. In this one-pot protocol, the desired products (3a-h) were obtained through the cyclocondensation of diverse synthesized 2-amino-*N*-alkylbenzamides (1a-h) with 6-bromo-7-chloro-2-(ethylthio)-5-methylpyrazolo[1,5-*a*]pyrimidine-3-carbonitrile (2) in the presence of K_2CO_3 in DMF. The true regioisomers of heterocyclization were also investigated.



R: Et, *n*-Pr, *i*-Pr, *n*-Bu, *i*-Bu, Bn, *Cyclo*-Hexyl, *p*-Me-Phenyl

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Paper code: 96

A regioselective synthesis of novel oxo-thioxo[3.3.3]propellanes

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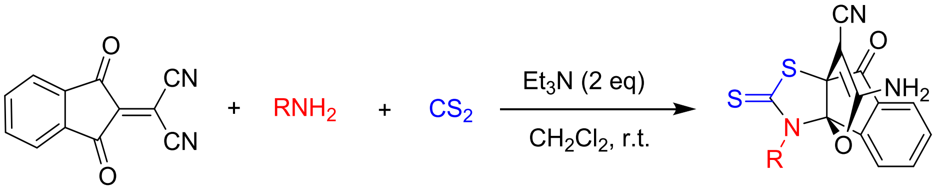
Propellane is a special kind of fused tricyclic system containing three non-zero bridges and one zero bridge between a pair of bridgehead carbon atoms [1]. This skeleton has received much attention in synthetic organic chemistry due to their fascinating topology, significant chemical and physical properties and their presence in several natural products and bioactive compounds [2]. In recent years, various protocols for the synthesis of propellanes have been described [3]. Herein, we report a new method for the synthesis of novel oxo-thioxo[3.3.3]propellanes **3** by a one pot three-component reaction involving aliphatic and aromatic amines **2**, carbon disulfide, and the Knoevenagel condensation product of ninhydrin and malononitrile **1** in CH_2Cl_2, in the presence of Et_3N, at room temperature (Fig. 1). The structures of products were characterized by their IR, ^1H NMR, ^{13}C NMR and mass spectral data. Various advantages of these transformations will be presented and discussed.



1 **2** **3**

Fig. 1 Synthesis of oxo-thioxo[3.3.3]propellanes.

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Paper code: 108

Synthesis of the Cu (II) Schiff base complexes supported on alumina nanoparticle; for preparation of 5-Substituted-1*h*-tetrazoles derivatives

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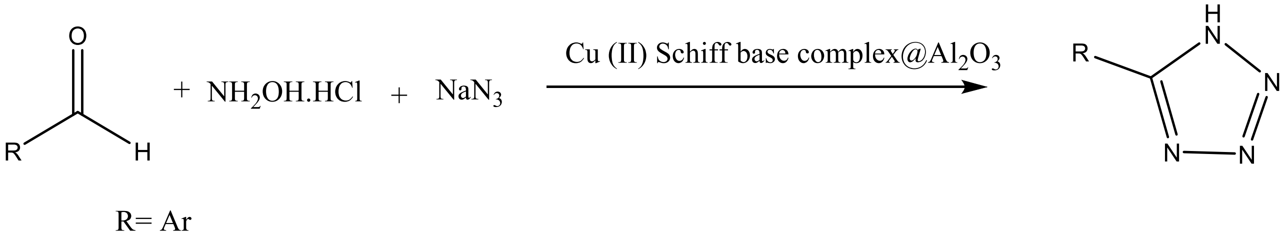
Schiff bases and their complexes are versatile compounds synthesized from the condensation of an amino compound with carbonyl compounds and widely used for industrial purposes and also exhibit a broad range of biological activities including antifungal, antibacterial, antimalarial, antiproliferative, anti-inflammatory, antiviral, and antipyretic properties. Many Schiff base complexes show excellent catalytic activity in various reactions and in the presence of moisture[1]. Complexes of Schiff bases have been used as antibacterial, antifungal, anticancer, antitubercular, hypertensive, and hypothermic agents[2]. Tetrazoles are an important class of heterocyclic nitrogen-rich compounds, due to their wide range of applications in agriculture, pharmacy, medicine, chemistry and material science, So the preparation of various tetrazole derivatives over the past few years has been developed rapidly.In pharmacy, they are employed as antidiabetics, antibiotics and HIV-inhibitor Owing to lower toxicity and higher lipophilicity of tetrazoles, they can be used as isosteric replacements in drugs Furthermore, they are applied as ligands in coordination chemistry [3]. In this research, the Cu (II) Schiff base complexes supported on alumina nanoparticle were used for the preparation of 5-Substituted-1*h*-tetrazoles. In this case (1/5mmol) NaN_3 (1/5mmol) $NH_2OH.HCl$ were treated with (1mmol) benzaldehyde derivatives through one-pot method in green solvent at short times and very good yields (Scheme1).



Scheme 1. Preparation of 5-subsituted 1*h*-tetrazole by using of Cu (II) Schiff base complex @Al_2O_3.

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Paper code: 125

One-Pot Synthesis Of 1,4-Benzodiazepine Derivatives Using Hetropoly acid Ionic Liquids Supported On Magnetic Nanoparticles Of $CoFe_2O_4$

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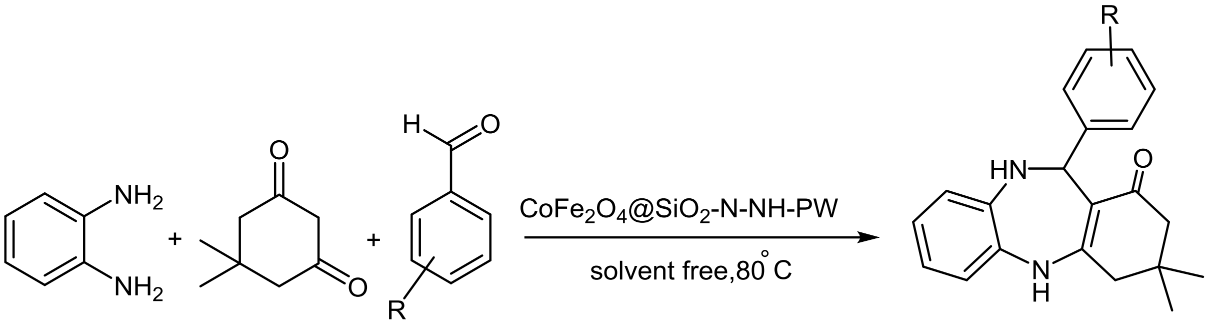
Benzodiazepine derivatives are a highly valuable class of heterocyclic compound that possess various medicinal, biological and pharmaceutical activities such as anticonvulsant, anti-anxiety, antitumor, antipyretic and anti-inflammatory [1].The heteropoly anions are heterogeneous acid catalysts that used for dehydration reactions from diols, rearrangement, friedel-craftts alkylation and the synthesis of antioxidants, vitamins and biologically active substances. Research has shown that immobilization of heteropolyacids (HPAs) on a suitable support can eliminate its encountered major drawbacks, including very low surface area and instability in polar solvents. However, immobilization of heteropoly acids have more than acidic sites available for their crude state, thus exhibiting more catalytic activity [2].Introducing HPAs supported on magnetic nanoparticles can provide a means for effective separation of the catalyst from the reaction mixture, and it can be easily separated from the reaction by applying a simple permanent magnet [3]. We now wish to report, easy and efficient one pot synthesis of 1,4-benzodiazepine derivatives directly from dimedone, *o*-phenylenediamine and an aromatic aldehyde in high yields over short reaction times, easy work-up, reusability of the nanocatalyst using heteropolyacids ionic liquids supported on magnetic nanoparticles of $CoFe_2O_4$ under one-pot solvent-free conditions.



R=CH_3, OMe, NO_2, Cl, CN

PW=$H_5PW_{11}CuO_{39}$

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Paper code: 130

Synthesis of new tetrahydropyridines catalyzed by Fe_3O_4@S-doped TiO_2 *via* one-pot multi component Mannich reaction

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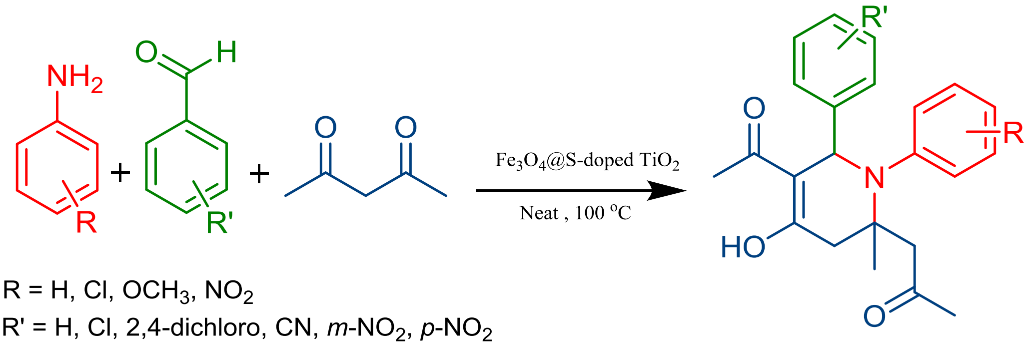
Organic reactions promoted by recyclable solid catalysts have attracted much attention for their great economic and environmental importance in the chemical and pharmaceutical industries. Synthesis of highly substituted tetrahydropyridines has been developed using several approaches such as intramolecular Mannich reaction onto iminium ions. These compounds are biologically active and important in pharmaceutics [1-3].

In this study, synthesis of new tetrahydropyridines from the one-pot three component Mannich reaction between acetyl acetone, aromatic aldehydes and amines under neat conditions is described. This reaction catalyzed by Fe_3O_4@S-doped TiO_2, as an efficient, reusable and heterogeneous catalyst (Scheme 1).

The results showed that catalyst affected both on the rate of reaction and purity of products. Design and preparation of Fe_3O_4@S-doped TiO_2 hollow nanospheres and optimization of the condition of the given reaction will be discussed in the congress.



R = H, Cl, OCH_3, NO_2
R' = H, Cl, 2,4-dichloro, CN, *m*-NO_2, *p*-NO_2

Scheme 1. Pseudo four component reaction for preparation of new tetrahydropyridines.

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Paper code: 140

Oxidation of alcohols and trimethylsilyl ethers by molybdic acid supported on $NaHSO_4.H_2O$ under solvent-free conditions

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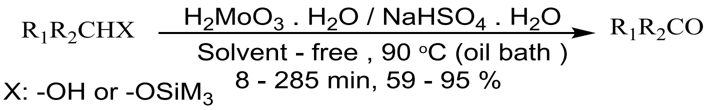
The oxidation of alcohols to their corresponding aldehydes and ketones is an important transformation in organic chemistry, which has received great attention in the past and also in recent years.Numerous oxidizing reagents are available to achieve this key transformation which of them chromium (VI)-based oxidants, ruthenium-based oxidants, activated dimethylsulfoxide and hypervalent iodine are examples. Although these methods are useful in organic synthesis, most of them suffer from disadvantages such as use of expensive or toxic reagents, long reaction times, low yields of the products, tedious work-up procedure and strongly acidic conditions. In this research,$H_2MoO_3.H_2O/NaHSO_4.H_2O$ has been used as an efficient reagent system for the oxidation of alcohols and trimetylsilyl ethers to their corresponding carbonyl compounds. high yields of the products and relatively short reaction times are important advantages of this reagent.



$$R_1R_2CHX \xrightarrow[\text{Solvent - free , 90 °C (oil bath)}]{H_2MoO_3\ .\ H_2O\ /\ NaHSO_4\ .\ H_2O} R_1R_2CO$$

X: -OH or $-OSiM_3$ 8 - 285 min, 59 - 95 %

Fig1: The oxidation of alcohols and trimetylsilyl ethers with molybdic acid supported on NaHSO4.H2O under solvent-free conditions.

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Paper code: 141

L-Prolin anchored on mesoporous SBA-15: A new recyclable catalyst to the synthesis of pyrimidines

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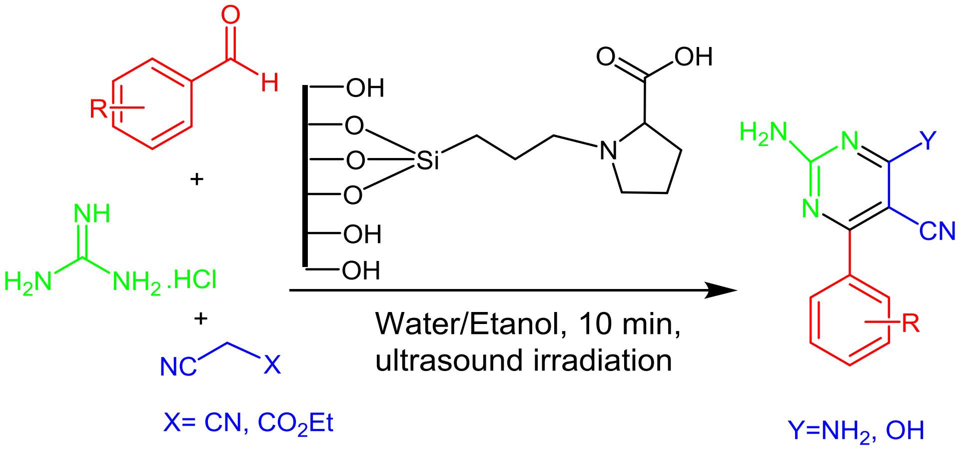
The Heterogenization of catalyst prospers the recycling properties along with improving the performance of them. Ordered mesoporous silica show high ability to be an environmentally benign catalyst.[1] They have a robust structure with high surface area to use in the industries. As regard to the pore size of them, especially SBA/15 can be functionalized by organic compound in order to develop the application in catalysis.[2] In this research the novel organic–inorganic hybrid catalyst by N-Functionalized L-Proline anchored SBA/15 was synthesized**.** The structure of 2D-hexagonally ordered mesophases of catalyst characterized by FTIR spectroscopy, N_2 adsorption analysis, scanning electron microscope, X-ray diffraction spectroscopy. The activity of catalyst has been scrutinized by synthesizing pyrimidine that showed biological anti-bacterial activities.[3] The process of the synthesis of these compounds might be followed by tautomeric interconversion but in the presence of L-proline@SBA-15 catalyst, the reaction stopped at this stage. small angle X-ray diffraction pattern of prior and after the incorporation of the bidentate complex shows an intense diffraction peak at (1 0 0), (1 1 0) and (2 0 0).



Scheme. Synthesize of pyrimidines in the presence of L-proline@SBA-15 under ultrasound irradiation

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Paper code: 148

Nano-$SnCl_4/SiO_2$ as a Green and Reusable Catalyst for the Synthesis of Azo Dyes Based on 2- Naphtol under Grinding Conditions

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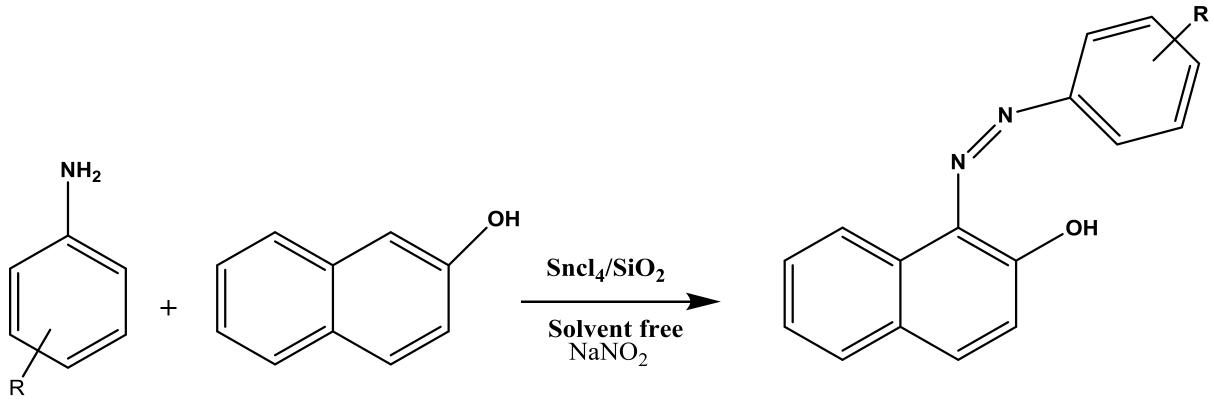
It is well known that azo compounds are the most widely class of industrial synthesized organic dyes due to their versatile application in various fields, such as dyeing textile fibers, biological and pharmacological properties[1]. Azo dyes are generally synthesized in two steps: the diazotization of aromatic primary amines, followed by the coupling reaction between diazonium salts and activated aromatic compounds [2]. Previously, aromatic amines have been converted to diazonium salts in the presence of $NaNO_2$ and a mineral acid at 0-5 °C[3]. Herein, we wish to report a convenient and one-pot method for diazotization and diazo coupling reaction with 2-naphoi by using nano-$SnCl_4/SiO_2$ under solvent-free conditions by grinding (Scheme1).The advantages of this work are simple work-up, mild condition, short reaction time and high yields.



Scheme1

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Paper code: 149

Facile and one-pot synthesis of pyrimido[4,5-*b*]quinolines catalyzed by [PVP- SO_3H]HSO_4

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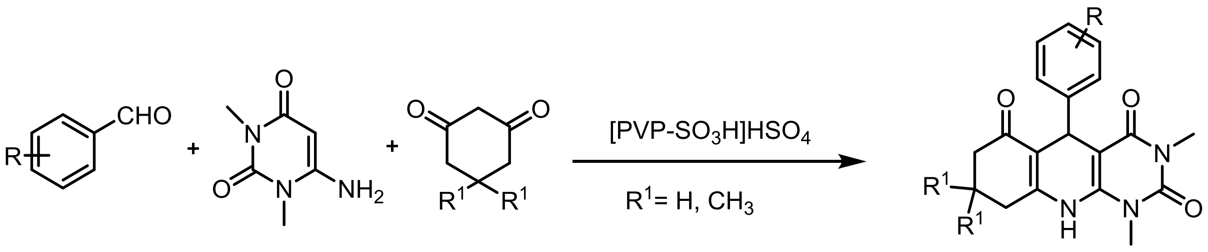
Recently, much attention has been paid to the development of new procedures for the synthesis of heterocyclic compounds such as quinoline. Quinoline derivatives are of interest in medicinal chemistry and chemical biology due to their wide range of biological activities such as antibacterial, antimalarial, antitumor, antiasthmatic, anthelmintic and antiplatelet [1-2].

Herein, we report the synthesis of pyrimido[4,5-*b*]quinoline derivatives *via* a three-component, one-pot condensation of aldehyde derivatives, 1,3-diketone, and 6-amino-1,3-dimethyl uracil in the presence of [PVP- SO_3H]HSO_4 as catalyst. The procedure gave the products in excellent yields in short reaction times and good to high yields. Also this catalyst can be reused several times without loss of its catalytic activity.



Scheme 1 Synthesis of pyrimido[4,5-*b*]quinoline derivatives using [PVP- SO_3H]HSO_4 as the catalyst.

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Paper code: 152

Isonicotinic acid as an efficient catalyst for the synthesis of hexahydroquinolines

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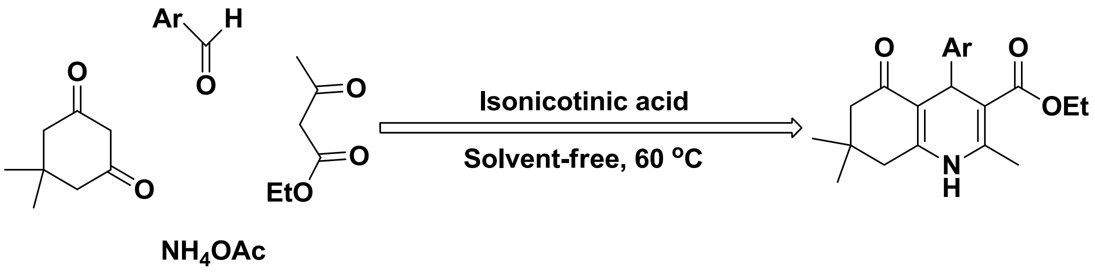
Quinolines with a 1,4-dihydropyridine structure are promising scaffolds due to their pharmacological activities. This part of quinoline derivatives has very utilizations in medicinal chemistry and applied as antiasthamatic, anti-inflammatory, antimalarial, antibacterial, antihypertensive, and tyrosine kinase inhibiting compounds [1-3]. One of the important classes of DHPs with a modified structural scaffold is hexahydroquinolines (HHQs) which could be synthesized by the reaction of various aromatic aldehydes, dimedone, *β*-ketoesters and ammonium acetate using different catalysts. Herein, we have reported the preparation of hexahydroquinolines using isonicotinic acid, at 60 °C under solvent-free conditions (Scheme 1).



Scheme 1. The preparation of hexahydroquinolines catalyzed by isonicotinic acid.

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Paper code: 156

Synthesis of cyclopropane derivatives via an efficient stereoselective trimerization procedure

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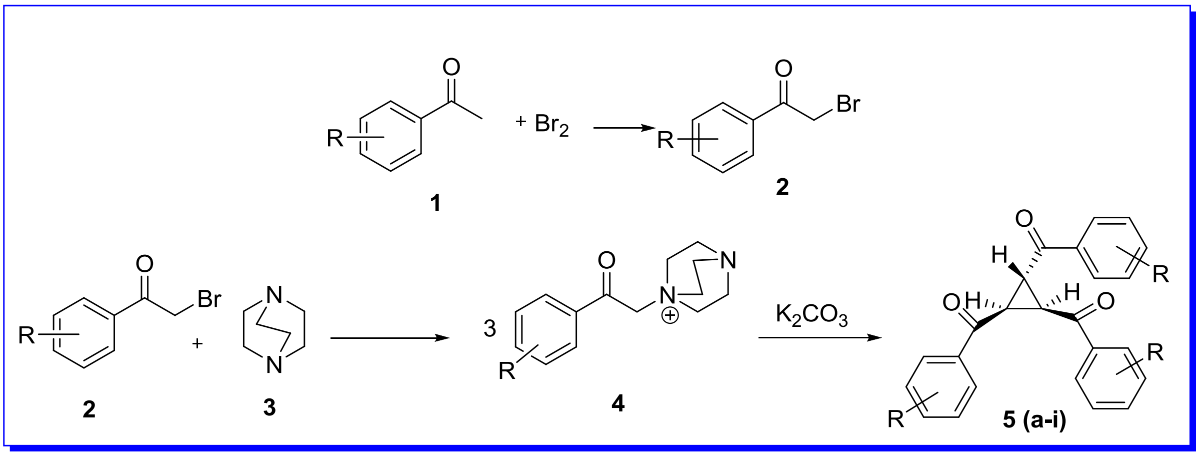
Cyclopropanes are valuable intermediates that can be used in a wide array of biochemical process and in medicinal chemistry owing to a unique combination of reactivity and structural properties [1,2].

In this work, quaternary ammonium salts (**4**) is prepared by the reaction of phenacyl bromides (**2**) with the 1,4-Diazabicyclo[2.2.2]octane (**3**). Deprotonation with potassium carbonate as a mild base forms the corresponding ylide, which undergoes trimerization reaction to give (2,3-bis-(aroyl)cyclopropyl)aryl methanone derivatives (**5a-5i**) efficiently in a stereoselective manner (Scheme 1). The reaction mixture was purified by using column chromatography to afford the desired pure product. The structures of the products were identified by spectral data. The *cis* configurations of the products were confirmed by the coupling constant of the vicinal protons of cyclopropane ring [3].



Scheme 1. Synthesis of cyclopropane derivatives via a trimerization reaction

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Paper code: 163

Bromination of Phenol and Anillin derivatives in Presence of $[MdPd](Br_3)_2$

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Mono(6,7-dihydrodipyrido[1,2-a:2',1'-c]pyrazine-5,8-diium)hexabromide$[MdPd].(Br_3)_2$ was quantitatively prepared and used for the bromination of anilines and phenols in the presence of a mixed solvent system (e.g., Acetonitril or DCM/MeOH 2:1) and under solvent free conditions [1-2]. Also it has been done selective oxidation of Benzyl alcohols to their corresponding carbonyl compounds in presence of Mono (6,7-dihydrodipyrido[1,2-a:2',1'-c]pyrazine-5,8-diium) diperchlorate.

This new ionic liquid has advantages over similar brominating agents in terms of short reaction time, simple workup, regioselectivity and high yields.

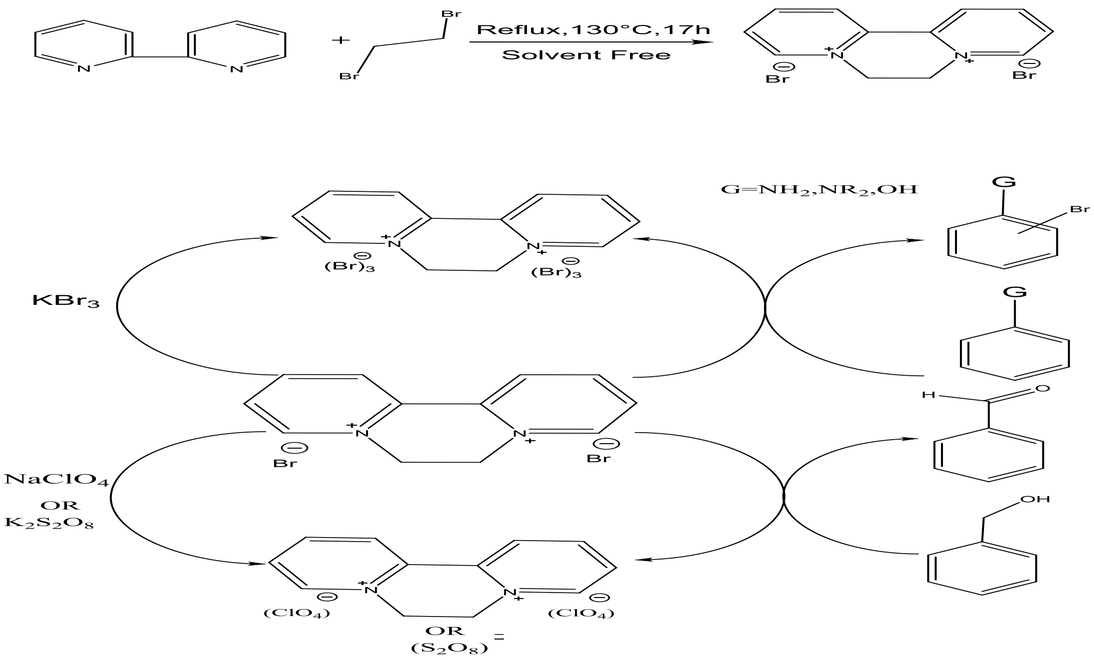

Fig. 1 Synthesis and mechanism reaction of Bromination and selective oxidation.

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Paper code: 164

Highly efficient three-component synthesis of 5-substituted-1H-tetrazoles, in the presence of Cu(II) heterogeneous complex catalyst

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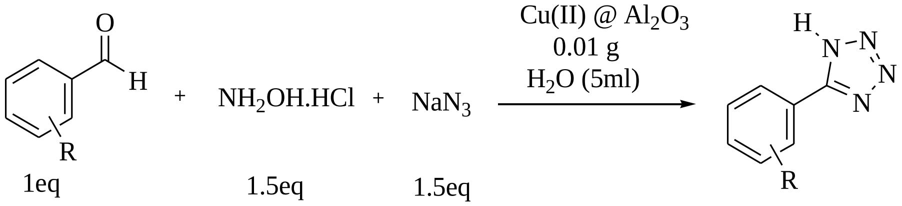
Tetrazoles as one of the most important synthetic heterocyclic compounds exhibit numerous applications in different areas of sciences especially in chemistry, material, and medicinal sciences. Tetrazoles have displayed important pharmacological and biological properties such as anticancer, antiviral, anti-HIV, anti-inflammatory, antifungal, and antibacterial activities. In addition, tetrazolyl moieties are present in the structures of several famous drugs such as candesartan, losartan, valsartan, and zolarsartan [1]. The use of heterogeneous catalysts for organic synthesis is rapidly growing over homogeneous catalytic systems because of their several advantages such as high stability and tolerant to harsh reaction conditions, reusability of the catalyst, environmental friendliness and easy to purify of the products [2].

In this research, we used Cu(II) complex on poly(methyl acrylate) supported on alumina nanoparticles as a substrate for the preparation of a heterogeneous catalyst. Then, a small amount of the catalyst was used to one pot reactions between benzaldehyde (1 mmol), hydroxylamine hydrochloride (1.5 mmol) and sodium azide (1.5 mmol) in the presence of green solvent (water) at room temperature to produce 5-substituted-1H-tetrazoles derivatives, the related products were obtained with high efficiency in a short time (Scheme 1).



Scheme 1 Synthesis of 5-substituted-1H-tetrazoles derivatives using Cu(II) @ Al_2O_3 catalyst

References

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Paper code: 165

Hantzch reaction for the synthesis of 4-(2-pyrrolyl)-dihydropyridines in the presence of Fe_3O_4@Chitosan–SO_3H nanoparticles as catalyst

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1,4-Dihydropyridines belong to an important class of organic compounds which include unique structural motifs in a wide range of natural products and biologically active molecules [1]. They are an important class of heterocyclic compounds that have a broad scope of pharmacological and biological activities such as antidiabetic, antitumor, vasodilator, bronchodilator, geroprotective and anti-atherosclerotic properties. Therefore, the use of dihydropyridine moiety in the skeletons of heterocyclic and biological molecules is of great interest [2-4]. One of the methods for the synthesis of this compounds is the Hantzch reaction. Among the several methodologies of this reaction, using of heterogeneous magnetic catalysts has been widely considered. In this study, the efficacy of magnetic sulfonated chitosan as catalyst for synthesis of dihydropyridines via one-pot three-component condensation reaction has been examined. Treatment of N-substituted-pyrrole-2-carbaldehyde (1 eq.), 1,3-dicarbonyls (2 eq.) and ammonium acetate (1 eq.) in the presence of Fe_3O_4@Chitosan–SO_3H (10 mol%) as a heterogeneous catalyst at 70ºC gave the desired products in good yields. (Figure 1). The merits of this method include mild reaction conditions, high yield of products, short reaction times, and reusability of the catalyst.

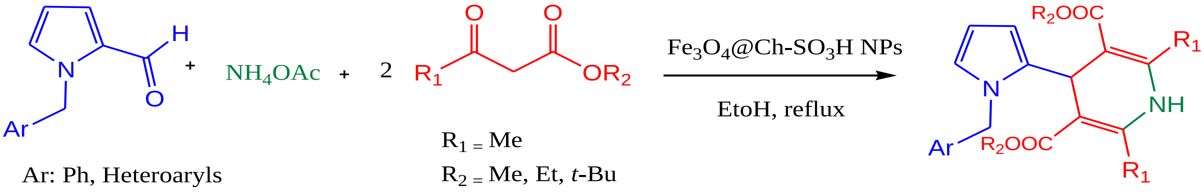

Fig. 1 one-pot three-component Hantzch reaction for the synthesis of 4-(2-pyrrolyl)-dihydropyridines

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Paper code: 168

Tandem cyclocondensation-Knoevenagel–Michael reaction of phenylhydrazine, acetoacetate derivatives and arylaldehydes, in the presence of isonicotinic

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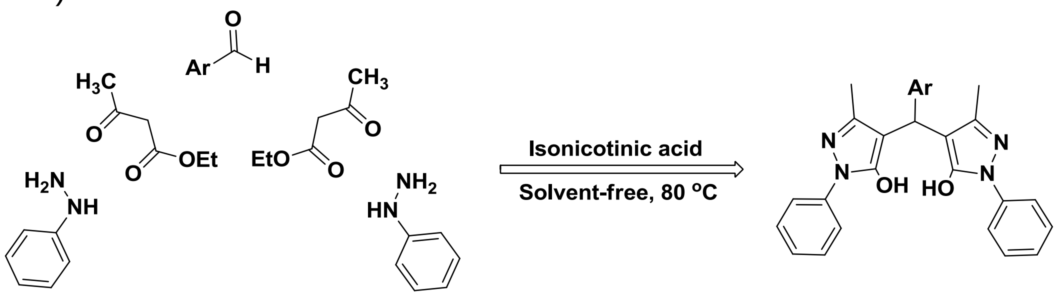
Bis(pyrazolyl)methanes such as 4,4′-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s being used as anti-inflammatory, antipyretic, gastric secretion stimulatory, antidepressant, antibacterial and antifilarial agents [1, 2]. Moreover, these compounds have been applied as fungicides [3], pesticides [4] and insecticides [5, 6]. The most common protocols for the synthesis of 4,4´-(arylmethylene)bis(1H-pyrazol-5-ol)s is one-pot three-component condensation reaction of various aldehydes with 3-methyl-1-phenyl-5-pyrazolone using different catalysts [6]. Having this issue in mind, we have introduced isonicotinic acid as an efficient and homogeneous catalyst for the preparation of 4,4´-(arylmethylene)bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s via one-pot pseudo five component condensation reaction of phenylhydrazine and ethyl acetoacetate with various aromatic aldehydes at 80 ˚C under solvent-free conditions (scheme 1).



Scheme 1. The preparation of bis(pyrazolyl)methanes catalyzed by isonicotinic acid.

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Paper code: 169

Synthesis and spectroanalytical studies of a new heterocyclic acid-base indicator

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The new purple dyes of the imidazopyridine series were synthesized by the reaction of 6-chloro-3-nitroimidazo [1, 2-a] pyridine with (4-methylphenyl) acetonitrile in basic MeOH solution via nucleophilic substitution of hydrogen atom. The reagent solution shows a reproducible change in its color due to the addition of acid or base. A UV-Vis spectroscopic characterization and acid-base equilibrium study of the reagent for its possible use as an indicator were investigated. The results show that the reagent is an amphoteric which possesses two ionization constants Kb and Ka of weak basic and acidic properties. The dissociation constants of the indicator in aqueous solution which are determined by spectrophotometric method are pKb, 11.57 and pKa, 9.73. This indicator is compared with existing acid-base indicators effective over the same pH range. Furthermore, conversion of these dyes to new 8-chloro-3-methylpyrido [2',1':2,3] imidazo [4,5-b]quinoline-,12-carbonitriles is reported.

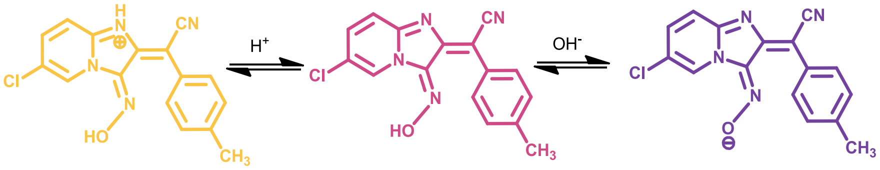

Fig. 1 The equilibriums at low and high pH.

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Paper code: 170

Using a new magnetically separable nanocatalyst in the synthesis of [1,2,4]triazolo quinazolinone derivatives

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The quinazolinones derivatives as nitrogen-containing heterocycles has drawn a huge consideration because of their biological activities and various applications in pharmaceutical industries and their important role in research, medicinal and industrial societies. [1,2]. in this study Immobilized $NaHSO_4$ on core/shell phenylene bridged Periodic mesoporous organosilica magnetic nanoparticles (Fe_3O_4@Ph-PMO-$NaHSO_4$) as a new acidic magnetically separable nanocatalyst was successfully prepared in three steps: (i) preparation of Fe_3O_4 nanoparticles by a precipitation method, (ii) synthesis of an organic-inorganic periodic mesoporous organosilica structure with phenyl groups on the surface of Fe_3O_4 magnetic nanoparticles (MNPs) and (iii) finally adsorption of $NaHSO_4$ on periodic mesoporous organosilica (PMO) network and it was used as a a new magnetically separable solid acid nanocatalyst for the synthesis of [1,2,4]triazolo quinazolinone [3].

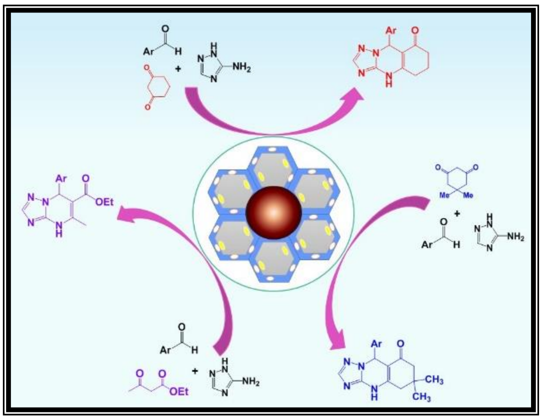

Fig. 1 Synthesis of [1,2,4]triazolo quinazolinone derivatives.

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Paper code: 171

Using a new superparamagnetic nanocatalyst for the N-Boc protection of amines

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Functional group protection and deprotection methods are important in the multistep organic synthesis. The presence of an amino group in various biologically active compounds makes its protection as a necessity during their synthesis [1]. The N-amine protecting groups have been used extensively across a wide range of chemical fields, such as peptide, nucleotide, polymer, and ligand preparations. Several methods and reagents have been reported for the protection of amine and amin and amine derivatives [2]. Among them, N-tert-butoxycarbonylation has received the greatest attention because of the stability of the N-Boc group against nucleophilic attack or alkali media and catalytic hydrogenation [3].

The challenge of designing a protocol for efficient Boc protection of amines, which is mild as well as environment-friendly and which has the advantages of solid catalysts, encouraged us to investigate the applicability of a new stable and highly active superparamagnetic nanocatalyst for the preparation of N-Boc derivatives. In this regard, a simple, green, and efficient method for the N-tert-butoxycarbonylation of amines was accomplished at 50˚C and neat conditions. The green conditions, excellent yields, practicability, operational simplicity, product purity, cost efficiency and environmentally profits are the considerable advantages of this protocol.

$$R^1R^2NH \xrightarrow[\text{Solvent-free, 50 °C}]{Boc_2O,\ Fe_3O_4/MCM\text{-}41\text{-}Zr/piperazine} R^1R^2N\text{-}Boc$$

Scheme 1 N-Boc protection of amines.

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Paper code: 172

The synthesis of 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s using boric acid aqueous solution system

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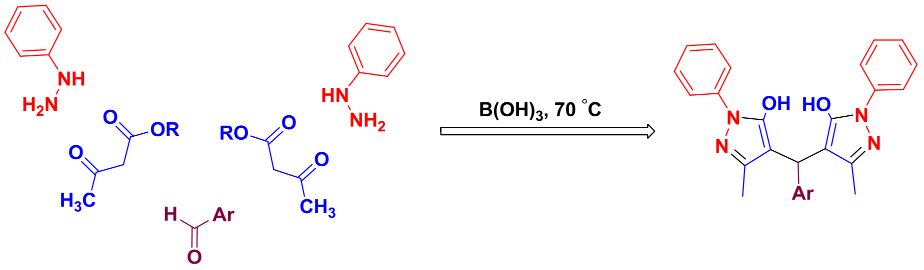
Bis(pyrazolyl)methanes (BPMs) including 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s have a broad spectrum of approved biological activity, being used as anti-inflammatory, antipyretic, gastric secretion stimulatory, antidepressant, antibacterial, and antifilarial agents [1]. 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s, were prepared by various methods including application of piperidine in ethanolic solution [2], tandem Knoevenagel-Michael reaction in benzene solutions [3], application of sodium dodecyl sulfate in aqueous media [4], and electrocatalytic synthesis [5]. Having above facts, we have reported the preparation of bis(pyrazolyl)methanes by the condensation reaction of phenylhydrazine, ethyl acetoacetate and aryl aldehydes in the presence of boric acid, at 70 °C under aqueous conditions as a mild and green reaction condition (Scheme 1).



Scheme 1: Synthesis of 4,4´-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s

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Paper code: 179

Application of Fe_3O_4@Chitosan–SO_3H nanoparticles as efficient catalyst for synthesis of 4*H*-isoxazol-5-ones in aqueous medium

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Isoxazoles are a class of heterocyclic compounds having a remarkable number of applications and have been demonstrated to be very versatile building blocks in organic synthesis [1]. They have a wide range of biological activities including hypoglycemic, analgesic, antiinflammatory, anti-bacterial and HIV-inhibitory activities, as well as some agrochemical properties such as herbicidal and soil fungicidal activities [2]. Isoxazoles have also been used as dyes, electric insulating oils and high temperature lubricants. The key feature of these heterocycles is that they possess the typical properties of an aromatic system but contain a weak nitrogen-oxygen bond which is a potential site of ring cleavage under certain reaction conditions, particularly in reducing or basic conditions. Thus, isoxazoles are very useful intermediates, since the ring system stability allows the manipulation of substituents to give functionally complex derivatives [3]. Among the several methodologies for synthesis of this compounds, using of heterogeneous magnetic catalysts in multicomponent reactions have been widely considered. Herein, we report the using of sulfonated magnetic chitosan (10 mol%) for synthesis of 4*H*-isoxazol-5-ones via one-pot three-component condensation of various aromatic aldehydes, hydroxylamine hydrochloride and 1,3-dicarbonyls at room temperature in aqueous medium (Figure 1).

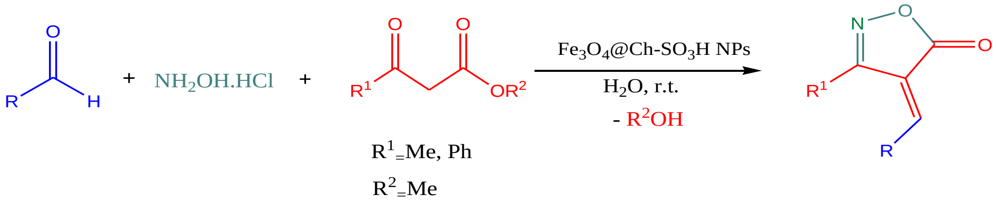

Fig. 1 Synthesis of 4*H*-isoxazol-5-ones via one-pot three-component condensation of various aromatic aldehydes, hydroxylamine hydrochloride and 1,3-dicarbonyls

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Paper code: 192

One-pot Synthesis of Some Novel 1,8-dioxooctahydroxanthenes Catalyzed by PVPP-OXA

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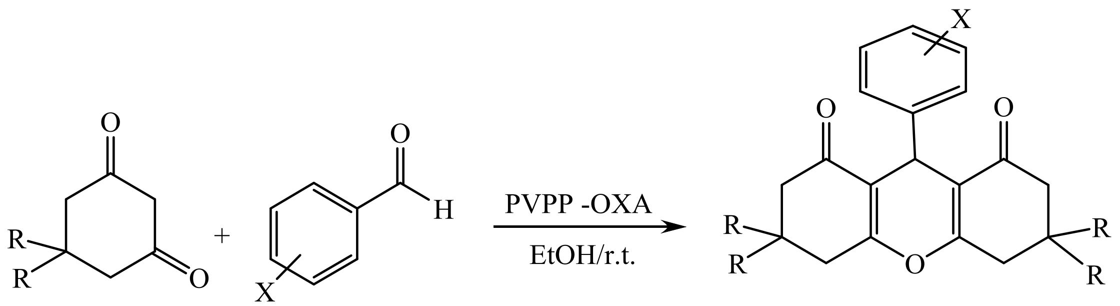
Xanthenes have pharmacological properties such as antibacterial, antiviral, and anti-inflammatory activities [1]. The synthesis of 1,8-dioxooctahydroxanthenes can be carried out in the presence of amberlyst-15 [2], Fe^{3+}–montmorillonite [3], and SiO_2-R-SO_3H [4]. In this research, a convenient and an efficient method was developed for the synthesis of some new 1,8-dioxooctahydroxanthene derivatives. The reaction proceeded via condensation of arylaldehydes with dimedon or 1,3-cyclohexadione in the presence of polyvinylpolypyrrolidone-supported oxalic acid (PVPP-OXA). In terms of reaction time and yields, the optimum results were obtained for the synthesis of 1,8-dioxooctahydroxanthenes in ethanol at room temperature. Clean methodologies, easy work-up procedure, high yield and simple preparation of the catalyst are some advantages of this work.



R = Me, H

X = H, *p*-Cl, *m*-NO_2, *p*-OH, *o*-OH, *p*-O-$(CH_2)_4$-O-C_6H_5-CHO, *o*-O-$(CH_2)_4$-O-C_6H_5-CHO, *p*-C_6H_5-CHO, *p*-O-$(CH_2)_2$-O-C_6H_5-CHO

Scheme 1. One-pot synthesis of 1,8-dioxooctahydroxanthenes derivatives

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Paper code: 196

Facile synthesis of aryl-azo dyes using a nano sized dicationic acidic catalyst

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Nano-scale catalysts have considerable attention due to large proportion of atoms at their surface and good activity [1]. On the other hand, dicationic catalysts because of the great variety of harmonious interactions, high thermal stabilities and broader selectivity are a rapidly growing field [2-3]. The understanding of dicationic ionic liquids (DILs), which consist of two head groups linked by a rigid or flexible spacer and two monoanions, is an interesting research topic because the numbers of possible combinations of cations and anions in dicationic ILs are greater than in monocationic ILs.

In this work, a mild and efficient procedure have been reported for the synthesis of Azo dyes from corresponding amines using a nano sized dicationic acidic catalyst under green conditions at room temperature, which carried out *via* aryldiazonium salts intermediates. Easy work-up only with water is one of the important features of this method. In addition, all reactions are performed under mild conditions during acceptable reaction times in excellent yields.

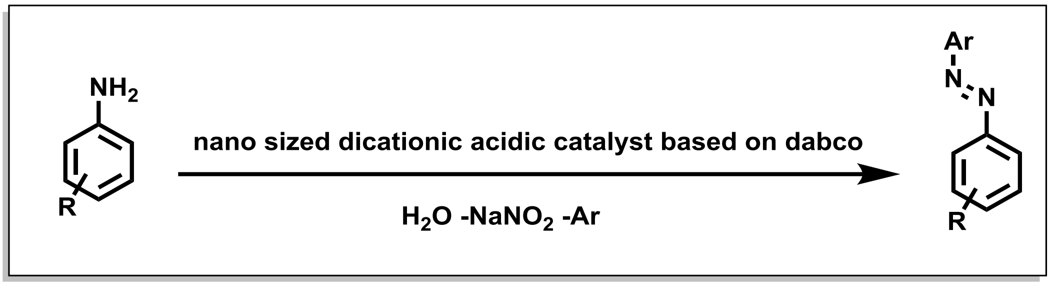

Fig.1 Diazotization of anilines using ionic liquid and azo-coupling.

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Paper code: 200

Synthesis of 2-substituted Perimidine Derivatives using Nanosawdust/ $TiCl_4$ as a Green Catalyst under Solvent-free Condition

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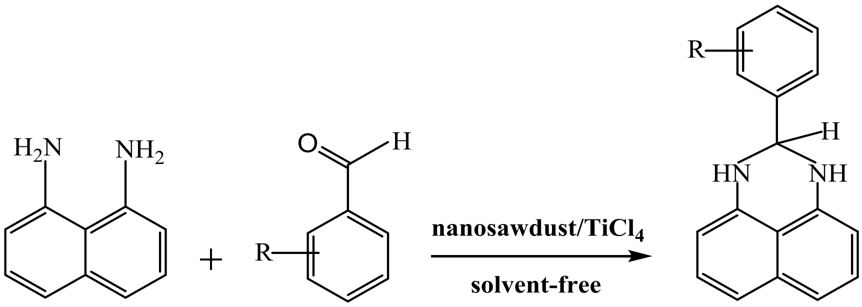
Perimidines are a kind of heterocycles containing a dihydropyrimidine ring and peri-fused to the naphthalene structure [1]. Multinuclear N-heterocyclic compounds, such as perimidines, are of wide interest because they exhibit a diverse range of biological activities. Among their multiple applications in pharmaceutics, including also activity as antiulcer, antifungal, antimicrobial, immunosuppres- sive agents and enzyme inhibitors, a particular interest is assumed by the established chemotherapeutic, anti-cancer and anti-proliferative properties of perimidine derivatives [2]. The most commonly method for the preparation of perimidines is the condensation reaction of 1, 8-diaminonaphthalene with a carbonyl group, which requires a special reagent or force reaction conditions [3]. Many procedures for the synthesis of dihydroperimidines have been reported in the presence of various catalysts. . In comparison within solid acid catalysts and others, the liquid acid catalysts such as sulfuric acid are corrosion properties. On the other hand, BF_3 is a gaseous material. Thus, working with it is not simple. Herein, we wish report the synthesis of dihydroperimidines using various aromatic aldehydes and 1,8- diaminonaphthalene in the presence of nanosawdust/$TiCl_4$ as a green catalyst under solvent-free conditions (Scheme1).The advantages of this work are simple work-up, mild condition, short reaction time and high yields.



Scheme1

References

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Paper code: 201

Introduction of a new piperazine-based ionic liquid as an efficient catalyst for the biginelli reaction

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Catalytic systems in organic synthesis are constantly developing and expanding. Meanwhile, ionic liquids are very much considered for some reason, including reasonable prices, environmental compatibility, high reactivity, recyclability and selectivity [1]. So far, ionic liquids have been used successfully as a catalyst in many of the major synthetic reactions such as aldol condensation, protection of carbonyls, Koch carbonylation, Diels-Alder reactions, Mannich reaction, Heck reaction, Knoevenagel reaction and heterocyclic synthesis [2].

3,4-Dihydropyrimidin-2(1*H*)-ones (DHPMs) and their derivatives, due to their significant biological properties, are important compounds in the pharmaceutical field. These compounds are used as medicines for antihypertensive, antibacterial, antiviral, anti-cancer and anti-HIV drugs in medicine [3].

In this work, a piperazine-based ionic liquid is synthesized and after characterization with FT-IR, Mass and NMR spectroscopy, is used as a catalyst for the Biginelli reaction. The main advantages of using this ionic liquid is high efficiency, acceptable reaction times, excellent yields of the achieved products and reusability of the catalyst.

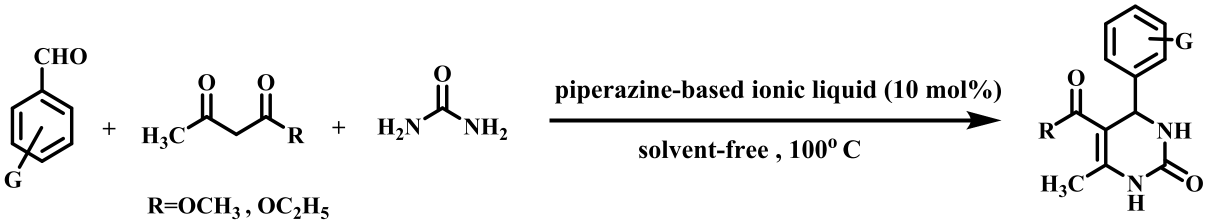

Fig. 1 Synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones.

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Paper code: 206

Synthesis of Substituted Pyrroles by using Choline Carboxylate Deep Eutectic Solvent

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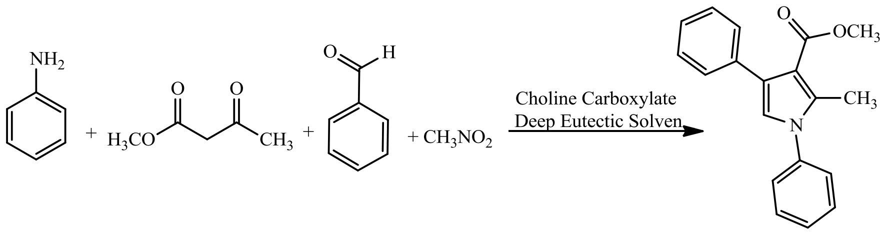
Pyrroles and their derivatives are the most important group of heterocyclic aromatic components, which exist in many synthetic pharmaceuticals and natural substances [1]. They are the core unit of many complex macrocycles, including the porphyrins of heme, bacteriochlorins, chlorophyll, and porphyrinogens [2]. They have significant biological properties such as antitumor, antibacterial, antioxidant, and antifungal. Pyrroles also have wide applications in materials science; therefore, several methods have been developed for the synthesis of the construction of pyrroles. These methods include some useful reactions such as Hantzsch, Knorr, or Paal-Knorr. Deep Eutectic Solvent Choline Carboxylate (DES) was synthesized. DES was characterized by XRD, FT-IR and NMR techniques for their surface area, surface acidity, crystallinity and functionality. The catalytic activity of the DES was determined in synthesis of substituted pyrroles with acetic anhydride. The influential parameters of the reaction such as molar ratio of the reactants, reaction temperature and amount of the DES were optimized. Herein, we wish to report the synthesis of substituted pyrroles using DES as a green and recyclable catalyst between an amine, an aldehyde, a 1,3-dicarbonyl compound, and nitromethane (Scheme 1). The catalyst can be recycled easily and reused several times without significant loss in its activity. The reaction time was decreased from several hours in other methods to some minutes using DES, in the present work.



Scheme 1: synthesis of substituted pyrroles using DES between amine, aldehyde, 1,3-dicarbonyl compound, and nitromethane.

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Paper code: 208

Application of a new dicationic ionic liquid catalyst in the efficient synthesis of 4*H*-pyran and pyrano[2,3-*d*]pyrimidinone derivatives

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4*H*-pyrans and pyrano[2,3-*d*] pyrimidinones are two important classes of heterocyclic compounds which constitute the structural unit of many natural products. The simplest and the most straightforward protocol for the preparation of 4*H*-pyrans and pyrano[2,3-*d*] pyrimidinones is based on the acceleration of three-component reaction of aromatic aldehydes, malononitrile, dimedone or barbituric acid in the presence of different types of catalysts. Although the introduced catalysts and procedures are effective, they have some disadvantages. Herein we wish to report an efficient and green procedure for the preparation of 4*H*- pyrans [1] and pyrano[2,3- *d*]pyrimidinones [2] via a domino Knoevenagel-cyclocondensation reaction using a nowel dicationic ionic liquid catalyst as a highly efficient, general and homogeneous catalyst, in a mixture of EtOH/water as a solvent. The promising reasons for the presented protocol are efficiency, generality, high yields of the products, short reaction times, cleaner reaction profile, simplicity, low cost and recyclability of the catalyst.

Fig. 1 Synthesis of 4*H*-pyrans and pyrano[2,3-*d*] pyrimidinone derivatives

Table. Comparison of the activity of $[C_4(MIm)_2].2Cl$ with other reported catalysts in the synthesis 4*H*-pyrans (entries 1-2) and pyrano[2,3-*d*]pyrimidines (entries 3-4).

Entry	Catalyst	Amount (mol)	Conditions	Time (min)	Yield (%)	TOF (min^{-1})	[Ref.]
1	$[H_2\text{-DABCO}][H_2PO_4]_2$	1.6×10^{-4}	H_2O : C_2H_5OH (1:2) / reflux	15	95	39583.33	[3]
2	$[C_4(MIm)_2].2Cl$	7×10^{-5}	H_2O: C_2H_5OH (1:1) / 90 ºC	5	98	280000	[This work]
3	$[BMIm]BF_4$	7×10^{-3}	90 ºC	180	92	73.02	[4]
4	$[C_4(MIm)_2].2Cl$	1×10^{-4}	H_2O/ 90 ºC	5	95	190000	[This work]

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Paper code: 212

Synthesis (perchloropyridin-4-yl)(aryl)methanones

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Perhalogenated aromatic and heteroaromatic compounds are important starting materials for the synthesis of other heterocyclic and macrocyclic compounds. The great number of review articles and monographs for the synthesis and applications of pyridines, reflects the important role of substituted pyridines in organic chemistry, biochemistry, and pharmaceutical chemistry [1]

In this work we investigated the synthesis of (perchloropyridin-4-yl)(aryl)methanones. Firstly we synthesized (perchloropyridin-4-yl)copper reagent from the reaction of 4-iodotetrachloropyridine with Cd and Cu powders, respectively, then followed by reaction with benzoyl chloride derivatives. Products confirmed by IR, ^{1}H-NMR and ^{13}C-NMR spectroscopy data.Perhalogenated heteroaromatic compounds are highly regarded toward nucleophilice reaction and few researches conducted on electrophilic reaction.[2]

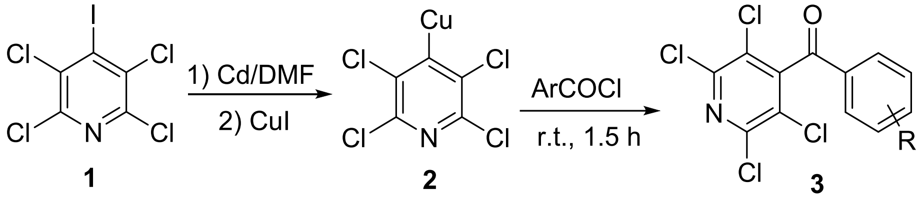

Fig 1. The synthesis (perchloropyridin-4-yl)(aryl)methanones

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Paper code: 213

Solvent-Controlled Highly Dehydration-Selective Synthesis of Indenone-Fused Thiazolo[3,2-*a*]pyridines Using Ketene Dithioacetals

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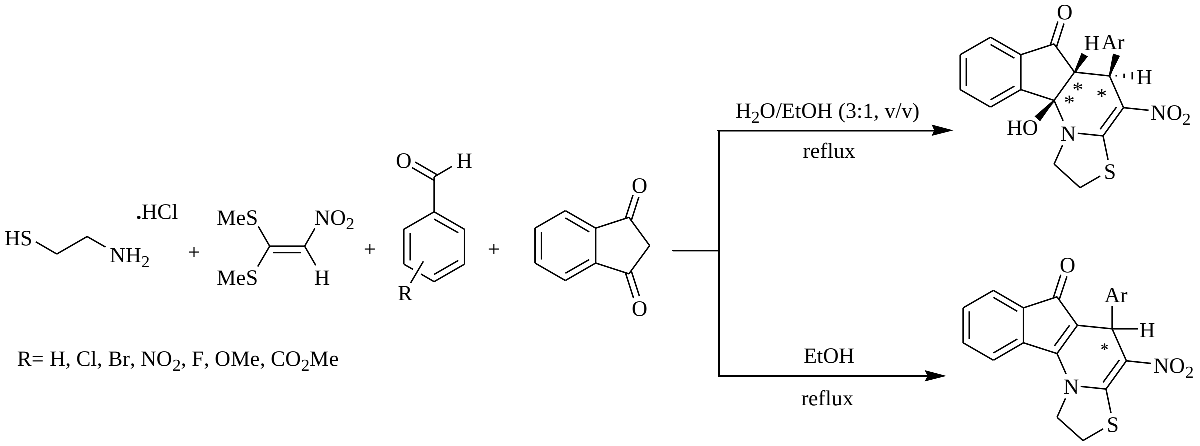
Over the past decade, sulfur-nitrogen heterocyclic compounds have attracted much attention of an increasing number of pharmaceutical and agrochemical researchers, due to their versatile biological activity, unusual physical properties and also existence these groups in a broad range of pharmaceuticals and natural products [1]. For the synthesis of sulfur-nitrogen containing molecules, β-nitro-thiazolidine as an enamine analogue moiety is a chemically useful precursor which electron-donating of nitrogen and sulfur atoms increased electron density of the carbon at β-position to nitrogen acts as a nucleophile [2,3].

Herein we would like to report a rapid and efficient one-pot catalyst-free protocol for the synthesis of either hydroxy-tetrahydro-thiaza-cyclopenta[*c*]fluoren-6-one or dihydro-thiaza-cyclopenta[*c*]fluoren-6-one *via* one-pot condensation of β-nitro-thiazolidine as an enamine analogue, 1,3-indandione and aromatic aldehydes by simply changing the reaction medium from mixture of water/ethanol to ethanol (Scheme 1). The structural diversities showed that the solvents play key roles in the construction of products. The structural diversities have been confirmed spectroscopically, which agree with the proposed structures.



Scheme. 1 Synthetic scheme for the formation of hydroxy-tetrahydro-thiaza-cyclopenta[*c*]fluoren-6-one and dihydro-thiaza-cyclopenta[*c*]fluoren-6-one.

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Paper code: 214

Graphene Oxide Immobilized Zr-Organic-Framework: A New and Efficient Catalyst for Biginelli Reaction

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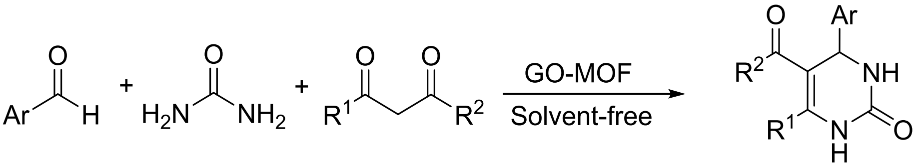
Multicomponent reactions (MCRs) have become current research interest to the synthetic organic chemist owing to their synthetic efficiency, atom economy and procedural simplicity [1]. MCRs are also an important tool to the modern drug development research so as to achieve a synthetic target in an expeditious way [2]. In this study a new zirconium-purphirine was immobilized on the edge of graphene oxide via covalent bond and the its catalytic activity has been tested in synthesis of 3,4-dihydropyrimidine-2-one via Biginelly reaction. The structure of catalyst was characterized with different techniques (TEM, SEM, FT-IR, TGA, EDX, XRD, ICP and Raman). According to FT-IR, SEM, TEM, EDS, TGA, XRD and Raman techniques, the structure of the catalyst has been approved and successful immobilization of Metal-Organic-Framework has been confirmed. Also ICP analysis shows that, the amount of zirconium is about 2 percent. This reaction was carried out from the reaction of aromatic and aliphatic aldehyde, ethylacetoacetate and urea in presence of catalytic amount of prepared catalyst. The catalyst could proceed the reaction in short reaction time and good to excellent yields. The reusability of the prepared nanocatalyst was examined five times with only a very slight loss of its catalytic activity.



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Paper code: 215

A Catalyst-free Approach to Synthesis of Polysubstituted Pyrano[3,2-*c*]chromene and Benzo[*g*]chromene Derivatives

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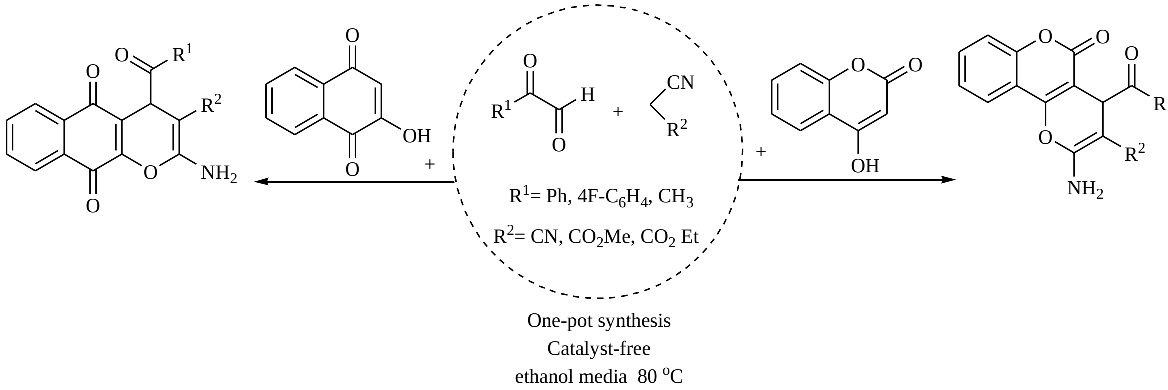
Nowadays, the rapid development of new drugs with diverse and unique structures and with novel mechanisms of action from that of existing widely used drugs seems essential. In the meantime, the development of heterocycles for drug design continues to be crucial in addressing this phenomenon [1]. Two class of the most important oxygen-containing heterocyclic compounds are pyrano[3,2-*c*]chromene and benzo[*g*]chromenes derivatives with a wide range of biological properties and applications in pigments and agrochemicals [2,3].

Hence, Because of their importance in pharmaceuticals and materials sciences, we were interested to synthesize a new library of pharmacologically relevant pyrano[3,2-*c*]chromene and benzo[*g*]chromene *via* the one-pot, multicomponent reaction of phenylglyoxal monohydrate, malononitrile/ethyl cyanoacetate/methyl cyanoacetate/cyanoacetamide and 4-hydroxycumarine or 2-hydroxy-1,4-naphthoquinone, at reflux in ethanol without the use of any catalyst (Scheme 1). These polysubstituted heterocyclic ring systems substituted with an amino group at C-2, carbonitrile group at C-3 and aroyl or acetyl group at C-4, which highlighted the effect of the substituents on the biological activity. This protocol is distinguished by its high atom-economy, good to high yields, mild condition without the use of any activator or metal promoters, simple workup and easy purification.



Scheme. 1 Synthesis of the pyrano[3,2-*c*]chromene and benzo[*g*]chromene derivatives.

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Paper code: 218

Hydrogen Production from Biomass derived-Formic acid Catalyzed by Pt-TiO_2: A Periodic DFT Analysis

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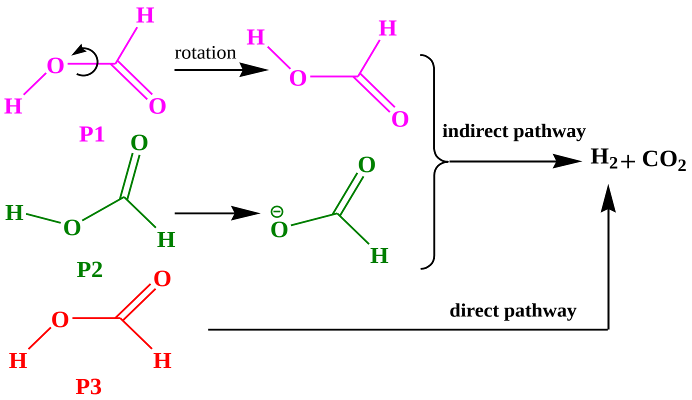
Hydrogen is a valuable gas as a clean energy source. It can easily be used in fuel cells for generation of electricity [1]. Currently, many researchers have focused on sustainable and environmental friendly energy from biomass to replace conventional fossil fuels [2]**.** TiO_2 based photocatalysts have the potential for the direct conversion and storage solar energy via production of hydrogen as the cleanest sources on Earth [3]. In this work, we have discussed the formation of hydrogen from decomposition of formic acid on a Pt-TiO_2 (101) surface by DFT. The anatase TiO_2 (101) surface was modeled as a periodic slab with four layers of oxide. Transition state search was performed at the same theoretical level with the complete LST/QST method implemented in DMol^3. Interestingly, formic acid absorption in the state of P2 (Scheme 1) on the Pt-TiO_2 surface has happened via a complete proton transfer reaction. From calculated results, the greatest amount of activation energy related to the third route of decomposition reaction of *cis*-formic acid on Pt-TiO_2 surface in gas phase condition (77.9 kcal/mol).



Scheme 1. Mechanistic Scheme for formic acid decomposition.

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Paper code: 220

Immobilized Cu(II) Schiff-base complex supported on Fe_3O_4 magnetic nanoparticles: A highly efficient and reusable new catalyst for the synthesis of pyranopyridine derivatives

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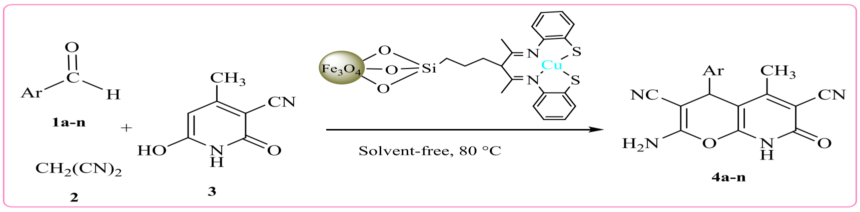
A new heterogeneous cupper (II) Schiff-base complex immobilized on silica-coated nanomagnetic Fe_3O_4 was synthesized from acetylacetonate (acac) and 2-aminothiophenol (ATP). The newly composed nanocatalyst Fe_3O_4@SiO_2-acac-2ATP-Cu(II) was structurally characterized by several analytical techniques such as Fourier transform infrared spectroscopy (FT-IR), vibrating sample magnetometer (VSM), energy dispersive X-ray spectroscopy (EDX), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The catalytic activity of Fe_3O_4@SiO_2-acac-2ATP-Cu(II) nanoparticles was investigated for the synthesis of pyrano[2,3-b]pyridine derivatives from one-pot three-component reaction of aldehydes, malononitrile, and 3-cyano-6-hydroxy-4-methyl-pyridin-2(1H)-one. A high catalytic performance was exhibited by this nanocatalyst under solvent-free conditions and excellent yields of the products were achieved from this reaction in reasonably short reaction times. The nanoparticles can be easily separated from the reaction mixture simply by magnetic decantation and reused for several fresh consecutive runs without significant loss of catalytic activity.



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Paper code: 230

$Fe_3O_4@SiO_2$-$SnCl_4$ promoted synthesis and screening of Pyrimido[4,5-b]quinolins as antifungal agents

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Multicomponent reactions are one-pot processes in which several easily accessible components react to from a single product [1]. Multicomponent reactions (MCRs) occupy an outstanding position in organic and medicinal chemistry for their high degree of atom economy and applications in combinatorial chemistry. Heterocycles containing the pyrimidine ring are important targets in synthetic and medicinal chemistry because this fragment is a key moiety in numerous biologically active compounds [2]. In connection with our continued interests in the synthetic benign protocols for biologically important products [3], we have extended our studies to the synthesis of new derivatives of pyridopyrimidines.

In order to expand the application of $Fe_3O_4@SiO_2$-$SnCl_4$ in the synthesis of heterocyclic compounds, in this study, we wish to report, one-pot synthesis of pyrimido[4,5-*b*]quinolone derivatives. These compounds were synthesized *via* reaction of 6-amino-2-(methylthio)pyrimidin-4(3*H*)-one, dimedone, or 1,3- cyclohexadione and aldehydes in the presence of $Fe_3O_4@SiO_2$-$SnCl_4$ as an efficient eco-friendly catalyst under ultrasound irradiation (Fig. 1). The final aim of this study is evaluation of antifungal activity of resulted products. All the compounds were screened for antifungal activity by broth microdilution methods as recommended by CLSI.

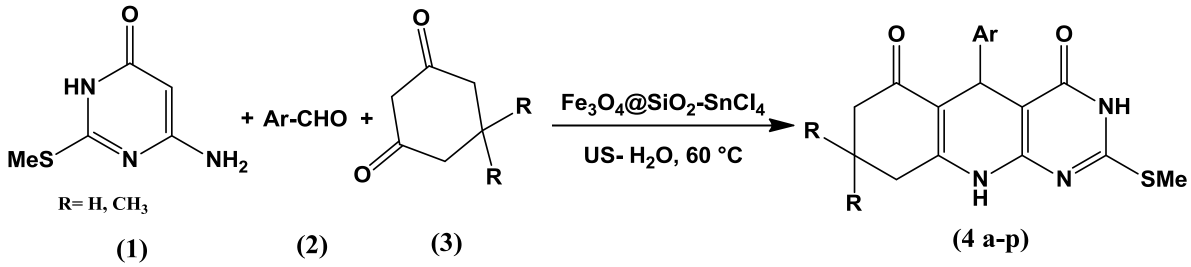

Fig. 1

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Paper code: 231

synthesis of 1-and 5- substituted 1H tetrazoles catalyzed by separable ligand complex of copper (||) supported on Fe3O_4@SiO_2 nanoparticles

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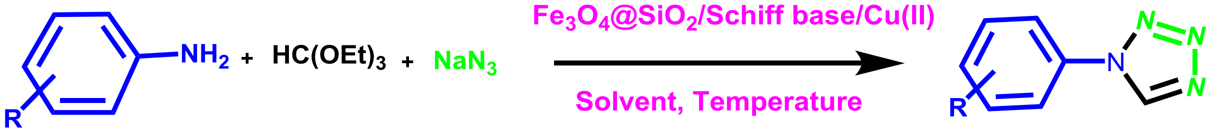
Simple and efficient procedure for the synthesis of 5-substituted 1H-tetrazole derivatives has been developed by one-pot three-component reaction with (0.05 gr, 2mmol, 2mmol, 2mmol) ratio of Fe3O_4@SiO_2/ liganad /cu (Ⅱ) catalyst, amin, sodium azide and triethyl ortho-formate under solvent free conditions at 100 ˚C.This catalyst is thermally stable, green, recyclable, inexpensive, and easy to prepare. In addition, it can be easily separated from the reaction mixture and recycled up to five times without any significant impact on its activity or the reaction yield. The operational simplicity, high yields, and facile work-up procedures associated with this catalytic process give it advantages over.



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Paper code: 232

A New Multi-Component Synthetic Route to Hexahydropyrido[2,3-*d*]pyrimidine Derivatives

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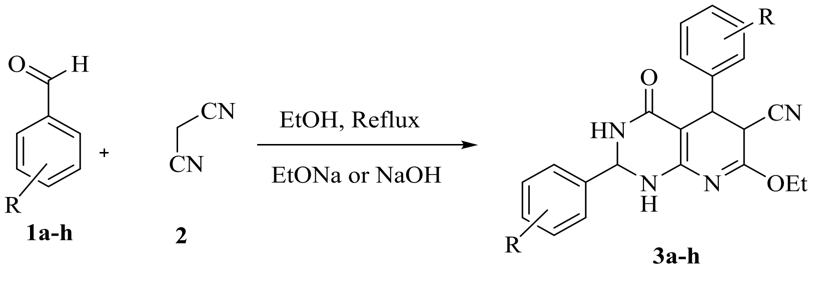
Pyrido[2,3-*d*]pyrimidine and some of its derivatives are an important class of heterocyclic compounds displaying diverse range of biological activities including antiviral, antifolate, antimicrobial, antitumor, antifungal, anti-inflammatory, anticonvulsive, antipyretic, anti-proliferative CDK2 and antihistaminic activity [1]. The synthesis of various pyridopyrimidines in view of their structural relation to pteridine has attracted the interest of numerous researchers. But the commen synthetic routes to these bicyclic compounds are limited and mainly involve either construction of pyrimidine ring onto pyridine derivatives or pyridine ring onto pyrimidine core. Both routes require the initial synthesis of the decent precursors before construction of the second ring to obtain the desired products [2].

In this work we wish to report a new, simple, convenient and highly efficient one-pot multi-component route for the synthesis of new hexahydropyrido[2,3-*d*]pyrimidine derivatives from malononitrile and benzaldehyde through manipulation of their molar ratios. The reaction presumably proceeds by a sequence of Knoevenagel condensation, Michael addition and ANRORC process. The generality of the reaction was surveyed by applying the one-pot multi component reaction (MCR) to a number of substituted benzaldehydes. The aromatic aldehydes with electron-withdrawing groups as substrates reacted very well at faster rate with shorter reaction time in comparison to aromatic aldehydes with electron-donating groups. The structural assignments of all the newly synthesized compounds **3a-h** was based upon spectroscopic and micro-analytical data and ^{2}D-NOESY spectrum, as well.



3a: R = H
3b: R = 2-OMe
3c: R = 4-OMe
3d: R = 2-Cl
3e: R = 4-Cl
3f: R = 4-Me
3g: R = 4-Ipr
3h: R = 3-NO_2

Synthesis of new hexahydropyrido[2,3-*d*]pyrimidine derivatives

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Paper code: 234

An efficient three-component synthesis of triazolo[2,1-*b*]quinazolinone derivatives catalyzed by reusable DABCO-based dicathionic ionic liquid

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Various biological and pharmacological properties of triazolo[2,1-b] quinazolinones derivatives have attracted wide interest for the preparation of these compounds. Fluconazole, itraconazole, and albaconazole are some examples antifungal drugs which possess triazole moiety in their structures. [1]

In recent years, Ionic liquids have been utilized as alternatives to hazardous, volatile and flammable solvents and catalysts, and due to their distinctive physico-chemical properties such as polarity, solvating activity, melting point, density, and viscosity. Furthermore, dicationic ionic liquids are attractive new category of ionic liquids that represent higher melting point, wider liquid range and better thermal stability in comparison with traditional ionic liquids. [2,3]

In this study, a convenient and straightforward method for the synthesis of triazolo-[2,1-*b*]quinazolinone derivatives, through a three-component reaction between aldehydes, *β*-diketones and 3-amino-1,2,4-triazole in the presence of an economical and reusable DABCO-based dicathionic ionic liquid has been reported (Fig. 1). The advantages of present methodology are ease of the preparation and handling of the catalysts, simple procedure, acceptable reaction times, non-column chromatographic separation, high yields, and recyclability of the catalyst.

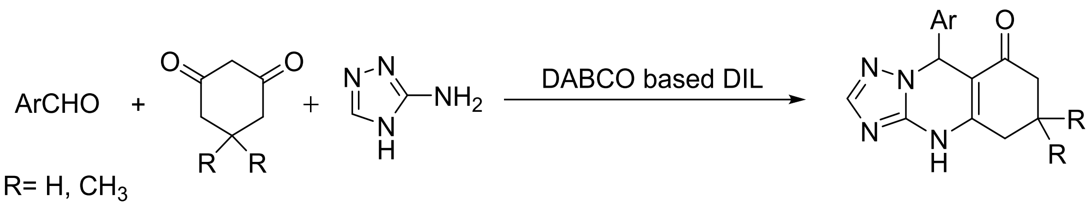

Fig.1 synthesis of triazolo[2,1-*b*]quinazolinone derivatives using DABCO-based DIL as the catalyst

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Paper code: 239

A simple and green approach for the synthesis of substituted dihydro oxypyrroles catalyzed by nano-Fe3O4@SiO2/SnCl4 super paramagnetic nanoparticles

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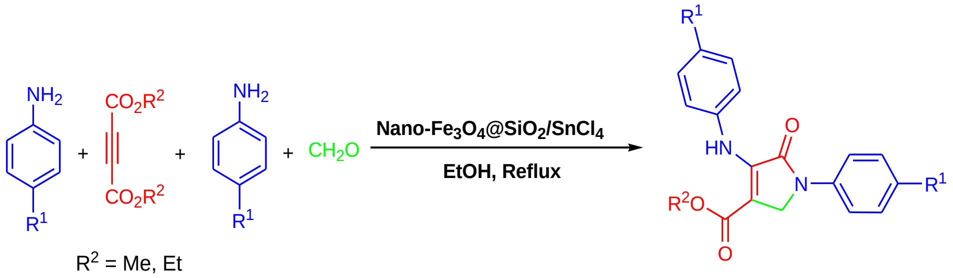
Heterocyclic rings are important fundamental cores in most biologically active compounds. As a significant class of these heterocycles, nitrogen-containing heterocycles as identified pharmacophores have received much attention in medicinal chemistry and drug discovery [1–2]. In this context, the presence of pyrrol-2-ones in pharmaceuticals and natural products has continued to stimulate much interest in the development of new methods for their synthesis [3].

To develop compound libraries based on this fused heterocyclic scaffold, we considered an efficient and green procedure for the synthesis of dihydro-2-oxypyrroles has been developed. One-pot four-component condensation reaction of aniline derivatives (2 mmol), dialkyl acetylene dicarboxylate (1 mmol), and aldehydes (1 mmol) was done in ethanol at 65 °C in the presence of nano-Fe_3O_4@SiO_2/$SnCl_4$ as a magnetically reusable heterogeneous acid catalyst (Fig. 1). The obtained dihydro-2-oxypyrroles were purified without any chromatography techniques. The structure of obtained pure products were identified by physical properties and spectroscopic data such as FT-IR, ^{1}H NMR, ^{13}C NMR and mass spectroscopy. This protocol, consistently has the advantages of excellent yields, short reaction time, simple workup, recyclability of the catalyst up to six runs without appreciable loss of activity.



R^2 = Me, Et

R^1 = 4-Me, 4-Et, 4-Br, 3-NO_2, 4-OMe, 4-Cl.

Fig. 1

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Paper code: 241

Novel efficient heterogeneous copper (||) nanoparticles for the synthesis of 1-and 5- substituted 1H tetrazoles

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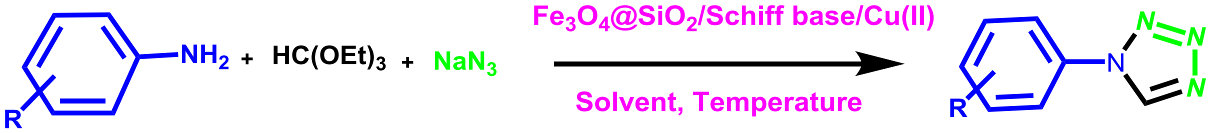
Tetrazoles are an important class of the synthetic heterocyclic compounds with wide range of practical applications in major areas of sciences such as medicine, chemistry and material sciences. From pharmaceutical chemistry viewpoint, tetrazole derivatives have many biological activities such as antihypertensive,1 anti-allergic,2 antibiotic,3 anti-diabetic,4 anti-arrhythmic,5 activity and have also potential for drug developmentas inhibitor for HIV or other immune diseases.tetrazole rings can be prepared in several ways.the most convenient rout for preparation of 5-substituted 1H-tetrazol is via mixture of amine (2 mmol),sodim azide (2 mmol),triethyl ortho –format(2 mmol), $Fe3O_4@SiO_2$/ liganad /cu (Ⅱ) catalyst(0.05 gr) was taken in a round- bottomed flask and stirred at 100 ˚C under solvent free condition.the stable, green, recyclable, inexpensive catalyst was removed by using magnetic field and then the resulting solution was washed with water.this method gives notable advantages such as easy separation, excellent yields, short reaction times,non- toxic metal catalyst and simplicity of operation make method a facile tool for the synthesis of tetrazoles.



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Paper code: 255

Synthesis of Novel Thiazolo[2,3-*b*]pyrimidine Derivatives Catalyzed by Nano−SiO_2 as a Reusable Heterogeneous Catalyst

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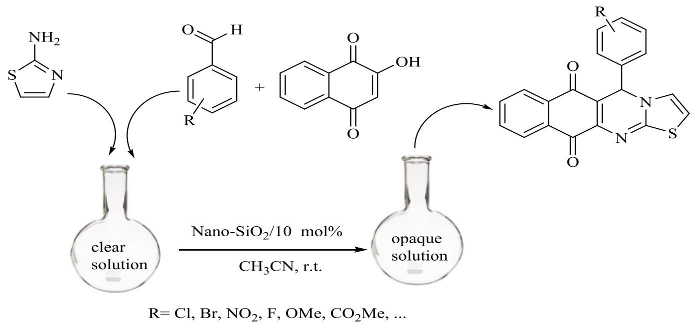
Thiazolo[2,3-*b*]pyrimidine is an important class of compounds with two different sulfur-nitrogen containing fused heterocycles, which specific strategies have been reported for the synthesis of thiazolo[2,3-*b*]pyrimidine derivatives as follows: In 2014 Wu et al. synthesized this scaffold *via* the reaction of 2-aminobenzothiazole, aromatic aldehydes and 2-hydroxy-1,4-naphthoquinone in the presence of amberlyst-15 [1]. In 2017, Keshari et al. utilized a *p*-TSA-catalyzed domino approach for the synthesis of novel thiazolo[2,3-*b*]pyrimidines [2].
In addition, the field of silica nanocatalysis has attracted the attention of researchers working, because of their stability, high surface area, and non-toxicity which made the silica nanoparticles ideal candidates for catalyst support [3].

In the view of above-mentioned points, a new series of thiazolo[2,3-*b*]pyrimidines derivatives were designed and prepared, by the three-component reaction of 2-aminothiazole, aromatic aldehydes and 2-hydroxy-1-4-naphthoquinone in the presence of nano−SiO_2 as a heterogeneous catalyst which used commercially (CAB-O-SIL M5) with characteristic properties in acetonitrile at room temperature (Scheme 1). The direction of heterocyclization and the structure of final products identified spectroscopically. The significant advantages of this protocol include simplicity, regioselectivity, good yields, use of a recyclable catalyst and simple work-up.



Scheme. 1 Synthetic scheme for the formation of naphthoquinone-fused thiazolo[2,3-*b*]pyrimidines.

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Paper code: 268

Magnetic based piconaldehyde-melamine copper complex for the one-pot synthesis of hexahydroquinolines via Hantzsch four component reactions

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In the present work, piconaldehyde-melamine copper complex was loaded on the magnetic Fe_3O_4 core, so that it contains 0.33 mmol Cu per g of the catalyst and used as an efficient catalyst. The catalyst was used to motivate the raw materials in the synthesis of hexahydroquinoline derivatives by the one-pot four component reaction. Reaction between various aryl aldehydes, dimedone, ethyl acetoacetate and ammonium acetate was carried out at the optimum condition. Different aryl aldehyde derivatives with electron withdrawing and electron donating groups on the benzene ring were successfully examined.Low reaction time (minutes vs. half an hour), solvent free condition, and magnetically separable catalyst are some salient features of the developed catalyst. Besides, the optimum amount of the catalyst and temperature was obtained 0.07 g, and 87.6 °C, respectively, which was determined using response surface methodology (RSM) and optimization techniques. The proposed and plausible mechanism based on FT-IR is shown in the Fig. 1. As it shown (Fig. 1), and based on the FT-IR investigations, the as prepared catalyst interacts only with benzaldehyde and reduces the carbonyl wave number from 1703.92 cm^{-1} to 1687.49 cm^{-1}.

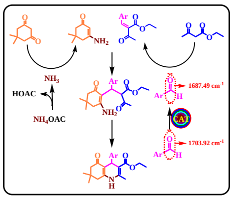

Fig.1 The plausible mechanism for the synthesis of hexahydroquinoline using as synthesized catalyst

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Paper code: 273

Synthesis of N, N′-bis (tetra fluoropyridyl) sulfonic diamid

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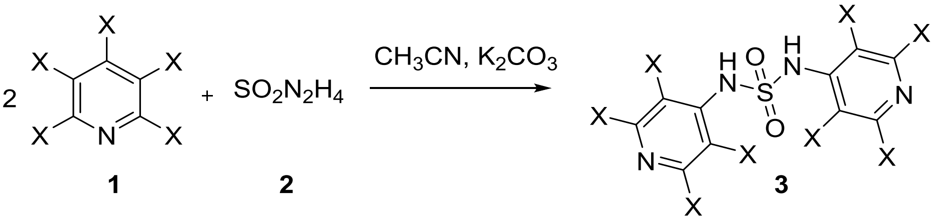
There has been an increasing interest in discovering and developing small molecules that are of pharmaceutical importance. Heterocyclic compounds are known to be the most versatile class of these types of molecules, either prepared synthetically or occurring in nature. However, in some cases, it has been reported that the activity is enhanced to a larger extent when these heterocycles are repeated in the molecule separated by a suitable spacer, bis-heterocycle. Thus, the synthesis of new bis-heterocyclic compounds has become an eye-catchy field to explore in the recent past owing to their pharmacological, biological and industrial importance [1]. The synthesis of bis-heterocycles is mainly achieved by joining heterocyclic nuclei together using a variety of linkers and points of linkages. Pentafluoropyridine has attracted considerable interest due to its synthetic utility [2].

In this work, we report our investigations on reaction of pentafluoropyridine 1 with Sulfamide 2 in the presence of potassium carbonate base and acetonitrile solvent following a literature procedure (Scheme 1). Various derivatives of these compounds were synthesized in good to excellent yields. The products were purified by plate chromatograghy using appropriate solvent systems, and the structures were established by NMR and IR spectral data.



X = F, Cl

Fig. 1 reaction of pentafluoropyridine with Sulfamide

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Paper code: 275

Facile and Efficient Multicomponent Synthesis of Some Trisubstituted 1,3,5-Triazine Derivatives Catalyzed by Various Nanocatalysts

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1,3,5-triazine derivatives have played a distinguished role in medicinal and biological chemistry. These derivatives have participated in the structure of some novel potent chemicals showing diverse medicinal effects such as 5-HT6 serotonin receptor agonists [1], antimycobacterial and antimicrobial agents [2]. Therefore, the multicomponent synthesis of 1,3,5-triazine derivatives under novel green conditions using magnetic Fe_2O_3-MCM-41 and modified zeolite nanocatalysts was studied in the present research study (Fig. 1). This protocol has been previously examined under uncatalyzed conditions [3,4]. The most important drawbacks of these previous methods include long reaction times and low to moderate yields of the products.

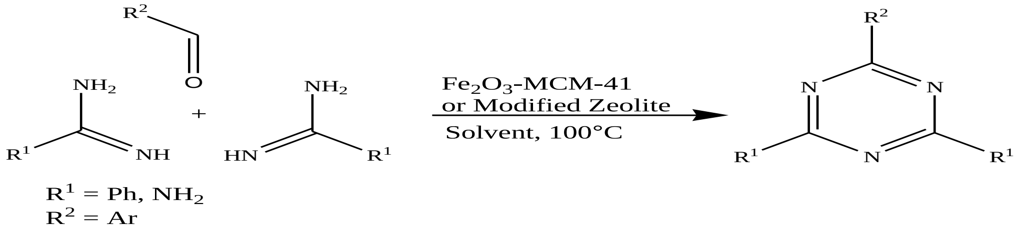

Fig. 1 Multicomponent synthesis of trisubstituted 1,3,5-triazines catalyzed by various nanocatalysts

Our introduced procedure led to the formation of ther desired 1,3,5-triazine derivatives with a broad range of substitutes at positions 2, 4 and 6 of the ring. Moreover, the reactions were proceeded smoothly under the defined reaction conditions and the products were obtained within short reaction times and good to excellent yields. The products were also easily purified without using laborious purification methods by aqueous dilution of the reaction mixture.

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Paper code: 277

Conformational analysis of bistetrazole energetic compound in neutral and anionic forms

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The synthesis of modern energetic materials such as bistetrazole is an area of intense research both in terms of synthetic and computational investigations. 5,5′-bistetrazole is composed from two tetrazole rings which are directly attached to one another either by one C atom (Fig. 1). This compound has low sensitivity, high performance, and high thermal stability as well as being environmentally friendly [1]. In this study, the conformational analysis of 5,5′-bistetrazole compound in neutral and anionic forms was performed by density functional theory (DFT) calculations at M06-2X/AUG-cc-pVTZ level of theory. New evidences about the stability and rotational energy barrier of these valuable energetic compounds were reported.

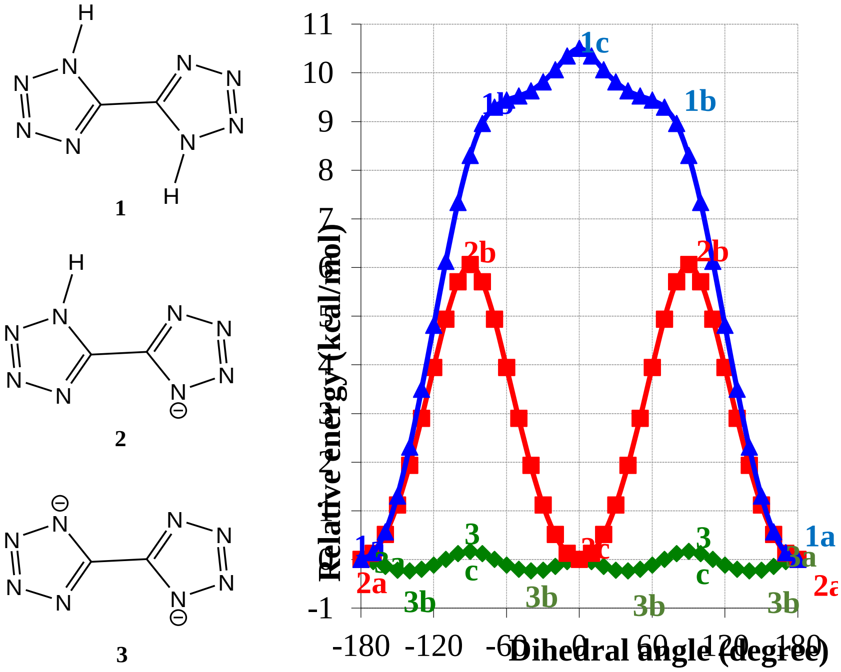

Fig. 1. The molecular energy profile calculated for compounds 1-3.

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Paper code: 291

Copper-catalyzed coupling of aryl boronic acids with hydrazine hydrate

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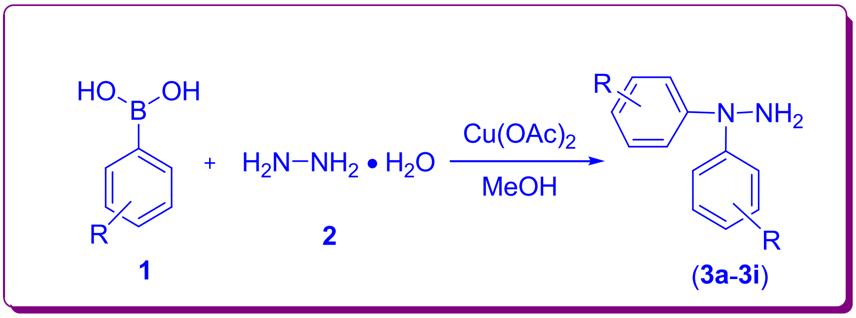
N-Arylation is one of the most challenging C-X coupling reactions. Despite the revolutionary achievements of palladium catalysis, classical Ullmann and Goldberg reactions are still very useful [1]. Arylation of hydrazines, which are a special class of nitrogen compounds, is of high interest because it is widely used in the synthesis of natural products, pharmaceutical ,and agrochemical compounds, as well as polymers and materials [2].

Arylboronic acids have been widely used in *N*-arylation of arylamines through the amination strategies developed by the various research groups [3]. The development of new processes using cheap and abundant amino sources as feedstocks in the synthesis of aromatic amines remains a highly attractive goal.

In this work, a copper-catalyzed *N*-arylation process for the synthesis of 1,1-diphenyl hydrazine derivatives (**3a-3i**) by reaction of aryl boronic acids (**1**) with hydrazine hydrate (**2**) has been developed (Scheme 1). Importantly, this transformation is very practical and it does not require the use of strong bases, expensive ligands or rigorous exclusion of air and moisture.



Scheme 1. Synthesis of 1,1-diphenyl hydrazine derivatives

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Paper code: 301

Efficiet one-pot synthesis of pyrazoles catalyzed by Nano silica sulfamic acid, Graphene oxide and Cobalt titanate(III) using green chemistry

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Pyrazole derivatives have become increasingly important in the past few years because they have proven to be extremely useful intermediate for the preparation of new biological materials. The pyrazole ring is present in numerous pharmacological compounds [1-4]. Pyrazoles are an important structural subunit found in a variety of biologically active agents, including major drugs such as Viagra, Xalkori, Lexiscan, and Celebrex. The prevalence of the pyrazole motif in medicinally relevant compounds, dyes, and ligands for metal catalysts has inspired the development of many novel methods for their preparation. Many procedures for the synthesis of pyrazoles derivatives have been developed during the last two decades. But the most efficient method of choice is the reaction of 1,3-diketones with hydrazines and their derivatives. For the synthesis of pyrazole reactions between 1,3-diketones and hydrazines with catalyst Nano silica sulfamic acid, Graphene oxide and Cobalt titanate(III) solvent-free condition using green chemistry have been reported.

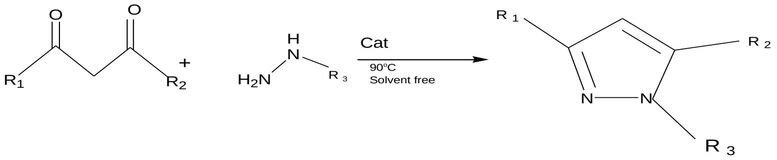

Fig. 1 The synthesis of pyrazole derivatives

Obtaining the product in the short reaction time and good to excellent yields, using catalytic amount of catalyst, easy work up and avoidance of using solvent are notable advantages of this method. The experiments a number of substituted Pyrazole derivatives is prepared by melting point and spectroscopic techniques, have been identified

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Paper code: 305

Synthesis of Tocopherol succinate-Polyoxomolybdate Hybride Bio-Conjugate as potential anti-cancer agent

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Polyoxometalates (POMs) are typical clusters of nanometer-sized transition metal oxides. They can play the unique roles as anticancer agents. Some of the antitumor mechanisms of POMs are as follows; the induction of cell apoptosis, weak nonspecific interactions with DNA and the inhibition of ATP generation (1). The conjugation of an organic ligand onto the POMs offers additional advantages, such as better stability and desirable ligand orientation. Most importantly, the attachment of bio-active ligands to POMs might improve their biocompatibility, allow selective recognition of biological targets, as well as tune the bioactivity and cytotoxicity. We hypothesize that the conjugation of tocopherol succinate to the Anderson-type POM $\{MnMo_6O_{18}[(OCH_2)_3CNH_2]_2\}^{3-}$ (Fig1) can boost the anti-tumor function and impart targeted chemotherapy for cancer treatment due to the selectivity of the resulting conjugates (2). We investigated the structure of POM conjugate using FTIR and HNMR spectra. These techniques indicated the successful synthesis of the POM-tocopherol succinate conjugate. We have prepared a new bioconjugate that can enhance anti-tumor activity and selectivity in comparison with the parent cluster and tocopherol succinate. The in-vitro studies on how this conjugate kills MCF-7, LNCAP and HUVEC cells are currently undergoing in our laboratory.

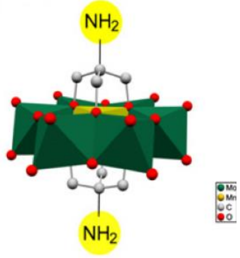

Fig1: $\{MnMo_6O_{18}[(OCH_2)_3CNH_2]_2\}^{3-}$

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Paper code: 310

Pomegranate juice as a green catalyst for the synthesis of 2-aminochromenes-3-carbinitriles

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Densely functionalized 2-aminochromenes have become a key class of heterocyclic compounds because of their noticeable biological and pharmacological activities, such as antibacterial, antiviral, and antitumor [1]. Therefore, many efforts have been made by researchers to achieve efficient catalysts for their synthesis [2-7].

In this contribution, pomegranate juice was employed as a green and efficient catalyst for the one-pot, three-component cyclocondensation reaction of 4-hydroxycoumarin (or naphthols), malononitrile/ethyl cyanoacetate, and aryl/hetero-aryl aldehydes. These compounds underwent Knoevenagel-Michael-Thorpe-Ziegler heterocyclization upon heating at 50 °C to give the respective medicinally relevant 2-aminochromene-3-carbonitriles (Fig. 1). Pomegranate juice contains compounds such as citric acid, maleic acid, ascorbic acid. The method is versatile and amenable to many substrates as it requires no specialized devices such as microwave, ultrasound and ball-milling. Also, the salient features of this high-yielding protocol are green reaction conditions, safe, simple purification processes, and relatively shorter reaction times.

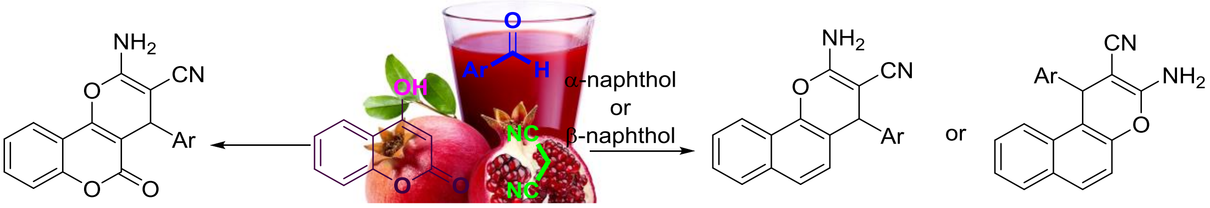

Fig. 1 Pomegranate juice catalyzed synthesis of densely 2-aminochromenes.

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Paper code: 311

Application of Cellulose/Clay/ZnO/CeO_2 nanocomposite as a catalyst for oxidation of aniline derivatives

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Today, lanthanide oxides are widely considered by researchers in composite structures and food industry. Using these nanocomposites as an active packaging, in addition to increasing the shelf life of food products, eliminates chemical and microbial harmful contaminants on the behavior of a food coating based on catalytic oxidation of aniline derivatives allows them to be removed from food. Also nanocomposites can be used as a catalyst and mediator. Cerium oxide (CeO_2) has good mechanical and conductive properties. Its stability and convenient synthesis have led to catalytic oxidation and reduction reactions [1]. In recent years, the development of environmentally friendly materials obtained from renewable resources has attracted immense interest due to the new sustainable development policies. Carboxymethyl Cellulose is a readily available, naturally occurring biodegradable and biocompatible linear polysaccharide [2].

Nano ZnO/CeO_2 supported on Cellulose/Clay nanocomposite is introduced as a catalyst for the synthesis of azobenzen through oxidation of aniline and mostly derivatives as a green environmental reaction .In this reaction aniline was reacted with O_2 in the presence of various amounts of catalyst (Cellulose/Clay/ZnO/CeO_2) in various reaction times and different temperatures. Desired amounts of aniline and catalyst were stirred for 6 hours in130°C in the presence of O_2 and azobenzen was produced in 90% yield. At the end of the reaction catalyst was easily separated by centrifuge and the recovered catalyst was reused several times without any significant loss of activity.

The main objective of this work is to use Cellulose/Clay/ZnO/CeO_2 as a new nanocatalyst in the selective oxidation of aniline to azobenzen.

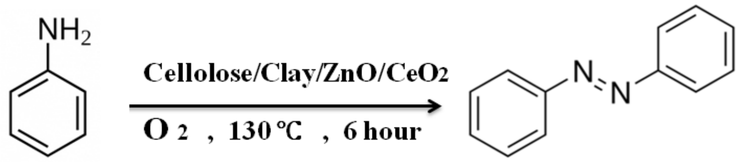

Fig. 1 selective oxidation of aniline to azobenzen in the presence of Cellulose/Clay/ZnO/CeO_2 nanocatalyst.

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Paper code: 312

Reaction of 2-cyano-acetamides with tetrafluoro-4-(phenylsulfonyl)pyridine

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Polysubstituted pyridines play an important role in organic chemistry, biochemistry, and pharmaceutical chemistry, this shown in numerous of review papers and monographs for the synthesis and applications of pyridines [1–2]. Many researchers are interested in the reactions of various N, O, S, C, and P nucleophiles with perhalogenated compounds [3]. The nature of nucleophile, reaction condition, and solvent have a basic role in the regiochemistry of the reactions.

In this paper, the reaction of 2-cyano-acetamides **1** with tetrafluoro-4-(phenylsulfonyl)pyridine **2** in the presence of potassium carbonate in CH_3CN as a solvent at reflux gave products **3a** and **3b**. The structure of products confirmed by IR,^{19}F-NMR, ^{1}H-NMR and ^{13}C- NMR.

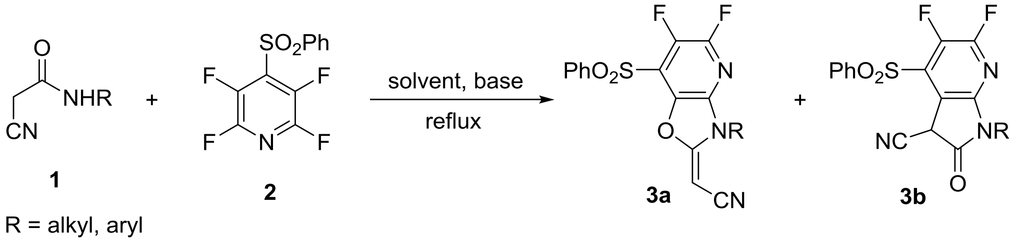

Fig. 1. Reaction of 2-cyano-acetamides with tetrafluoro-4-(phenylsulfonyl)pyridine

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Paper code: 316

Synthesis of Hyperbranched Polyglycerols using Ascorbic acid as an Activator

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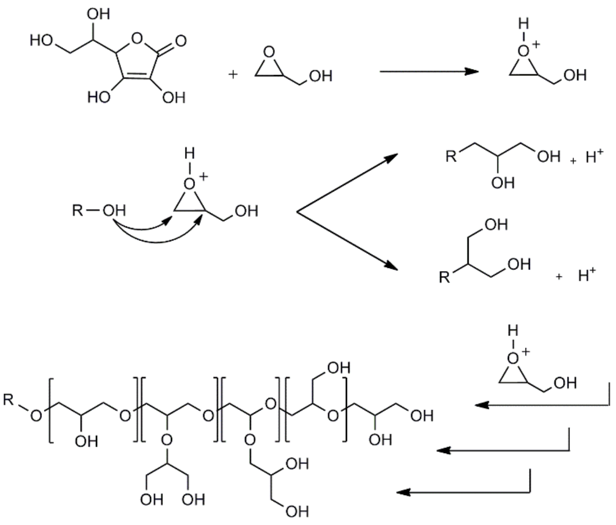
In this work, low molecular weight hyperbranched polyglycerols (LMPGs) are synthesized in bulk using ascorbic acid as an activator. Different molar ratios of glycidol and ascorbic acid were mixed and stirred at ambient conditions and LMPGs with different molecular weights, degree of branching and relative abundance of the structural units were obtained. According to spectroscopy data, ascorbic acid was not incorporated in the structure of polymer and plays the role of activating agent in the polymerization process. In this synthetic protocol, any other chemical reagent and organic solvents were not used. Therefore, products are free of toxic impurities and suitable for the future biomedical applications.



ROH is the monomer or a polymer chain

Fig. 1 Schematic representation of the proposed mechanism for the ring opening polymerization of glycidol by ascorbic acid.

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Paper code: 320

Iodine-catalyzed synthesis of 1,4-dihydropyridines and pyrido[1,2-a]quinoxalines

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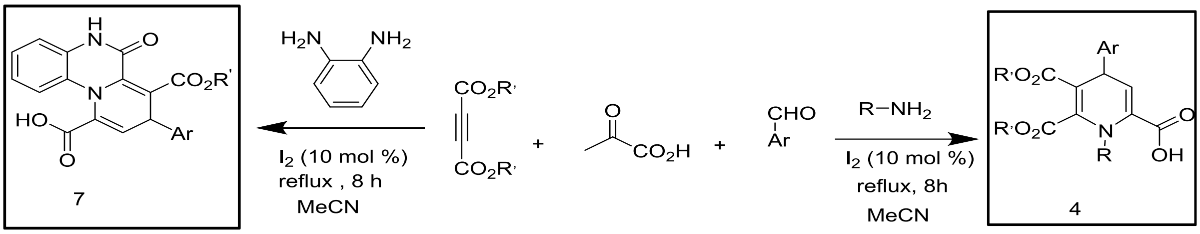
1,4-dihydropyridines (DHPs) have been broadly utilized in agricultural and pharmacological industries. The DHPs demonstrate therapeutic and pharmacological properties such as calcium channel blockers, antitumor, anti-inflammatory, antiallergics, antibacterial, antioxidant agent and analgesic activities [1].

Another aspect concerning enaminone chemistry leading to the one-pot synthesis of functionalized novel 1,4-dihydropyridines and pyrido[1,2-a]quinoxalines has been described. By highly efficient, onepot, iodine-catalyzed four-component reactions, combining one set of enamine intermediates and arylidene pyruvic acid (APA) in two procedures, heterocyclic skeletal diversity can be achieved. The synthesis involves reaction of the intermediates formed by the 1:1 interaction between primary amines (or o-phenylenediamine) and dialkyl acetylenedicarboxylate with pyruvic acid and benzaldehyde through an iodine-catalyzed Knoevenagel/Michael/cyclization sequence. The reaction is particularly attractive due to the following advantages: atom economy, optimum convergence, high bond-forming efficiency, and avoidance of tedious workup and purification of products. Significantly, the presence of an acidic group at the 9-position on the products make these compounds excellent precursors for further synthetic modifications to meet the need for diverse chemical inputs.



Scheme 1. One-pot domino synthesis of 1,4-dihydropyridines 4 and pyrido[1,2-a]quinoxalines 7

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Paper code: 323

Synthesis of Novel Nano 5, 5-diphenyl hydantoins with alkyl linkage Capped Metal Nanoparticles

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Hydantoins substituted at C-5 are important medicinal compounds. The most familiar derivative, 5,5-diphenyl hydantoin (phenytoin) is extensively used as an anti-convulsion and cardiac antiarrhythmic [1],[2]. Recently antidepressant, antiviral activities, antiepileptics as well as inhibited binding of HIV to lymphocytes were also reported for hydantoins [3].
In this study, for the first time a novel nano 5,5-diphenyl hydantoins were synthesized in the presence of $(NH_4)_2CO_3$ and KCN in EtOH 50% in rt, in 45-55 % yield from corresponding 4-hydroxy benzophenone with bromoalkyl linkage. The completion of the reaction was monitored by TLC and recrystallized from 95% EtOH, to achieve thiolated products at room temperature in good yield and short reaction time without any side product. The sulfur of alkyl-linkage of final hydantoin was then capped strongly to MNPs surface by self-assembly as confirmed by IR, UV-Vis, SEM, XRD, Ms, elemental analysis and TEM image. These M@Hydantoin system may provide an advantage model system for the development of new effective drugs especially antiepileptic drug.Fig.1

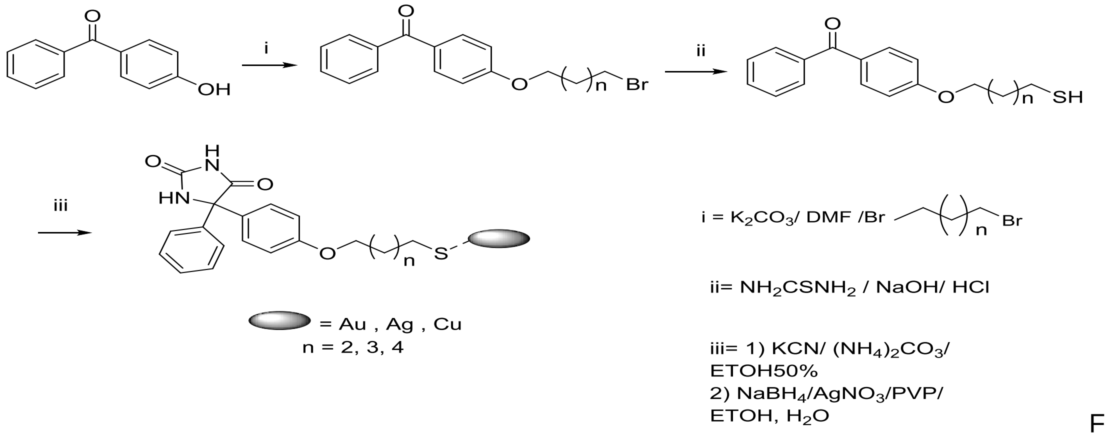

Fig. 1

Prepration of M@Hydantoin

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Paper code: 328

Selenopheno[2,3-*e*][1,2,4]triazolo[4,3-*c*]pyrimidine: A novel tricyclic selenium containing heterocyclic system

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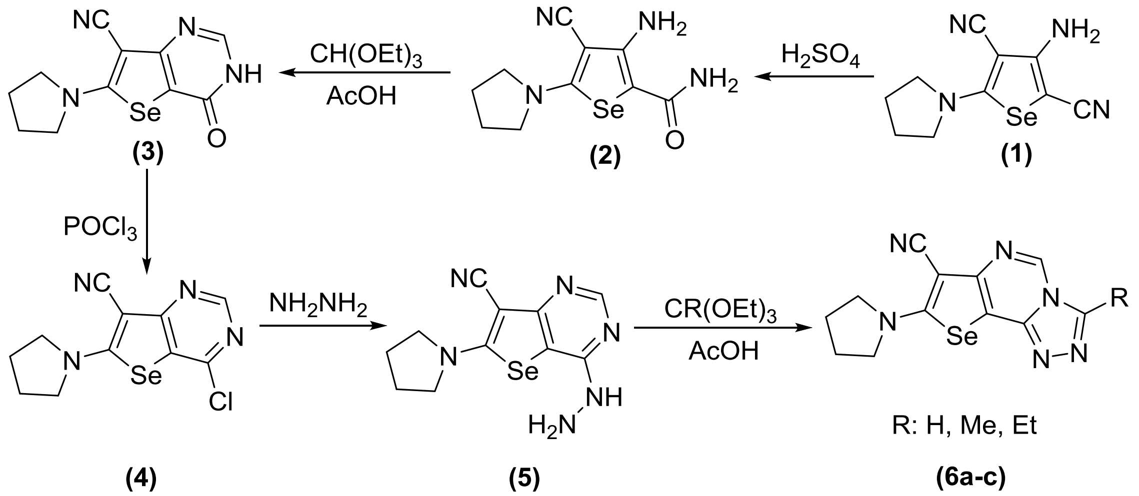
Selenium (Se) is an essential trace element for human, for example, many kinds of selenoproteins have an important role in human metabolism [1]. The interest in the synthesis of selenium-containing compounds has increased remarkably due to the discovery of various derivatives with potential biological and pharmaceutical activities. For instance, the practical application of such compounds in medicine for the treatment of tumors and cancers is a subject of current intense interest [2]. On the other hand, the synthesis of fused selenophenes has begun to play an important role in the design and synthesis of conducting, superconducting and magnetic materials [3].

Initially, concentrated sulfuric acid mediated hydrolysis of compound **(1)** gave the corresponding selenophene-2-carboxamide **(2)** which subsequently underwent the cyclization reaction with triethylorthoformate to give selenopheno[3,2-*d*]pyrimidine **(3)**. In continuation, compound **(3)** treated with $POCl_3$ and NH_2NH_2 to give the chlorinated and hydrazinated compounds **(4)** and **(5)**, respectively. The heterocyclization reaction of the latter compound with a few triethylorthoesters yielded quantitatively the desired tricyclic selenopheno[2,3-*e*][1,2,4]triazolo[4,3-*c*]pyrimidines **(6a-c)**.



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Paper code: 337

A Catalyst-Free Synthetic Route to Thiazolo[3,4-a]benzimidazol Dreivatives through a Three-Component Reaction

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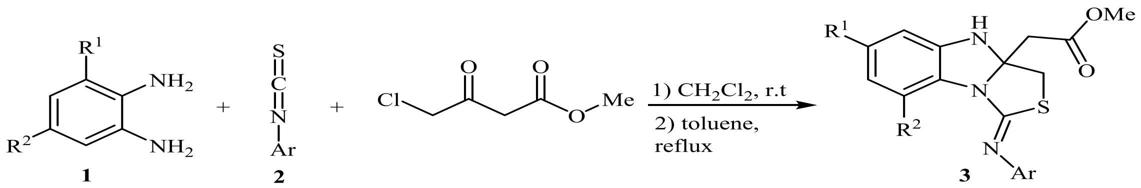
Thiazolo[3,4-*a*]benzimidazole and its derivatives were commonly synthesized through the condensation of *o*-phenylenediamines, 2-mercaptoacetic acid, and compounds containing a carbonyl group in the presence of various catalysts.[1,2] these methods have several shortcomings such as use of expensive or toxic transition metals as catalysts, moderate yields of products, and tedious workup.

As a part of our current studies on the synthesis of heterocylic compounds using multicomponent reactions,[3,4] we report herein a catalyst-free route for the synthesis of thiazolo[3,4-*a*][1,3]benzimidazol-3(4*H*)-yl]acetate 3 using the reaction of o-phenylenediamine derivatives 1, aryl isothiocyanate 2, and 4-chloro-3-oxo-butanoate in CH_2Cl_2-toluene under reflux (Scheme 1).



Scheme 1** multicomponent synthesis of thiazolo[3,4-a]benzimidazole **3

Initially, a mixture of *o*-phenylenediamine (**1a**) and phenyl isothiocyanate (**2a**) in CH_2Cl_2 was stirred at room temperature for ten minutes. After this time, 4-chloro-3-oxo-butanoate in toluene was added dropwise to the mixture and reaction was stirred under reflux for one hour, after completion of the reaction (monitored by TLC), compound 3 was separated by column chromatography (silica gel, *n*-hexane_EtOAC, 10:1).

In summary, we have described a convenient process for the synthesis of thiazolo[3,4-*a*]benzimidazole derivatives. Use of readily available starting materials and good yields of the products are the main advantages of this method. The reaction occurs under netrual conditions, and the starting materials can be mixed without any activation.

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Paper code: 340

Design and synthesis of SBA-15 with phosphorous acid tags as a new nanostrucured catalyst: Application in the synthesis of novel pyrido [2,3-*d*] pyrimidines

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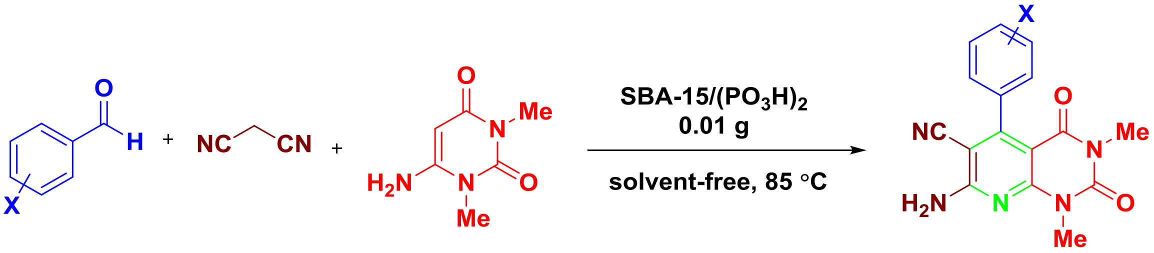
Uracil and its derivatives, such as pyrido [2,3-*d*] pyrimidines have received considerable attention over the past years because of their have biological activities such as, antibacterial, antiallergic, antimicrobial, tyrosine kinase, anti-inflammatory, analgesic, calcium channel antagonists, antihypertensive, tuberculostatic, antileishmanial, and antifungal [1-2]. A Mesoporous silica material (MSM), such as SBA-15, has surface area, good thermal stability, and potential for tunability due to its surface modifiable ability and nature of the MSM [3-6]. In this paper, there is growing interest in development of clean processes through involving green catalysts. Thus, in continuation of our pervious works on the application of reusable catalysts in organic synthesis, herein we decided to investigate the synthesis of pyrido [2,3-*d*] pyrimidines in the presence of SBA-15/$(PO_3H)_2$ as a recyclable green solid acidic catalyst (**Scheme 1**).



Scheme 1. Synthesis of pyrido [2,3-*d*] pyrimidines using SBA-15/$(PO_3H)_2$.

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Paper code: 341

Nanosilica sulfamic acid catalysed synthesis of 2-phenylbenzoxazole Derivatives as heterogeneous catalyst

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2-Arylbenzoxazoles are important heterocyclic motif widely found in bioactive molecules, pharmaceuticals and natural products [1]. 2-Substitued benzoxazoles are also fundamental scaffolds to construct novel ligands and materials. As such, four main strategies for their preparation have been reported such as transition metal-catalysed direct arylation of bezoxazoles with aryl halides; intermolecular cyclization of 2-aminophenol with aldehydes; intermolecular cyclization of halobenzanilides; and ring-opening-coupling-recyclization of benzoxazoles with aromatic aldehydes or benzoyl chloride [2-3]. Among them, acid-catalysed direct arylation of ortho-aminophenol presents an economically attractive strategy to afford diverse 2-arylbenzoxazoles [4].

In this study we reported mild synthesis of 2-arylbenzoxazole derivatives in the presence of nanosilica sulfamic acid as heterogeneous catalysts (fig 1).

We have demonstrated a nanosilica sulfamic acid-catalysed synthesis of benzoxazoles. The silica supported sulfamic acid catalysis promoted the condensation reaction in good to excellent yields with broad substrate scope, which provides a promising method for the synthesis of pharmacologically significant 2-aryl benzoxazole derivatives.

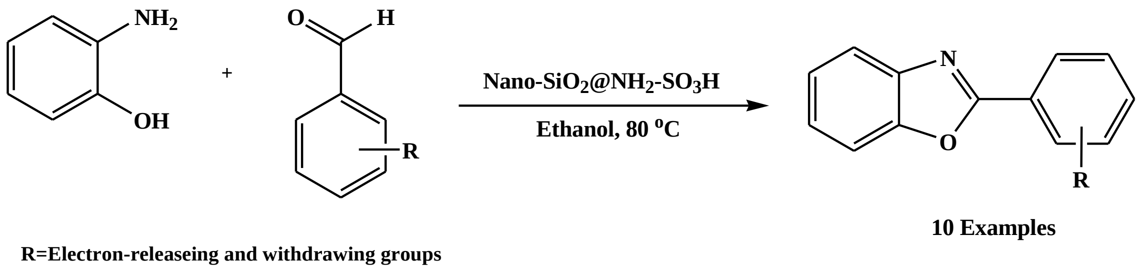

Fig. 1 Nanosilica sulfamic acid catalysed synthesis of 2-Aryl-benzooxazole

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Paper code: 344

Synthesis of quinazolines over recyclable Fe_3O_4@SiO_2-APTES-Fe^{3+} nanoparticles: A green, efficient, and solvent-free protocol

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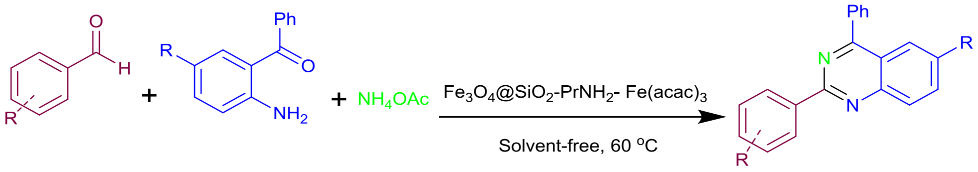
One of the most important nitrogen heterocycles found in a wide variety of natural products is quinazoline. It has received great attentions in organic synthesis and medicinal chemistry [1,2]. A practical and efficient method is developed for efficient synthesis of quinazoline derivatives through condensation reaction of 2-aminobenzophenone, an aldehyde, and ammonium acetate [3], over magnetic Fe_3O_4@SiO_2-APTES-Fe^{3+} NPs as a recyclable nanocatalyst, under solvent-free conditions. The as-prepared nanocatalyst is characterized using Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), thermogravimetry analysis (TGA), and vibrating sample magnetometer (VSM). The advantages of this protocol includes, avoiding the use of solvent, easy handling, short reaction time, simple experimental, product purity, and nontoxicity, economical and environmental friendly nature of the iron catalyst are the attractive features of this methodology. These together with the simple recovering of catalyst makes it a useful alternative for the scale-up for the synthesis of quinazoline derivatives [4,5].



Scheme 1. Synthesis of quinazoline derivatives using Fe_3O_4@SiO_2-$PrNH_2$-Fe(acac)$_3$.

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Paper code: 346

Introduction of benzimidazole-based ionic liquid as an efficient and reusable catalyst for the preparation of 1,8-dioxo xanthene derivatives

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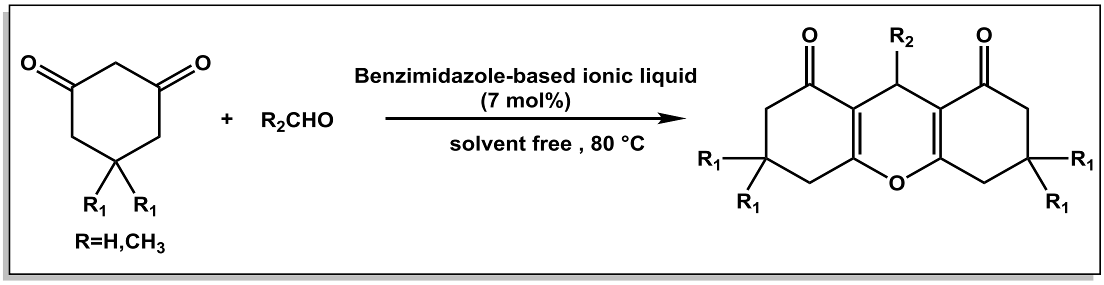
Xanthenes are biologically important drug intermediates for the synthesis of compounds having antibacterial, anti-inflammatory and antiviral activities [1]. Also, they were used as dyes in laser technologies, and in fluorescent materials for visualization of biomolecules. Because of these significant features there has been a continuous interest in the synthesis of these types of compounds and consequently numerous approaches have been reported for their synthesis [2].

Ionic liquids have received considerable interest as eco-friendly solvents, catalysts and reagents in organic synthesis because of their unique properties, such as low volatility, non-flammability, high thermal stability, negligible vapor pressure and ability to dissolve a wide range of materials [3].

In this work, a dicationic ionic liquid based on benzimidazole is simply prepared and after is used for the promotion of the synthesis of 1,8-dioxoxanthene derivatives. The main advantage for using this catalyst are ease of separation of the catalyst, high yields of achived products during low reaction times.



Scheme 1 Synthesis of 1,8-dioxo xanthene derivatives catalyzed by Benzimidazole-based ionic liquid

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Paper code: 351

Synthesis a new series of potential biological activities compounds by reaction of imidoyl chlorides and GBP drug

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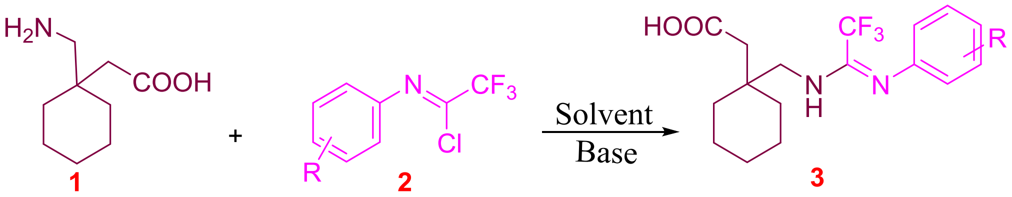
Gabapentin (GBP) is used as an anticonvulsant drug which displays analgesic effects in the therapy of a variety of chronic pain conditions, such as complex regional pain syndrome, inflammatory pain, central pain, trigeminal neuralgia, diabetic neuropathy, headaches, malignant pain, post-herpetic neuralgia, and HIV related neuropathy [1]. Fluorinated of imidoyl halides became a versatile tool in the synthesis of various and important fluorinecontaining molecules [2]. In the present work we synthesized a new series of potential biological activities compounds **3** by reaction of imidoyl chlorides **2** and GBP drug **1.** The structures of products were proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data and elemental analysis.



Scheme 1: Preparation of (2-(1-(2,2,2-trifluoro-N'-phenylacetimidamido)cyclohexyl)acetic acid derivatives.

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Paper code: 352

One-pot three-component synthesis of Acridine derivatives in glycerin media

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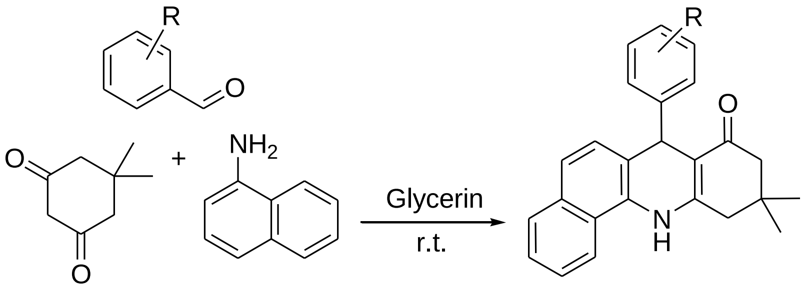
A plenty of natural and synthetic materials including the acridine skeleton display interesting biological and physical activities, such as antimalaria and antitumor agents, and multihydroacridineone derivatives have been reported to have high fluorescence efficiency and can be used as fluorescent molecular probes for monitoring of polymerization process [1-3]. In this project, naphthylamine, dimedone and aryl aldehydes compounds in glycerin media was stirred at room temperature. TLC indicated completion of the reaction. After completion of the reaction, water was added and the product was appeared as a solid compound. After filtration, the desired product was dried and recrystallized for more purification by ethanol and identified by Perkin Elmer FT-IR spectrometer and ^{1}H-NMR spectra on Bruker DRX- 300 MHZ NMR instrument. The condensation reaction between 1-naphthyl amine, dimedone and aryl aldehydes was promoted in glycerin media at ambient temperature to afford 7-aryl-7,10,11,12-tetrahydrobenzo[c]acridin-8(9H)-one derivatives (Scheme 1). To study the scope of the reaction, a series of aryl aldehydes carrying electron donating and electron withdrawing groups were subjected to produce their corresponding acridin-8(9H)-one derivatives in high yields. This method gives remarkable advantages such as simple work-up procedure, using of the green and inexpensive procedure with excellent yields.



Scheme1. Synthesis of 7-aryl-7,10,11,12-tetrahydrobenzo[c]acridin-8(9H)-one derivatives

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Paper code: 354

Ionic liquid-functionalized mesoporous silica nanoparticles ([pmim]$FeCl_4$/MSNs): Efficient nanocatalyst for solvent-free synthesis of N,N′-diaryl-substituted formamidines

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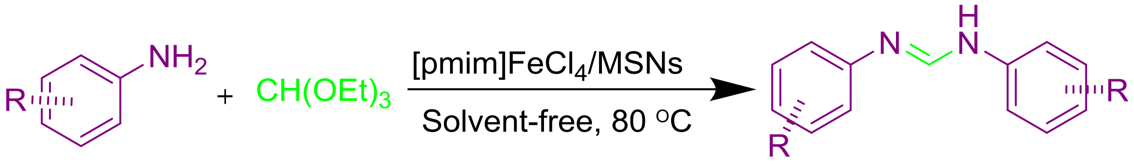
We report the synthesis of ionic liquid-functionalized mesoporous silica nanoparticles ([pmim]$FeCl_4$/MSNs) via a method of post-grafting on parent MSNs. This hybrid material was characterized using scanning and transmission electron microscopies, energy-dispersive X-ray spectroscopy, nitrogen adsorption–desorption analysis, Fourier transform infrared spectroscopy, powder X-ray diffraction and thermal analyses. The material was utilized as an efficient heterogeneous catalyst for the synthesis of *N,N′*-diaryl-substituted formamidines through the reaction of triethyl orthoformate with arylamines under solvent-free conditions. The catalyst was recovered easily and reused several times without significant loss of its catalytic activity [1-3].



Scheme 1. Synthesis of *N, N´*-diarylsubstituted formamidines.

References

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Paper code: 356

Synthesis of azo compounds by reaction between trifluoroacetimidoyl chlorides and hydrazinhydrat

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Trifiuoromethylated compounds have been receiving great interest in medicinal, agricultural, and material sciences [1]. Among the various trifluoromethylations, the preparation and utilization of trifluoromethylated building blocks involve one of the useful approaches to the goal, and have currently been receiving interest in synthetic organofluorine chemistries [2]. Azo compounds are the most common synthetic colourings used in foods, pharmaceuticals and cosmetics. Although they have been used in this way for many years, comparatively little work on their toxicity or metabolism was published before the last decade. With the increasing awareness of possible health hazards associated with their use, however, more attention has been focused recently on the biological activity of azo compounds [3]. Here we wish to report the result of our study on the reaction of trifluoroacetimidoyl chlorides **1** with $NH_2NH_2.H_2O$ **2** in the presence of base lead to azo-compounds **3**. The structures of this products were proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data and elemental analysisis.

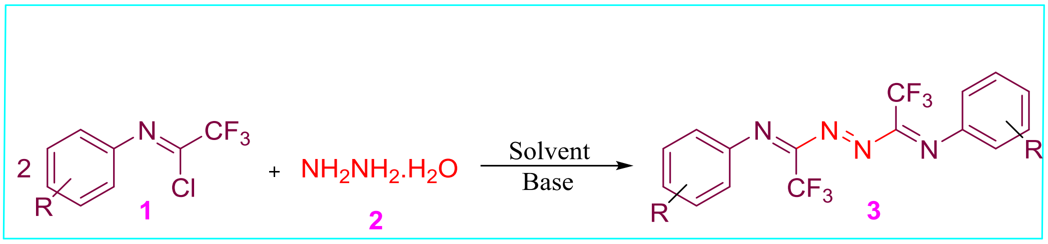

Fig. 1 Preparation of azo compounds.

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Paper code: 357

Nano BF_3/SiO_2: A Novel Acid Catalyst for the Synthesis of Pyrroles by the Paal–Knorr Condensation at Room Temperature

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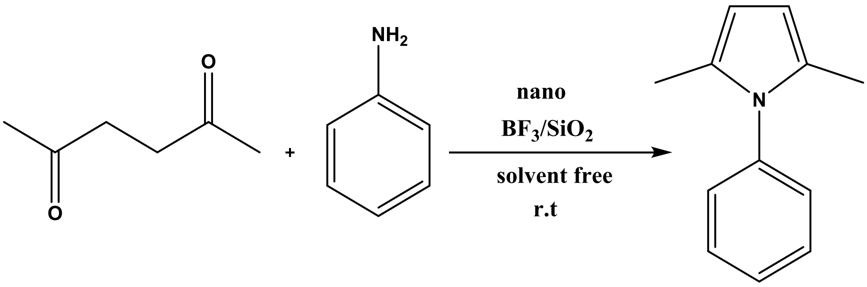
Pyrroles are the important five-membered nitrogen heterocyclic compounds, which can be used as intermediates in many organic reactions and are important in fine chemical industry, particularly in the synthesis of many important drugs[1]. The laboratory methods for pyrrole synthesis by many organic chemist such as Knorr[2]. Due to the efficient, mild reaction condition and facile reaction process, the Paal–Knorr condensation reaction remains the most frequently used one to generate pyrrole and its derivatives[3]. In this reaction, the N-substituted pyrrole could be obtained through condensation of 2,5-hexanedione with aniline derivatives in one step. We wish to report herein a simple, clean, and environmental eco friendly process for the synthesis of pyrrole derivatives by nano BF_3/SiO_2 as heterogenious catalyst under solvent-free condition at room temperature(Scheme1).



Scheme1

References

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Paper code: 360

Synthesis of pyrido[1,2-b][1,2,4]triazine-7,9-dicarbonitrile derivatives

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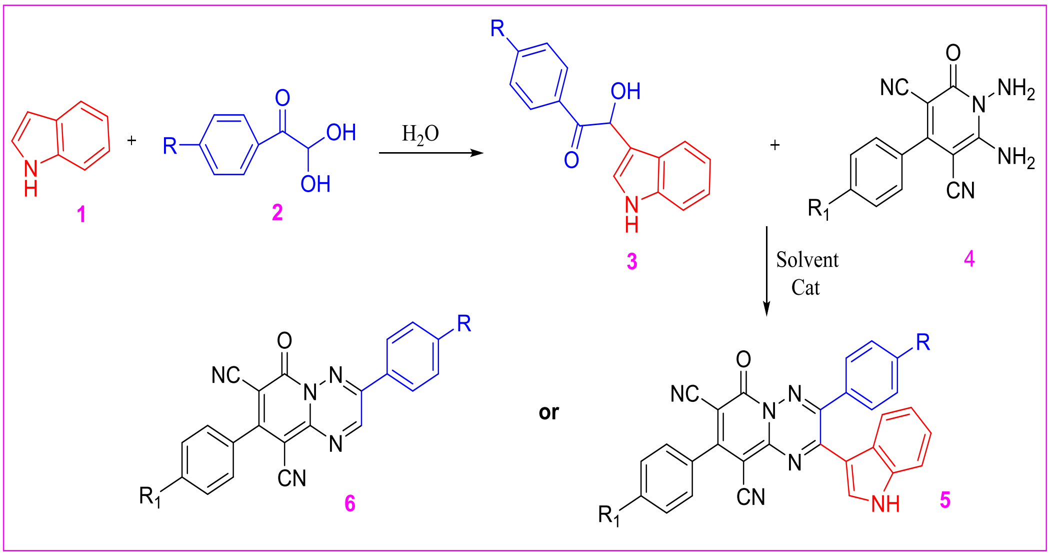
Heterocyclic compounds attract significant attention in the chemical literature due to their abundance in natural products and their diverse biological properties [1]. Indole is the most important chemical skeletons which existing as the main core in the structure of various physiologically, pharmaceutically, and industrially important compounds. For example indole derivatives involve beneficial estron metabolism promoter, inhibitor for human prostate cancer cells and radical scavengers [2,3]. In this investigation reaction of 2-hydroxy-2-(1H-indol-3-yl)-1-phenylethan-1-one derivatives 3 and 1,6-diamin derivatives 4 in the presence of acid catalyst lead to the corresponding products 5 and 6 in 85-92% yields. The structures of compounds were confirmed by spectroscopic and analytical data.



Scheme 1: Preparation of 2-(1H-indol-3-yl)-6-oxo-3,8-diphenyl-6H-pyrido[1,2-b][1,2,4]triazine-7,9-dicarbonitrile derivatives.

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Paper code: 363

An efficient, four-component reaction for synthesis of dihydropyrimidin derivatives from malononitrile, arylglyoxal, arylamine and benzonitrile

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Heterocycles are important, not only because of their abundance, but above all because of their chemical, biological and technical significance. Heterocycles count among their number many natural products, such as vitamins, hormones, antibiotics, alkaloids, as well as pharmaceuticals, herbicides, dyes, and other products of technical importance [1]. Classical methods for preparation of dihydropyrimidin derivtives via various intramolecular cyclization reactions of urea derivtives or amidine derivtives onto compounds such as 1,3-dicarbonyl, ketone, α,β-unsaturated and other have been described. The medicinal importance of dihydropyrimidin has been recognized for many decades and many compounds exhibit antiviral, antitumor, antibacterial, and anti-inflammatory properties [2]. Herein, we describe a simple four-component reaction on the addition of malononitrile **1** and arylglyoxal **2** with aryl amines **3** and benzonitrile derivativs **4** in ethanol solvent leading to dihydropyrimidin derivatives **5** (Fig. 1). The mild reaction conditions, catalyst-free, short reaction time, and excellent yields are advantages of the protocol.

All the synthesized compounds were unknown to the best of our knowledge and were characterized by ^{1}H and ^{13}C NMR, IR and melting points. For instance, the ^{1}H NMR spectrum one of the compound derivatives **5** (6-amino-4-(4-methylbenzoyl)-2-phenyl-1-(p-tolyl)-1,6-dihydropyrimidine-5-carbonitrile) consisted of two singlet at δ = 2.24 and 2.26 ppm for the methyl groups in the product. Carbon aliphatic proton's was observed as a singlet in δ = 4.92, the aromatic protons and NH_2 protons resonated in the region δ = 7.10-7.64 ppm. The ^{13}C NMR spectrum of compound 5a exhibited 20 distinct signals in agreement with the proposed structure. In the IR spectrum, the two carbonyl and nitrile group absorption were observed at 1707, 2245 cm^{-1}. Partial assignments of these resonances for the other products are given in the experimental section.

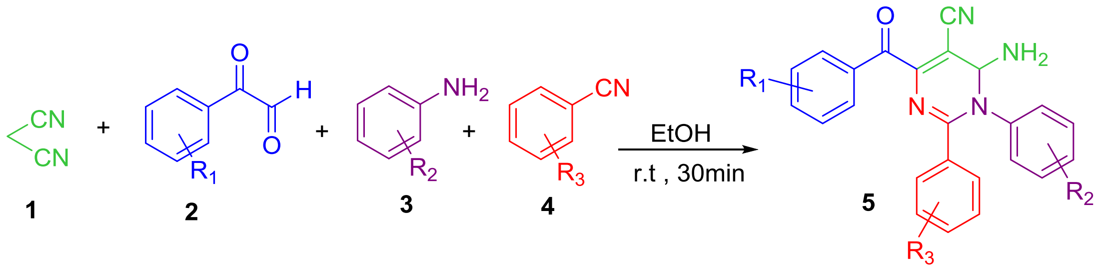

Fig. 1 Synthesis of dihydropyrimidin derivatives

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Paper code: 364

Efficiet one-pot synthesis of pyrazoles catalyzed by nono particles Graphine/iron oxid(hematite), Hollow zine ferrite nanosphere, Au nano particles using green chemistry

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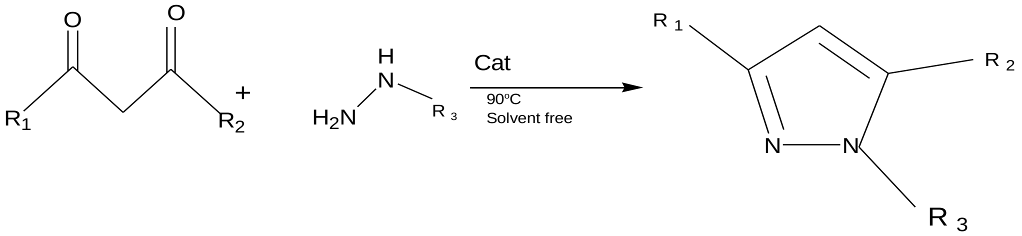
Pyrazoles are of significant synthetic targets in organic and pharmaceutical chemistry because of pyrazole motif generally acting as a core framework in numerous biologically active compounds [1–3]. As a part of our continuing effort towards the development of useful synthetic methodologies, here in we report an efficient process for synthesis of various pyrazoles, in the reaction of different 1,3-dicarbonyl compounds with hydrazines using nano particles Graphine/iron oxid(hematite), Hollow zine ferrite nanosphere, Au nano particles, as the catalyst solvent-free conditions have also been reported (Scheme1). This extensive application of heterogeneous catalysts in synthetic organic chemistry can make the synthetic process more efficient from both environmental and economic point of view and used-catalyst can be easily recycled. Performance of reaction under solvent-free conditions, short reaction times, and high returns are the benefits of this research work. The structure of the products was investigated by IR and ^{1}H-NMR.



Scheme1 The synthesis of pyrazole derivatives

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Paper code: 367

Synthesis of sucrose stearate and its application as emulsifier

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Sucrose Fatty acid esters are compounds that are mainly prepared from esterification of sucrose with fatty acids or glycerides. These compounds are used as emulsifiers in various industries such as food and cosmetic industries [1], [2]. In this study, the synthesis of this compound was carried out in two steps. In the first step, the methyl ester of stearic acid was synthesized. In the second step, sucrose stearates were synthesized from methyl ester and sucrose. Also optimization of temperature, solvent and ... was studied. Finally, the application of this compound was performed as an emulsifier.

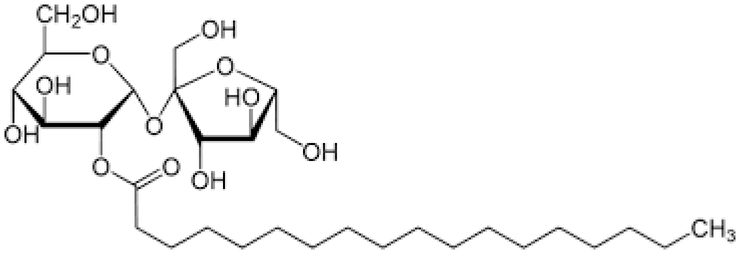

Fig. 1 The Structure of Sucrose Stearate

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Paper code: 369

Synthesis of new phenyl(3-(trifluoromethyl)-4H-furo[3,4-b]indol-1-yl)methanone derivatives

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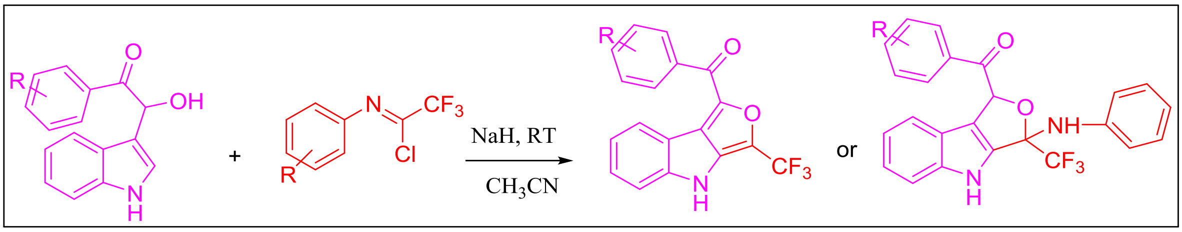
The synthesis of biologically active organofluorine heterocyclics has received more attention in the medicinal chemistry and materials sciences [1]. Among these derivatives synthesis and development of new methods for preparation of CF_3 containing heterocylic compounds have gained more attention, because of their physical and pharmaceutical properties and using in industry, medicinal and agriculture [2]. Our interest in fluorine chemistry and trifluoroacetimidoyl chloride reactions, and our attempt to synthesize bioactive organofluorine compounds led us to consider the reaction of trifluoroacetimidoyl chloride derivatives with 2-hydroxy-2-(1H-indol-3-yl)-1-phenylethan-1-one in acetonitrile and in the presence of NaH at ambient temperature for formation of phenyl(3-(trifluoromethyl)-4H-furo[3,4-b]indol-1-yl)methanone derivatives (Scheme 1). The structures of this products were proved by ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR and IR spectral data and elemental analysis. Reactions were clean and products were isolated by simple filtration.



Scheme1

References

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Paper code: 375

Synthesis of 2,2,2-trifluoro-N-phenyl-1-tosylethan-1-imine derivatives

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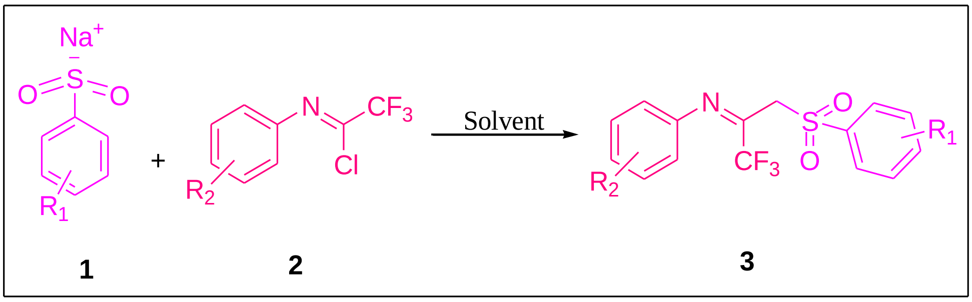
The progress in the field of fluorination organic compounds has been summarized in numerous review articles. It was considered that the fluorine atoms or fluorinated compounds play a pivotal role in bioactive compounds, because they provide an avenue for further structural elaboration. In recent years, various fluoroalkylation reagents and reactions such as trifluoromethylation, difluoromethylation, and monofluorome-thylation have been extensively investigated, in order to synthesis new organofluorine compounds [1]. Sodium aryl sulfinate are important structures in bioactive compounds [2]. Synthesis of such molecules, however, usually requires cumbersome synthetic routes. Herein a simple and an efficient for the synthesis of 2,2,2-trifluoro-N-phenyl-1-tosylethan-1-imine derivatives **3** (Scheme 1) from of trifluoroacetimidoyl chloride derivatives **2**, Sodium Aryl sulfinate **1** under mild reaction conditions has been developed.



Scheme 1: Preparation of 2,2,2-trifluoro-N-phenyl-1-tosylethan-1-imine derivatives

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Paper code: 378

An efficient synthesis of quinoxaline derivatives: one-pot three-component reaction of arylglyoxal, o- phenylenediamine, Meldrum's acid as catalyst

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Functionalized quinoxalines represent an important class of nitrogen-containing heterocycles as they constitute useful intermediates in organic synthesis and are useful dyes [1]. Quinoxaline derivatives have different pharamacological activities such as bacteriocides and insecticides, antibacterial, antifungal, antitubercular and analgesic [2]. Quinoxalines derivatives was prepared via stirring of Meldrum's acid as catalyst **1** and arylglyoxal **2** with o- phenylenediamine **3** in ethanol at room temperature for 1 h. After completion of the reaction, determined by TLC, the product **4** was precipitated from the reaction mixture. The precipitate was filtered and recrystallized from ethanol (Fig 1). The advantages of this method are base free, the high yields of products, short reaction times, easy of the work up, and green solvent. Quinoxaline derivatives were identified by spectroscopy techniques such as ^{1}H-NMR, ^{13}C-NMR, IR.

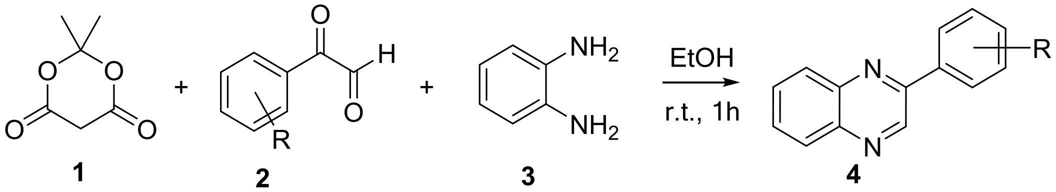

Fig. 1. Synthesis of quinoxaline derivatives

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Paper code: 380

An efficient synthesis of 1,8-dioxodecahydroacridine derivatives in the presence of glycerin

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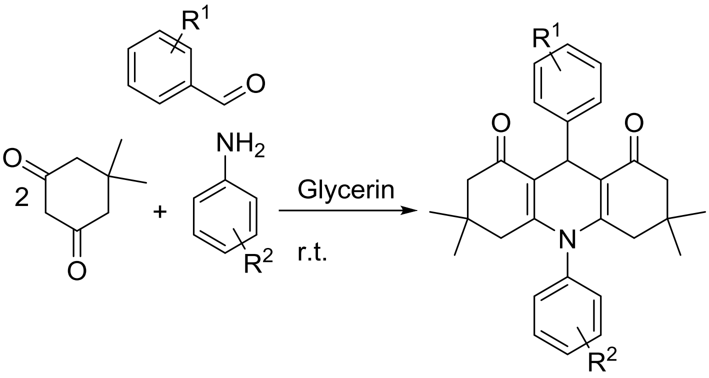
Substituted Acridines have been used as antimalarial for many years quite successfully and several of them have exhibited excellent results in chemotherapy of cancer. These derivatives are frequently used in industry, especially for the production of dyes [1-3]. The products identified by Perkin Elmer FT-IR spectrometer and ^{1}H-NMR spectra on Bruker DRX- 300 MHZ NMR instrument. Aromatic aldehydes, aryl amines and dimedone were used in the synthesis of 1,8-dioxodecahydroacridine derivatives in glycerin media at room temperature (Scheme 1). High yields, simple and comfortable separate operation provided several special advantages this protocol.



Scheme1. Synthesis of 1,8-dioxodecahydroacridine derivatives

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Paper code: 384

Synthesis of new selective ligand from N-Aryltrifluoroacetimidoyl chlorides and aniline derivatives

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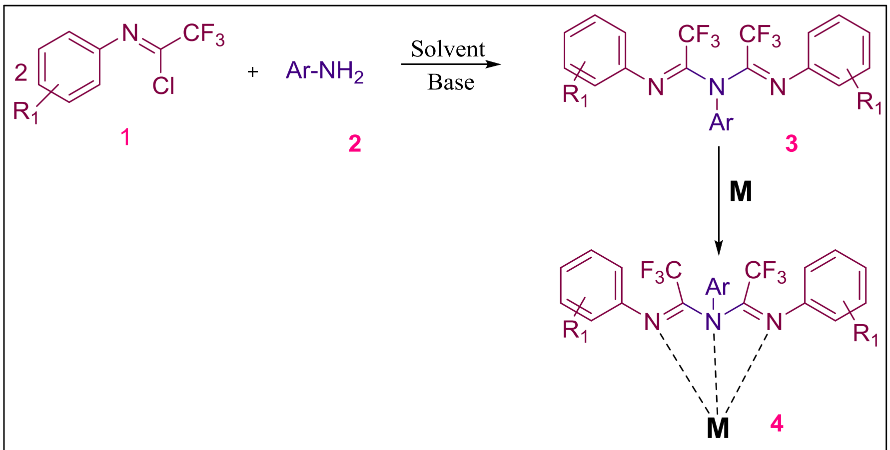
Trifluoromethylated compounds are of particular interest as the strong electron-withdrawing effect of the CF_3 group contributes to a number of biologically important molecular properties. For example, it results in a significant increase in the lipophilicity of the molecule, which is a very important feature in drug delivery. N-Aryltrifluoroacetimidoyl chlorides can be prepared by several procedures [1, 2]. Herein we wish to report we now report synthesis of new selective ligand 2,2,2-trifluoro-N,N'-diphenyl-N-((2,2,2-trifluoro-1-(phenylimino)ethyl)acetimidamide **3** based on the reaction of trifluoromethylimidoyl chlorides **1** with the aniline derivatives **2** in the presence of base (scheme 1). The structures of this products were proved by ^{1}H-NMR, ^{13}C-NMR, ^{19}F-NMR and IR spectral data and elemental analysis.



R_1: 4-CH_3, 4-OMe, 4-Br, 4-Cl, 3-CH_2CH_3
Ar: :4-CH_3-C_6H_5, 4-OMe-C_6H_5, 4-Br-C6H5, 4-Cl-C_6H_5, 3-Br-C_6H_5, 2-Cl-C_6H_5
M: Ni^{2+}, Cu^{2+}, Fe^{2+}

Scheme 1: Preparation of new selective ligand 2,2,2-trifluoro-N,N'-diphenyl-N-((2,2,2-trifluoro-1-(phenylimino)ethyl)acetimidamide derivatives.

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Paper code: 394

Regioselective Synthesis of New Aryloyl-Functional Thiazolo[3,2-*a*]pyridine Using Ketene Dithioacetals in Ethanol Media

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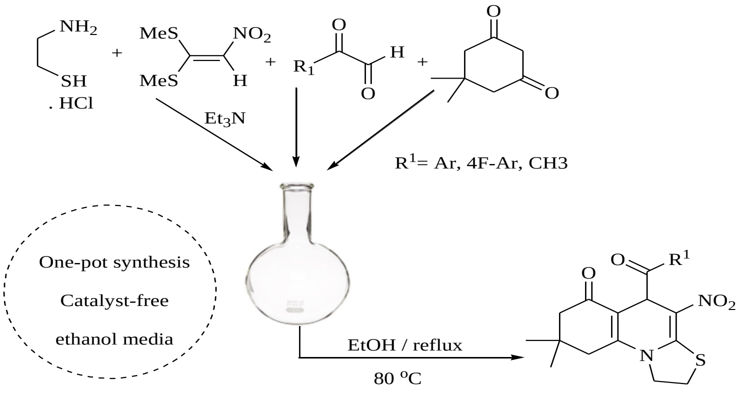
Thiazolo[3,2-*a*]pyridines are well known as an important class of sulfur-nitrogen containing heterocycles with two different fused heterocycles, which are found in a broad range of compounds possessing a variety of biological activities such as potent CDK2-cyclin A inhibitor, potential uterus stimulant, beta-amyloid production inhibitor, coronary dilator, antibacterial, antifungal, scavenge free radicals because of possessing electron acceptors and donors, and also these derivatives play an important role in drug development for chemotherapy of various cancers [1, 2].

We report a novel approach to prepare a series of heterocycles containing thiazole and pyridine rings which substituted with nitro and aryloyl groups. The title compounds are obtained from one-pot four-component reaction of nitroketene dithioacetals, cysteamine hydrochloride, dimedone and phenylglyoxal in ethanol (Scheme 1). These sulfur-nitrogen containing heterocycles with drug potential activity, synthesized through sequential Knoevenagel/Michael/intramolecular *N*-cyclization sequences. Environmentally benign procedure without the use of any catalyst or metal promoters, mild reaction conditions, easy work-up with superior atom economy are some advantages of this method.



Scheme. 1 Synthetic scheme for the generation of 5-aryloyl-4-nitro-thiazolo[3,2-*a*]quinolin-6-one.

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Paper code: 401

Synthesis pyrimidin- 5-yl-pyrroles derivatives

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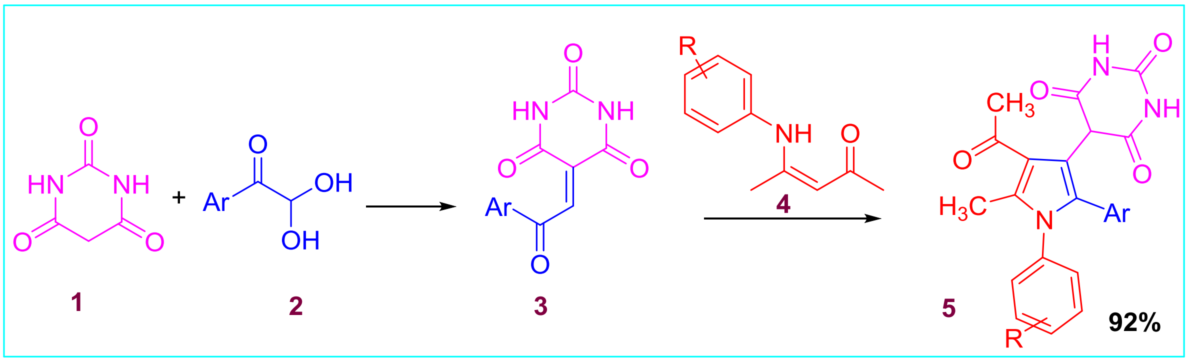
Barbiturates are related to pyrimidines and their activities vary by changing the alkyl groups present in the C-5 position [1]. Reactions modifying this position are therefore particularly useful. Scaffolds containing the pyrrole core are found in numerous drugs, natural products and biological systems. Several methods have been developed for the synthesis of pyrrole analogues [2] as a clear indication of the important role pyrrolyl heterocycles play in synthetic and medicinal chemistry [3]. Herein a simple and an efficient three-component domino method for the synthesis of poly-functionalized pyrimidin- 5-yl-pyrroles **5** (Scheme 1) from a three-component domino reaction of enaminone derivatives 4, barbituricacid **1** and arylglyoxalhydrates **2** under mild reaction conditions has been developed.



Scheme 1

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Paper code: 403

Solvothermal Synthesis of Surface-Passivated and Functionalized Carbon Quantum Dots with High Catalytic Activity for Selective Oxidation of Alcohols under Mild Conditions

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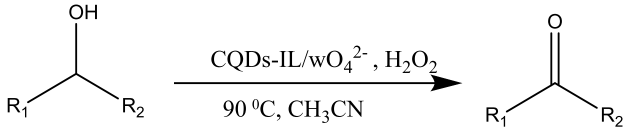
Selective oxidation of alcohols to their aldehydes and ketones is an important synthetic conversion both in the organic synthesis and industrial chemistry. Owing to the corresponding carbonyl compounds are exceedingly valuable intermediates in various industries. The collection of reagents that have been developed to accomplish this transformation is reflects its significance. However, noncatalytic oxidation of alcohols using stoichiometric quantities of oxidants such as chromium, ruthenium, manganese oxides, permanganate, dichromate, hypochlorite, Swern and Dess-Martin reagents are relatively expensive, highly toxic, time-consuming and pollute the environment. Hence, with increasing environmental concerns and in order to save time and money, enormous efforts have been assigned to the design of greener catalytic systems that employ H_2O_2 as a clean, cheap, eco-friendly co-catalyst oxidant. In this study, for the first time, we designed a novel heterogeneous catalyst (labeled as wo_4^{2-}@IL-CQDs) for selective oxidation of alcohols to aldehydes and ketones. In the resulting catalyst, ILs-modified carbon quantum dots act as a metal-free support for the immobilization of Tungstate ions ($wo_4^{=}$) which is necessary for oxidation. The above catalyst high activity and selectivity in alcohols oxidation in present H_2O_2 as oxidant.



R_1, R_2 = Alkyl or H

References

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Paper code: 405

Synthesis of polyhydroquinoline derivatives in the presence of [PVP-SO_3H] HSO_4 under solvent-free conditions

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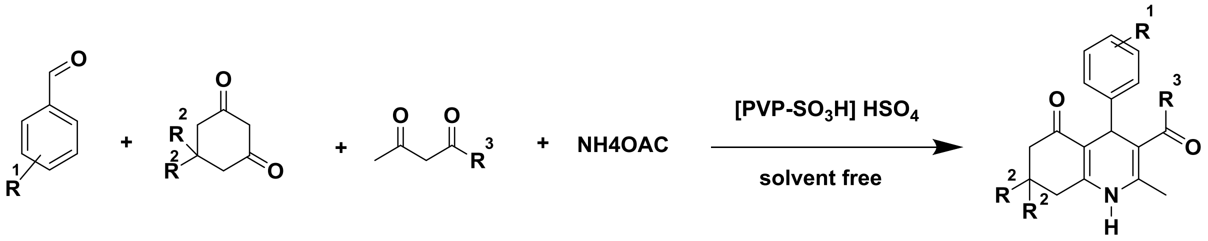
Quinolines have been identified as promising structure in medicinal chemistry because of their many pharmacological properties, including their antibacterial antihypertensive, anti-inflammatory, antimalarial, antiasthmatic, and tyrosine kinase inhibitory activity. In recent years, a number of methods have been reported on hantzsch. Many of the hantzsch methods have disadvantages such as expensive reagents, formation of side products, thermal instability, and difficult accessibility to reagents. Thus, a mild, convenient, and high yield procedure using inexpensive catalyst would be valuable [1].

[PVP-SO_3H] HSO_4 is a solid acid catalyst, which improves the reaction in solvent-free conditions [2]. In this work, [PVP-SO3H] HSO4 was used as catalyst in the hantzsch synthesis of polyhydroquinoline derivatives via four component reaction of aldehydes, ammonium acetate, diketone, and ethylacetoacetate. The procedure has several advantages such as shorter reaction time, higher purity and yields, high reaction rates, ease of preparation and handling of the catalyst, simple and green experimental procedure and use of inexpensive and reusable catalyst for five times without loss of its catalytic activity.



Scheme 1 Synthesis of polyhydroquinoline derivatives using [PVP- SO_3H] HSO_4 as the catalyst.

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Paper code: 407

Synthesis of spiro-fused heterocyclic scaffolds through multicomponent reactions involving nitro ketene aminal (HKA)

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Spiro heterocycles represent an important class of naturally occurring substances with biological properties. Spiro compounds having cyclic structures fused at a central carbon are of recent interest due to their interesting conformational features and their structural implications on biological systems. Spiro heterocycles have been found to play fundamental roles in biological processes. They have exhibited diversified pharmacological activities [1].

As a type of versatile building block for the synthesis of fused heterocycles, heterocyclic ketene aminals (HKAs) received much attention within the chemical community [2]. To continue our studies on the synthesis of pharmacologically active heterocyclic compounds using HKAs and considering the importance of spiro-fused frameworks in organic synthesis [3], herein we report an efficient synthesis of spiro-fused heterocyclic compounds **5** trough multi-component reactions of nitro ketene aminals derived from the addition of various diamines **1** to nitro ketene dithioacetal **2** with *o*-phthalaldehyde **3** and 2-hydroxy-1,4-naphthoquinone **4** (Fig 1). This reaction proceeded without any catalyst in excellent yield and the other advantages of this work are simple work-up, no toxic byproducts and milder reaction conditions. All structures were confirmed by IR, ^{1}H- and ^{13}C-NMR analyses.

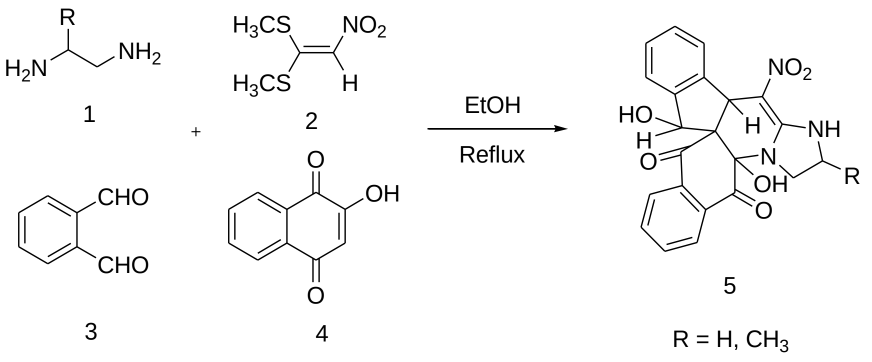

Fig. 1 Synthesis of spiro-fused heterocyclic compounds.

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Paper code: 408

New approaches for the synthesis of imidazopyridine carboxamide and pyridopyrimidine carboxamide derivatives

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Heterocyclic compounds, especially nitrogen containing heterocycles, are important natural and synthetic materials. Among them, imidazo[1,2-a]pyridine derivatives display a diverse range of biological activities such as antibacterial, antiinflammatory, antifungal, anthelmintic, antiviral, antiprotozoal, analgesic, antipyretic, hypnoselective, anxioselective [1], and pyrido[1,2-a]pyrimidine derivatives exhibit promising antiviral, antibacterial, anti-AIDS, and antinociceptive activities [2].

During recent years, the use of 1,1-bis(methylthio)-2-nitroethene in organic synthesis has attracted great interest from many chemists [3]. Herein we report an efficient synthesis of imidazopyridine carboxamide and pyridopyrimidine carboxamide derivatives, via a one-pot, four-component reaction of nitro ketene aminals derived from the addition of various 1,n-diamines **1** to 1,1-bis(methylthio)-2-nitroethene **2** with aromatic aldehydes **3** and cyanoacetamide **4** in EtOH as solvent under reflux condition in excellent yields (Fig 1). This protocol has the advantages of simple workup, mild reaction conditions, absence of catalyst and provides an entry point to fused heterocyclic structures. All structures were confirmed by IR, MS, ^{1}H- and ^{13}C-NMR analyses.

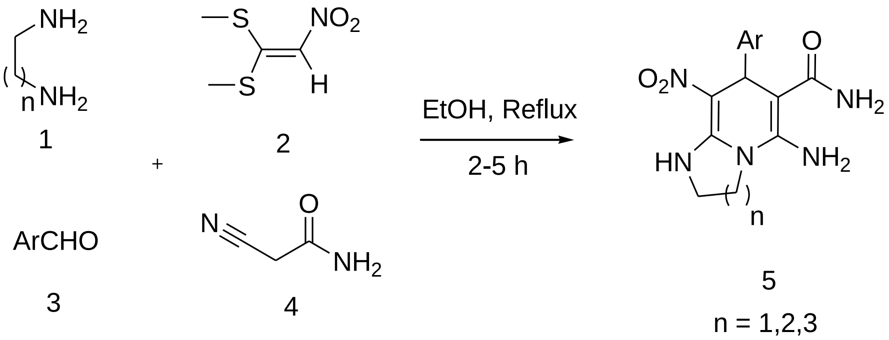

Fig. 1 Synthesis of imidazopyridine carboxamide and pyridopyrimidine carboxamide derivatives.

References

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Paper code: 411

An efficient and rapid synthesis of functionalized quinoline derivatives

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For more than a century, heterocycles have constituted one the largest areas of research in organic chemistry. Amongst the heterocycles, N-based heterocycles represent a highly important class of compounds which are widely used in materials science, agrochemistry, and medicinal chemistry [1]. Quinoline is one of the most popular N-heterocyclic compounds incorporated into the structures of many pharmaceuticals [2].

Enaminones and related compounds are versatile synthetic intermediates in organic chemistry. They are widely used for the synthesis of a variety of heterocycles especially N-heterocyclic compounds in the past several years [3]. herein we report an efficient synthesis of functionalized quinoline derivatives **5** through a multi-component reaction of enaminone derived from the addition of various anilines **1** to dimedone **2** with aromatic aldehydes **3** and cyanoacetohydrazide **4**, respectively in melt conditions and then in ethanol/water as a green medium (Fig 1). The significant features of this method are green methodology, easy work-up, readily available starting materials, high atom economy, compatibility with various functional groups and good product yields. All structures were confirmed by Mass, IR, ^{1}H- and ^{13}C-NMR analyses.

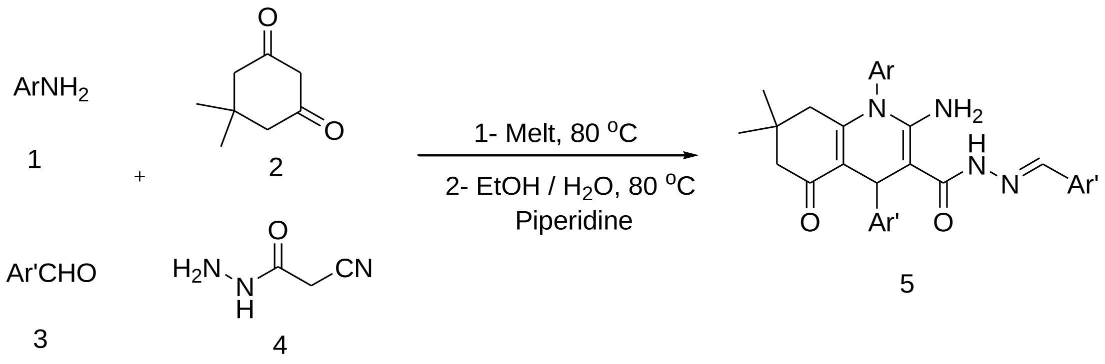

Fig. 1 Synthesis of functionalized quinoline derivatives.

References

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Paper code: 412

A mild and efficient one-pot synthesis of new indenone-fused heterocyclic compounds

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The development of new synthetic methods in the research of novel bioactive compounds, such as natural products and analogous, drugs, diagnostics and agrochemicals, in academic and industrial chemistry is closely connected to the efficient synthesis of such compounds [1]. Indenone frameworks are in a large number of natural and synthetic drugs. Indenone-fused heterocycles have attracted the attention of chemists and pharmacologists because of their broad range of bioactivities [2].

The presence of a trihalomethyl group in a molecule can result in significant changes in its physical, chemical, and biological properties. Many bioactive trihalomethylated compounds have found important applications in medicine and agriculture [3]. herein we report an efficient synthesis of indenone-fused heterocycles **5** trough multi-component reactions of trichloroacetamidine derivatives **3** derived from the addition of various amines **1** to trichloroacetonitrile **2** with ninhydrin **4** (Fig 1). This strategy includes some advantages, such as simple experimental procedures, easy accessibility of reactants, absence of catalyst, high atom economy, and good to excellent product yields. All structures were confirmed by IR, ^{1}H- and ^{13}C-NMR analyses

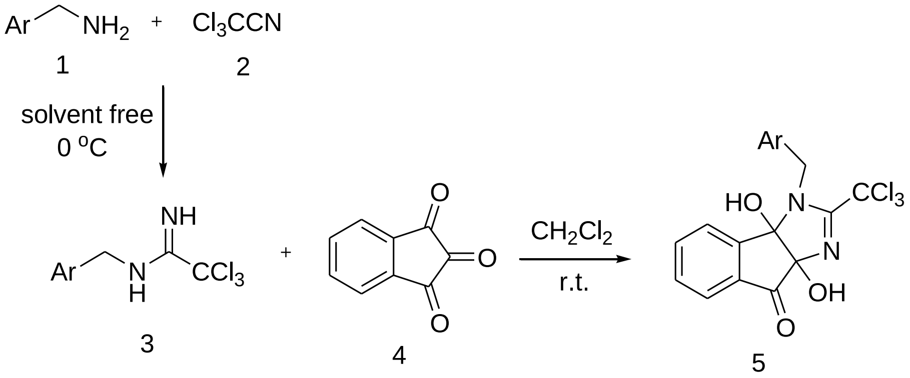

Fig. 1 Synthesis of indenone-fused heterocycles.

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Paper code: 420

Caffeine-based Acidic catalysts for the one-pot preparation of Some Multi-Component Reactions

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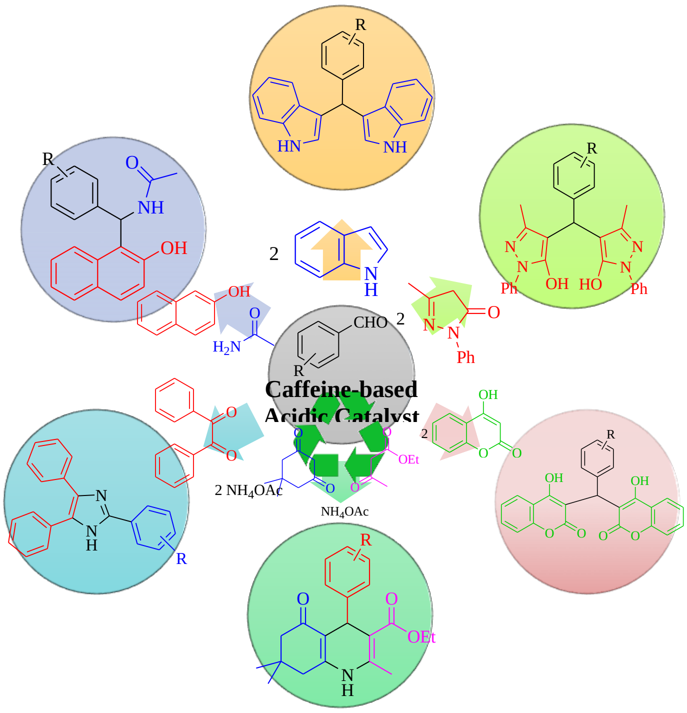
Multi-component reactions (MCRs), has been in the focus of concern recently by organic and medicinal chemists, due to the simplicity and the diversity these reactions provide. Apart from their applications in synthesis, MCRs have been utilized as a criteria for benchmarking novel catalysts. Caffeine-based acidic catalysts including caffeine-H_2SO_4, and caffeine-H_3PO_4 has been prepared and applied for the One-pot preparation of Bis(indolyl) methanes, 4, 4′-(arylmethylene) bis (1H-pyrazol-5-ols), 3,3'-(arylmethylene) bis (4-hydroxycoumarins), 2,4,5-Tri-substituted imidazoles, 1-amidoalkyl-2-naphthols, and Polyhydroquinolines. The Catalysts were characterized with FTIR, ^{1}HNMR, ^{13}CNMR, TGA, XRD and LC-Mass spectroscopy. According to the obtained results, including high yield of the products, short reaction Time, facile separation of the catalyst and easy work-up procedure, Caffeine-based catalysts can be considered as an efficient acidic catalyst for organic transformations [1, 2] (Scheme 1).



Scheme 1. One pot preparation of various MCRs in the presence of Caffeine-based acidic catalyst

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Paper code: 426

Magnetic mesoporous silica supported propyl amine: An efficient catalyst for Knoevenagel reaction

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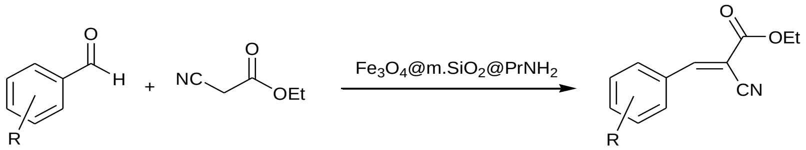
The Knoevenagel reaction is one of the most important method for formation of carbon–carbon double bond between activated methylenes and carbonyl compounds [1, 2]. Traditionally, several homogeneous catalysts such as pyridine, [Bmim][OH], diethyl amine and basic ionic liquids, benzimidazole, piperidine acetate and acetic acid were applied for this process [1-4]. However, these suffer from limitations of non-catalyst recoverability, difficult product separation and harsh reaction conditions. Accordingly, a set of different recoverable heterogeneous catalysts were designed and used for this reaction. In continuous of these studies, herein, a novel amine-functionalized magnetic mesoporous silica (Fe_3O_4@m.SiO_2@$PrNH_2$) is prepared, characterized and applied as an efficient nanocatalyst for the Knoevenagel condensation (Scheme 1). This catalyst was prepared *via* modification of magnetic iron oxide nanoparticles with mesoporous silica followed with treatment with 3-aminopropyl-triethoxysilane (APTES). The Fe_3O_4@m.SiO_2@$PrNH_2$ was characterized using scanning electron microscopy (SEM), vibrating sample magnetometer (VSM), Fourier transform infrared spectroscopy (FTIR) and energy-dispersive X-ray spectroscopy (EDX). This was successfully used as an effective catalyst in the condensation of aldehydes with ethylcyano-acetate to deliver corresponding Knoevenagel products. The recoverability, reusability and stability of the designed catalyst have been also studied under applied conditions.



Scheme 1. Preparation of Knoevenagel products using Fe_3O_4@m.SiO_2@$PrNH_2$ catalyst

References

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Paper code: 427

Nef/Perkow Cascade towards Imidazo Phosphate Derivatives

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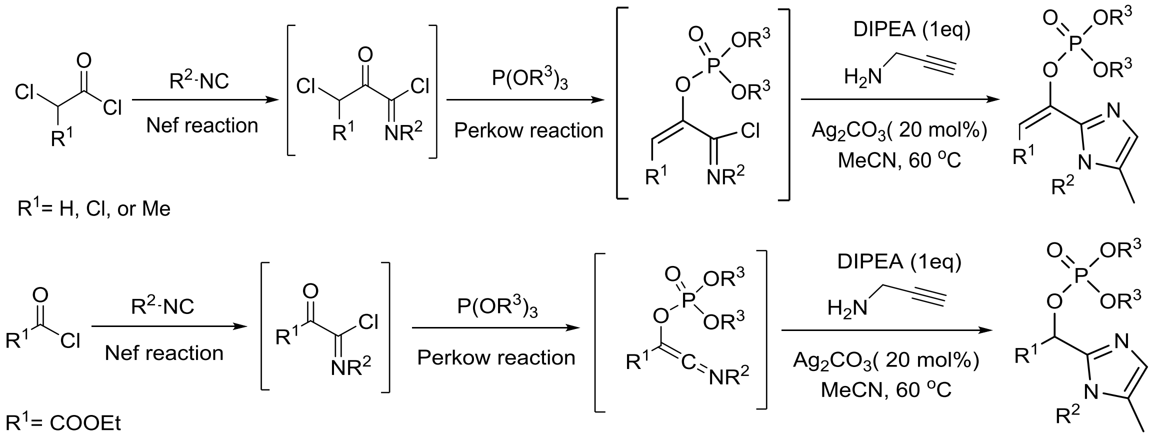
We report an efficient synthesis of imidazolyl vinyl phosphate and imidazolyl phosphate derivatives via a one-pot sequential four-component reaction. The addition of isocyanides to acyl chlorides (Nef reaction) leads to imidoyl chlorides which can later be treated with trialkylphosphites in a Perkow-type reaction [1]. The outcome of this reaction step depends of the nature of the starting acyl chloride.

For acyl chlorides possessing chloride atoms at the 2 position, the vinyl phosphate derivatives are obtained. However for acyl chlorides substituted by esters, the Perkow step leads to the formation of ketenimines phosphates [2].

Vinyl phosphate imidoyl chlorides and ketenimine phosphates obtained in Nef/Perkow sequence may be easily converted to imidazolyl vinyl phosphate and imidazolyl phosphate derivatives under addition of propargyl amine in basic condition and in the presence of silver carbonate as a catalyst at 60 ℃ [3].

We are currently exploring the potential addition of other nucleophiles to these Nef-Perkow phosphate intermediates.



Scheme 1. A one-pot four-component synthesis of imidazo phosphates using a Nef /Perkow sequence

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Paper code: 430

Survey reactivity of some bidentate nucleophile toward 2, 3, 5, 6-tetrafluoro-4-(phenyl sulfonyl) pyridine

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Polyfunctional heteroaromatic compounds are useful systems used to access a wide range of interesting compounds [1]. The introduction of fluorine atoms to heterocyclic systems has an important effect upon the biological and chemical properties of these compounds [2]. Additionally, perfluorinated heteroaromatics are useful scaffolds for the synthesis of a wide range of heterocycles due to their high reactivity toward nucleophilic attack as a result of their electron-deficient nature [3]. The order of nucleophilic attack on pentafluoropyridine follows the sequence 4- F > 2-F > 3-F.8–10 Perfluoropyridines are highly regarded for their synthetic utility.

In this paper, the reaction of 2-benzoxazolinone(**1**) as a model compound, with 4-phenyl sulfonyl tetrafluoro pyridine(**2**) in the presence on K_2CO_3, as a base in CH_3CN under reflux condition gave 2,3-difluoro-4-(phenylsulfonyl)-5aH-benzo[4, 5]oxazolo[2, 3: 2, 3] oxazolo[4, 5-b] pyridine(**3**) in moderate yield.

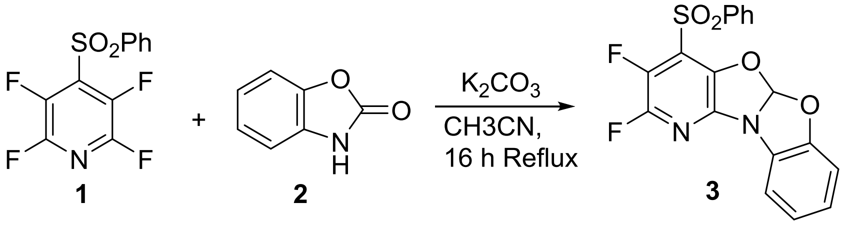

Fig. 1 Reaction of 4-phenyl sulfonyl tetrafluoropyridine with 2-benzoxazolinone

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Paper code: 431

The reaction of three component isoquinoline and dimethyl acetylenedicarboxylate with pentachloropyridine

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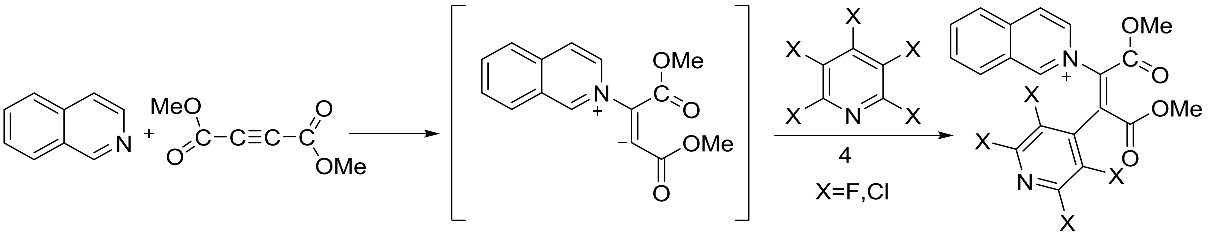
Heterocyclic compounds have occupied an important place in organic chemistry, and their derivatives have attracted considerable interests in recent years for their versatile properties in chemistry and medicine. In the context of the synthesis of novel families of polysubstituted heterocycles with useful biological properties and pharmaceutical applications, perfluorinated compounds, such as pentafluoropyridine, are important materials in organic chemistry and in the life science industries. Pentafluoro- and pentachloropyridines are most susceptible to nucleophilic attack by O-, S-, N-, and P-centered nucleophiles. Perhalogenated aromatic and heteroaromatic compounds are important starting materials for the synthesis of other heterocyclic.

In this work, three-component reaction of isoquinoline, dimethyl acetylenedicarboxylate (DMAD) and perhalopyridines were investigated. Nucleophilic reaction of anion **3**, derived from reaction of isoquinoline with DMAD, with perhaloropyridines gave corresponding products arising from the substitution of the most activated halogen at the 4-position of pyridine ring (Scheme 1). The structure of products were confirmed by IR, ^{1}H-NMR, ^{13}C-NMR spectroscopy data [1].



1 2 3 5

Scheme 1. three-component reaction of isoquinolines, dimethyl acetylenedicarboxylate (DMAD) and perhalopyridines

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Paper code: 442

A One-pot, efficient synthesis of polyfunctionalized 5-hydroxybenzo[a] phenazin-6-yl)-1,3-dimethylpyrimidines by nano-Fe_3O_4/PEG/succinic anhydride

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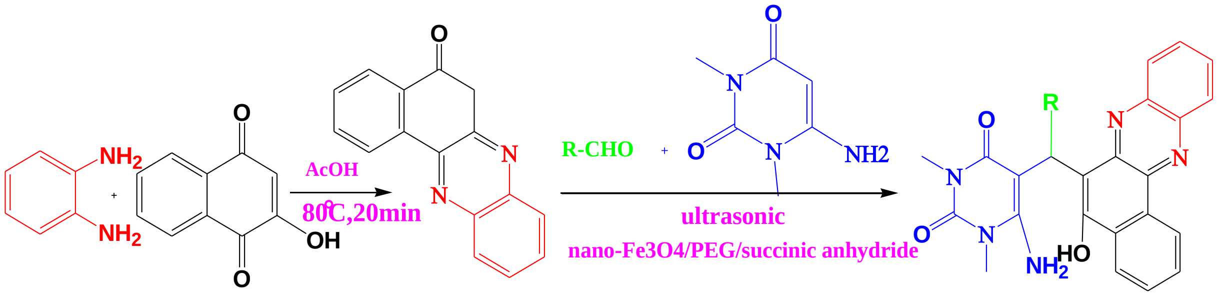
We envisage exploring the multicomponent reactions of 6-aminouracils in "green" solvents. Herein, we describe an efficient protocol for the formation of polyfunctionalized 5-hydroxybenzo[a]phenazin-6-yl)-1,3-dimethylpyrimidines adducts in AcOH by 6-aminouracils.[1]

Recently, magnetic nanoparticles (MNPs) have received significant attention due to their diverse applications in synthesis and catalysis. In the current work, we disclosed a novel methodology for the synthesis of polyfunctionalized 5-hydroxybenzo[a]phenazin-6-yl)-1,3-dimethylpyrimidines adducts by one-pot condensation of aldehydes,2-hydroxynaphthalene-1,4-dione,*o*-phenilendiamin, 6-aminouracils catalyzed by core/shell nano-Fe_3O_4/PEG/succinic anhydride as a magnetic nanocatalyst under ultrasonic irradiation. The remarkable advantages of this methodology are easy work-up, short reaction times, recycling of the catalyst, little catalyst loading and use of ultrasonic irradiation as a valuable and powerful technology. [2,3]



Scheme. Synthesis of of Polyfunctionalized Pyrido[2,3-d] pyrimidine by nano-Fe_3O_4/PEG/succinic anhydride

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Paper code: 443

A facile one-pot green synthesis of piperidines by acidic ionic liquid (4-sulfobutyl)-tris (4-sulfophenyl) phosphonium hydrogen sulfate

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Synthesis of six-membered nitrogen heterocyclic compounds such as piperidines and their analogues is very important owing to their biological activities such as antimalarial, antihypertensive, antibacterial, anticonvulsant and anti-inflammatory agents [1, 2]. Furthermore, green synthesis of these compounds is very important at this time. Ionic liquids are receiving a widespread attention as mediums, because of their unique properties for green chemistry reactions such as a wide liquid range, non-flammability, non-volatile, thermal stability, low vapor pressure, and the ease of handling [3, 4]. Thus, an efficient green and one-pot procedure for the preparation of piperidine derivatives from five-component reactions of aromatic aldehydes, substituted anilines, and ethyl/methyl acetoacetate (molar ratio: 2/2/1) in the presence of acidic ionic liquid (4-sulfobutyl)-tris (4-sulfophenyl) phosphonium hydrogen sulfate as the catalysts at 80°C under solvent-free conditions has been developed [5]. Piperidines were obtained in high yields with simple green procedure and short reaction time (Fig. 1).

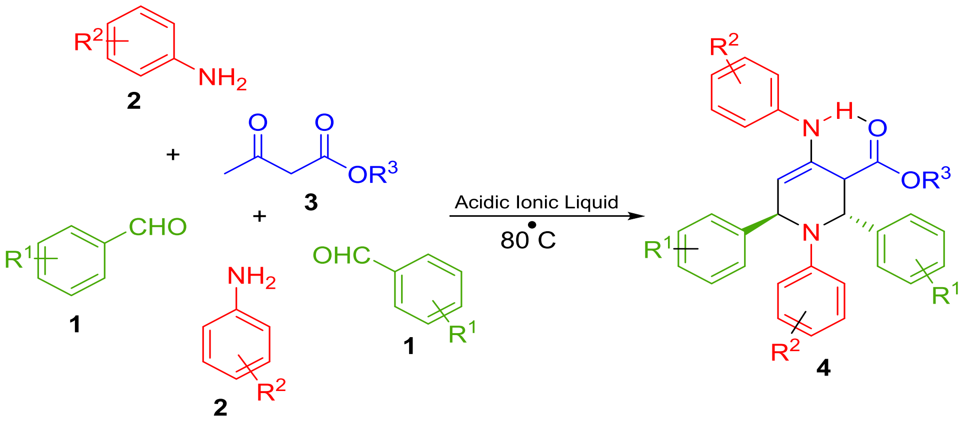

Fig. 1 Synthesis piperidines in the presence of acidic ionic liquid.

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Paper code: 447

A one-pot, efficient synthesis of non-cyclized adducts by aldehydes, 1,3-dicarbonyl compounds, and 6-aminouracils

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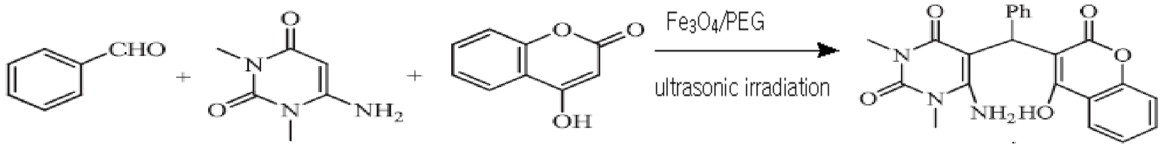
The possibility of accomplishing multicomponent reactions with a heterogeneous catalyst under ultrasonic irradiation could improve their effectiveness from operating cost and ecological points of view. In recent years core/shell nanoparticles have received considerable attention because of their unique properties. In the present paper, Fe_3O_4/ polyethylene glycol (PEG) magnetic composite nanoparticles with a core–shell structure were prepared [1]. A one-pot, efficient protocol for the synthesis of non-cyclized adducts by 6-aminouracils in poly (ethylene glycol) 200/H_2O was described (scheme 2). An interesting family of non-cyclized adducts bearing fused pharmacological active units are prepared. The reaction is free of toxic solvents and catalysts, has simple workup procedure, and has high atom economy, making it more environmentally friendly and suitable for large-scale operations [2,3].



Scheme 1. Synthesis of 6-Amino-5-((4-hydroxy-2-oxo-2H-chromen-3-yl)(phenyl)methyl)-1,3-dimethylpyrimidine-2,4(1H,3H)-dione

References

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Paper code: 449

Unexpected products in the multicomponent reaction of sodium azide, barbituric acid, and arylglyoxal

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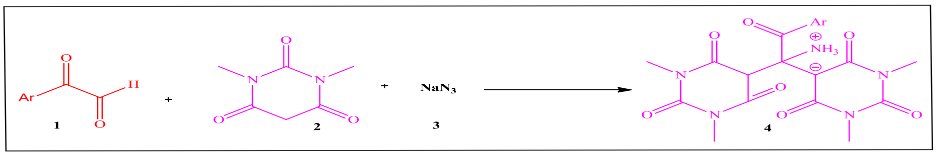
The derivatives of barbituric acid, commonly known as barbiturates, have a special place in pharmaceutical chemistry because of their biological activities such as hypnotic, sedative, anticonvulsant, antimicrobial, anaesthetic, anticancer and antitumor properties [1,2]. Substances of the barbituricacid group have been used thera-peutically for many years. Due to the chemical structure of barbituricacid and its capabilityto make keto–enol form, it has a unique potential to beusedas a valuable building block in various organic reactions. Here we wish to report the result of our study on the reaction of arylglyoxals **1**, barbituric acid **2** and sodium azide **3** in green solvent lead to products **4**. The structures of this products were proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data and elemental analysiss. To a mixture of â-dicarbonyl compound (1 mmol) in ethanol (5 mL), were added arylglyoxal (1 mmol), sodium azide (1 mmol) And room thempreture for 30 min . After removing the solvent under reduced pressure, the crude product was purified by washing with diethyl ether. 5-(1-ammonio-2-argio-1-(1,3-dimethyl-2,4,6-trioxohexahydropyrimidin-5-yl)-2-oxoethyl)-1,3-dimethyl-2,4,6-trioxohexahydropyrimidin-5-ide.Yellow powder Yield: 98%. IR (KBr) (ūmax, cm^{-1}):; 3372 (NH3), 1670 (C=O). 1H- NMR (400 MHz DMSO-d$_6$): δ 2.42 (12H, s, CH_3), 6.02 (1H, s, CH), 7.42 (2H, d, $^3J_{HH}$= 8 Hz, HAr), 7.71 (2H, d , $^3J_{HH}$= 8 Hz, HAr), 10.1 (3H, s, NH_3).



Scheme 1

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Paper code: 450

Survey of reaction between arylglyoxal derivatives, phenyl hydrazine, in the presence Meldrum's acid as catalyst

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The pyrazole cores are one of the most important heterocycles compound, they have been attention in recently years due can be found in many pharmaceutical field (such as the anti-anxiety, antipyretic, analgesic and anti-inflammatory drugs) [1]. Recently, some were reported to have non-nucleoside HIV-1 reverse transcriptase inhibitory activity [2]. Herein, we have developed a highly efficient, catalyst-free and green method for the one-pot three-component synthesis of (Z)-2-(aryl)-2-oxo-N',N''-diphenylacetohydrazonohydrazide derivatives **4** from Meldrum's acid as catalyst **1**, arylglyoxal derivatives **2** and phenyl hydrazine **3** in an environmentally favourable moderate (ethanol) (Fig. 1). The structures of the products were determined by means of IR, ^{1}H NMR, ^{13}C NMR.

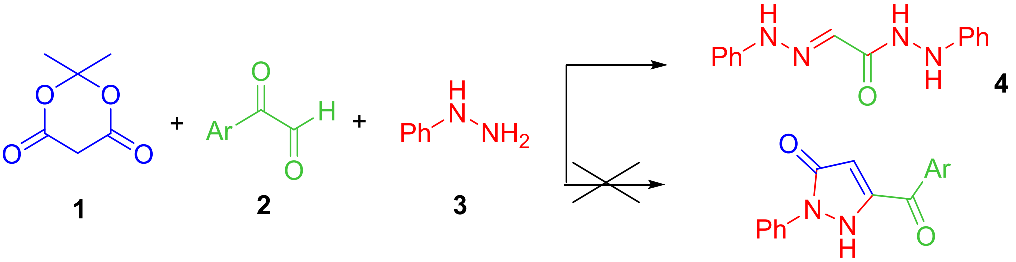

Fig. 1 Synthesis of pyrazole derivatives

References

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Paper code: 452

Investigation of Optical and Solution Properties of Azo-dyes Derived from Ethylacetoacetate and Aromatic Amines

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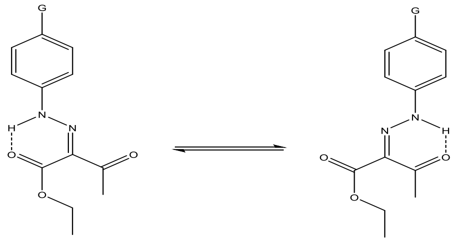
Rotamerism and tautomerism are phenomena being considered as processes of isomerization and proton exchanging between two or more forms, respectively leading to rearrangement of electronic density in whole molecule and therefore, to significant change in spectral and photophysical behavior [1, 2]. Individual rotamers and tautomers can exist in various isomeric forms differing in type of intramolecular hydrogen bonding [3, 4]. Existence of rotameric transformation in azo-hydrazone forms of azo dyes derived from β-dicarbonyl compounds is an interesting example of molecular switching [5].

In this work a series of azo dyes synthesized from benzenoeid aromatic amines and a β-keto-ester were firstly fully characterized by spectroscopic techiques, IR, NMR, and Mass. Due to switchable properties of the synthesized dyes, the effects of the substituents on rotameric equilibrium in solution along with solid state were investigated by Hammet correlation parameters based on their spectroscopic data, UV-vis, IR and NMR spectra, as well as electrochemical properties. Finally, theoretical calculations were carried out to determine the energy barrier of rotameric transformation in gas phase alongside HOMO-LUMO band gas.



G: OH, COOH, Cl, SO_3H, NO_2, Br, NO, NHOH, H, CH_3

Fig. 1 Switching equilibrium between possible rotamers.

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Paper code: 455

Diastereoselective synthesis of spirocyclopropane-linked pyrazolones from azomethine ylides *via* C(sp³)-H activation

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The cyclopropanation reactions of azomethine ylides are generally stereospecific, with the stereochemistry of the dipole and dipolarophile retained in the cycloadduct. In this work, a method has been developed for the generation of azomethine ylides *via* C-H activation of unreactive C(sp^3)–H bonds of 2-methylazaarenes. Molecular iodine-promoted metal-free C–H activation of alkyl azaarenes has been described [1].

Herein, we represent a novel diastereoselective synthesis of spirocyclopropane-linked pyrazolones from arylidenepyrazolone derivatives and azomethine ylides, prepared *in situ* from iodine-catalyzed reaction of 2-methylquinoline or acetophenones with pyridine in the presence of base. These transformations proceeded *via* the cyclopropanation reaction and followed by anti-elimination of pyridine. These methods offer several advantages, such as being inexpensive, moderate to high yield, short reaction time, with-out ligand or metal, ease of product isolation, which make them attractive processes for the synthesis of spirocyclopropane-linked pyrazolone derivatives. The spirans reported in this work may deserve further attention not only from a synthetic but also from a pharmacological point of view.

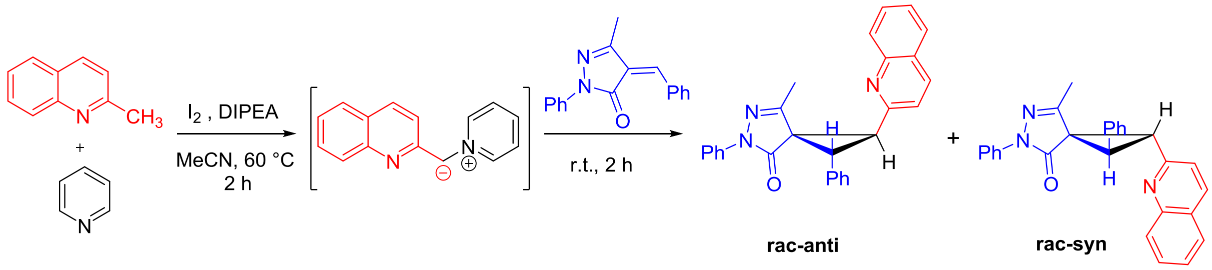

Fig. 1 Cyclopropanation reactions of azomethine ylides and arylidenepyrazolone derivatives.

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Paper code: 463

Synthesis of Thieno[2,3-*b*]quinolin-2-yl methanone Derivatives *via* Sequential Multi-component Reaction

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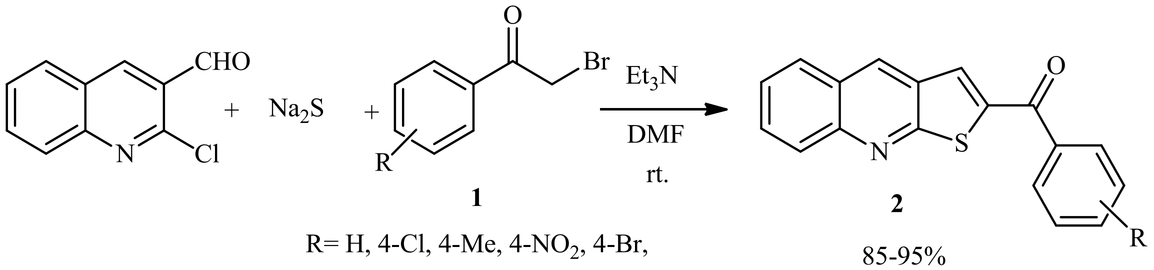
Thienoquinolines are substantial structural units in the domain of medicinal chemistry due to their myriad bioactivities. This class of compounds exhibits a wide array of biological properties including analgesic and anti-inflammatory activities. Some of them are useful as antagonist and antioxidant, memory enhancers, antipyretics, antianaphylactic, high affinity selective 5-HT$_{1A}$ receptor ligands, molluscicidal and larvicidal, and potential antihypertensive agents.

Accordingly, the development of convenient synthetic methods to access such heterocycles prompts us to examine the three-component reaction between 2-chloroquinoline-3-carbaldehyde, phenacyl bromide **1** and sodium sulfide. We used a one-pot sequential three-component procedure for the synthesis of thieno[2,3-*b*]quinolin-2-yl methanones **2** in DMF at room temperature which resulted in the products with excellent yields (85-95%) in short reaction times.



R= H, 4-Cl, 4-Me, 4-NO$_2$, 4-Br,
4-MeO, 3-MeO, 3-Br

85-95%

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Paper code: 473

Isatin: A versatile molecule in our laboratory

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Isatin (1*H*-indole-2,3-dione) has long been captivating scientists for its synthetic utilities and also its essential role responsible for several biological and physiological activities in many organisms. For this reason, we used this compound in our laboratory for the synthesis of oxindoles and spirooxindoles figure 1 [1-4].

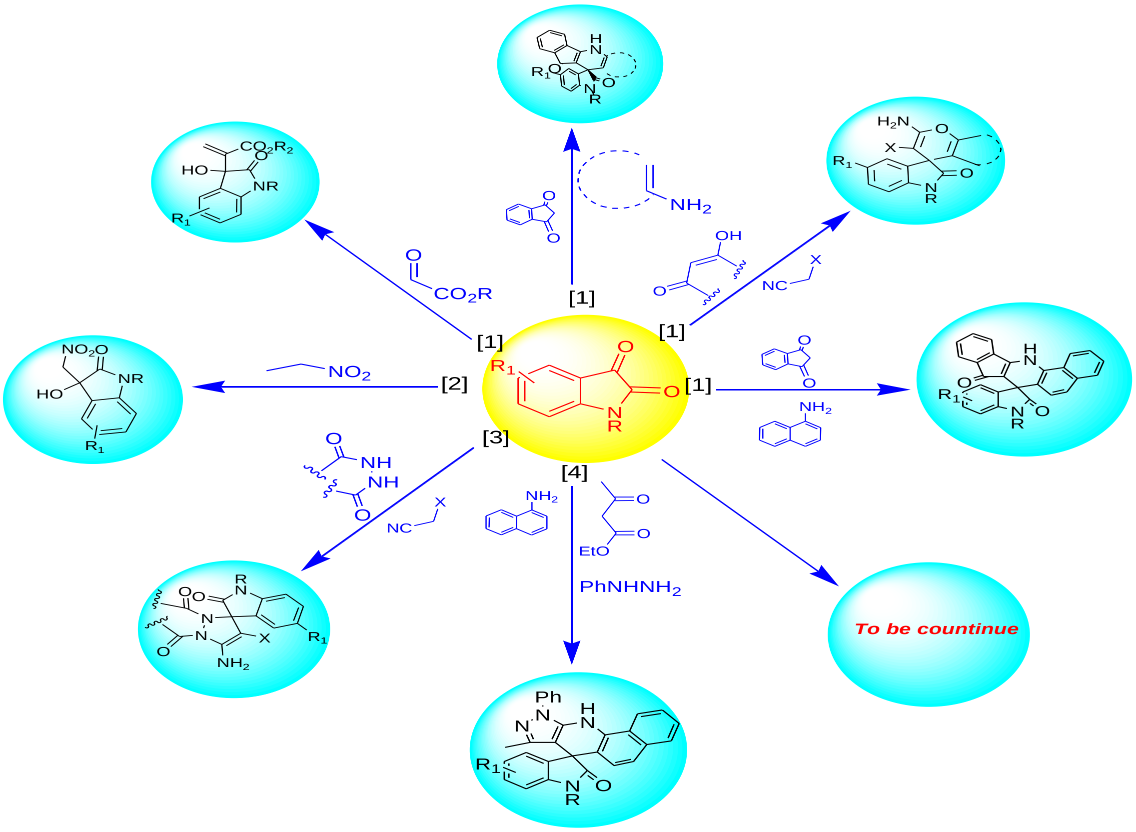

Fig. 1 Synthesis of oxindoles and spirooxindole

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Paper code: 481

Synthesis of various *S*-alkylated derivatives of newly synthesized tricyclic selenium containing heterocyclic system

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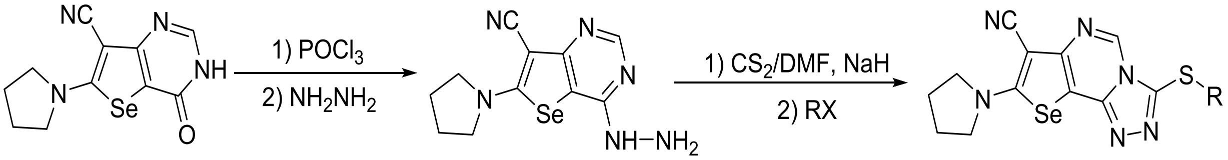
Selenium is a micronutrient essential for mammals. It plays a crucial role in the mammalian defense system against oxidative stress, since it is essential for the activity of glutathione peroxidase (GPx). It is also essential for the activity of various enzymes such as thioredoxin reductase, iodothyronine deiodinase, selenophosphate synthetase and selenoprotein P [1]. Moreover, some organoselenium compounds are known as effective insecticides, microbicides [2], prooxidants [3] and antimycobacterial agents [4].

Due to our interest for the synthesis of selenophens and selenolocondenced heterocyclic systems, in the present protocol, selenopheno[3,2-*d*]pyrimidine **(1)** was synthesized and subsequently treated with $POCl_3$ and hydrazine hydrate to give compound **(2)**. The hydrazinated compound **(2)** on treatment with CS_2 and subsequently various alkyl halides in the presence of NaH in DMF, converted to the corresponding desired *S*-alkylated selenopheno[2,3-*e*][1,2,4]triazolo[4,3-*c*]pyrimidines **(3a-e)**.



(1) **(2)** **(3a-e)**

R: Me, Et, n-Pr, n-Bu, Bn
50-70%

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Paper code: 482

Copper oxide supported on magnetic nanoparticles (CuO@γ-Fe2O3) for addition of amines to carbodiimides toward synthesis of guanidines.

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In this study, copper oxide supported on magnetic nanoparticle was used as an green magnetic nanocatalyst for hydroamination of carbodiimides towards synthesis of guanidines. Easy preparation and separation, Low price, non sensitive to moisture, and reusability of catalyst along with diversity and high yield of the products are silient features of this method.

Recently, we have reported the preparation, characterization, and catalytic evaluation of maghemite supported copper oxide nanocatalyst for the N–H insertion reaction with ethyl diazoacetate. Continuing our works in designing and using magnetic heterogeneous catalysts, herein we have tried to use this magnetic nanocatalyst for addition of amines to carbodiimides toward synthesis of substituted guanidines. Facile preparation of catalytic system from the low cost starting materials, easy separation from the reaction mixture, by using an external magnet, with the ability to re-use and recycling as well as the synthesis of various guanidines under mild reaction conditions are silient features of this procedure.

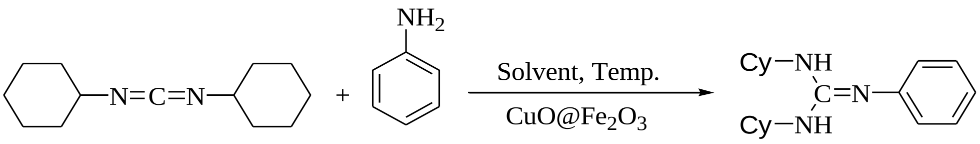

Fig. 1 Reaction conditions: *N,N*-dicyclohexyl carbodiimide, aniline, solvent and magnetic catalyst.

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Paper code: 486

A New Approach to the Synthesis of Acylals Using Nano Sawdust/BF_3 as Green Catalyst at Room Temperature under Solvent-free Condition

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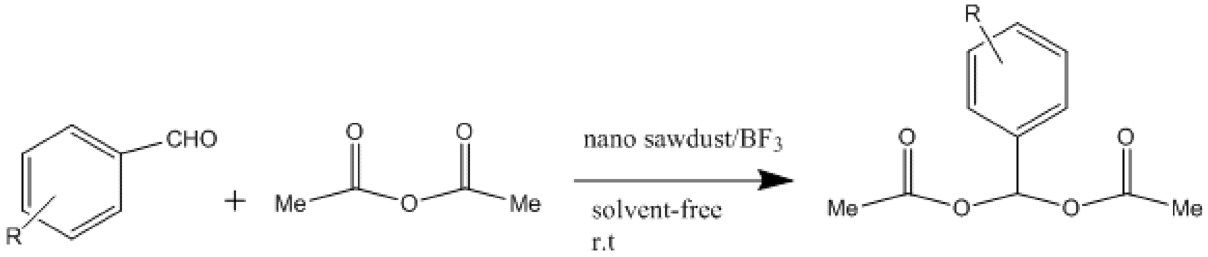
The selective protection and deprotection of carbonyl groups are one of the most important and versatile modern organic reactions [1]. The protection of aldehyde compounds such as acetals and acylals are one of the most important reactions in multi-step syntheses [2]. Among different methods for the protection of aldehyde, geminal diacetates (acylals) are appropriate candidates for this aim. Many methods have been developed for the chemoselective synthesis of 1,1-diacetates using various catalysts such as SiO_2.CTB, Fe_3O_4@SiO_2-imid-PMAn [3]. Herein, we wish report the synthesis of acylals using nano sawdust/BF_3 under solvent-free condition at room temperature (Scheme 1). The advantages of this work are simple work-up, short reaction time and high yeilds. The acylation of various aliphatic and aromatic aldehydes with acetic anhydride were done successfully in the presence of nano sawdust/BF_3 as an eco-friendly and green catalyst.



Scheme 1

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Paper code: 493

Three-component reaction between Indole with Arylglyoxals and amidines

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Indole is among the most important chemical skeletons existing as the main core in the structure of diverse pharmaceutically important compounds. For example indole derivatives involve beneficial estron metabolism promoter [1], inhibitor for human prostate cancer cells and radical scavengers. The primary antitumor screening essay showed that some indole derivatives exhibited the inhibitory activities to some tumor cell growth at relatively high concentration [2, 3]. In this project we report a new and highly efficient method for synthesis of imidazolyl indole derivatives 4 by reaction between indole 1 with arylglyoxals 2 and amidine derivatives 3 in acetonitrile at room temperature in the presence of $FeBr_3$ as a catalyst. The compound 4 can exist in equilibrium with compound 5.

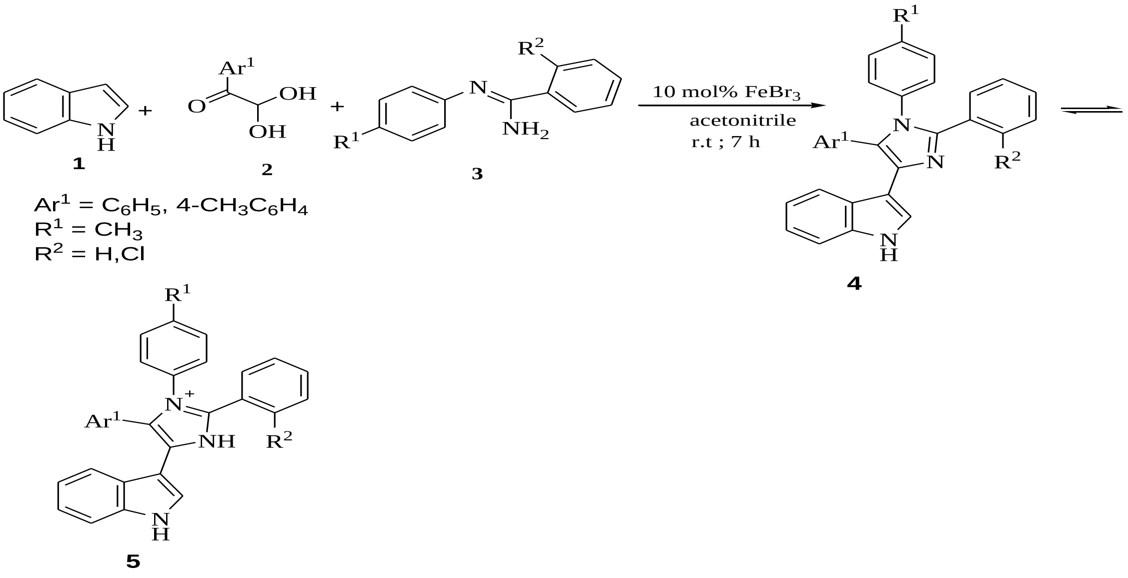

Fig. 1 Reaction between indole, arylglyoxals and amidines.

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Paper code: 494

Reaction of arylglyoxals with acetylacetone in aqueous media: facile synthesis of 3-acetyl-1-argiopent-2-ene-1,4-dione

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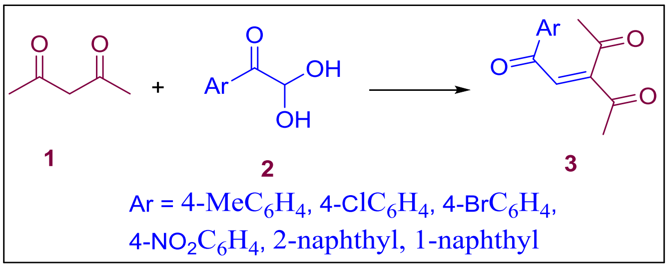
While for a long time water has mostly been banished from organic synthetic protocols, it has recently become popular again as a solvent for synthetic reactions in light of the search for "green" chemical processes. Water is a very cheap and the most environmentally benign solvent, as it is abundant in nature, and nonhazardous (inflammable, nontoxic). It also possesses a strong solvation ability especially for polar and ionic substances. In turn, this also implies that nonpolar substances, which represent the major part of reactants and products for reactions in organic synthesis, are not miscible with water and will cluster or separate to build a second liquid or solid phase. Hydrophobic reaction products can, thus, be easily separated by filtration or phase separation, while polar side products, especially saline products, are carried away with the water phase. In recent years, a surprising accelerating effect has also been observed when reactions between water-immiscible reactants were performed under stirring with water. This effect has led to the new field termed "on-water chemistry [1,2]. Here we wish to report that acetylacetone react with arylglyoxals in aqueous media in the absence of any catalyst to produce 3-acetyl-1-argiopent-2-ene-1,4-dione derivatives in high yields as the only product. Reactions are clean and products are isolated as pure compounds by simple filtration.



Scheme 1

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Paper code: 496

The synthesis of new boronic acid fluorescent chemosensors based on carbazole for sugars

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Biological molecules such as sugars are very important in living systems. They are the main source of energy for our bodies, building blocks for polysaccharides, DNA, RNA, glycolipids, glycoproteins, etc. Therefore, identification and determination of sugars for their monitoring attracts many attentions. Towards that goal, boronic acids have been explored as synthetic receptors for sugars. The boronic acid group interacts strongly and reversibly to cis-1,2-diols of saccharides to form the corresponding cyclic boronate esters [1]. Many fluorogenic units are used for reporting this event. The resulting fluorescent chemosensor has many advantages such as high sensitivity and quick response that leads to various applications in chemical, biological and environmental science. Therefore, many researchers are attracted to synthesize new fluorescent chemosensors for sugars that they are more sensitive and more selective [2]. Anthracene, naphthalimide, pyrene, quinoline and fluorene were employed in the synthesis of fluorescent chemosensors [3].

In our current work to synthesize efficient fluorescent chemosensors for sugars, carbazole was used as fluorophore and different spacers were employed to connect the fluorophore to receptor as illustrated in Fig. 1. The synthesis of desired fluorescent chemosensors will be reported in details and their structures will be characterized by melting point, ^{1}H NMR, and ^{13}C NMR spectroscopy.

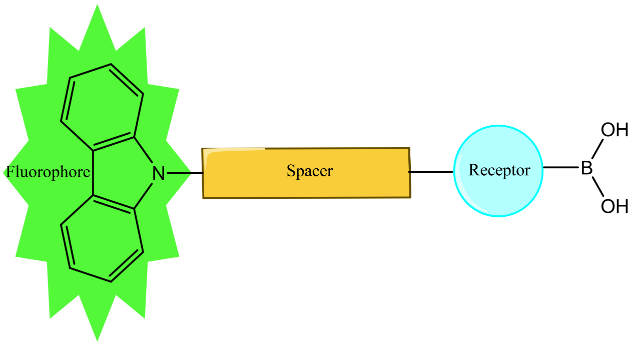

Fig. 1 Carbazole-boronic acid chemosensors

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Paper code: 497

L (+) Arabinose as a catalyst for efficient and simple synthesis of dibenzo [a, c] phenazine in ethanol

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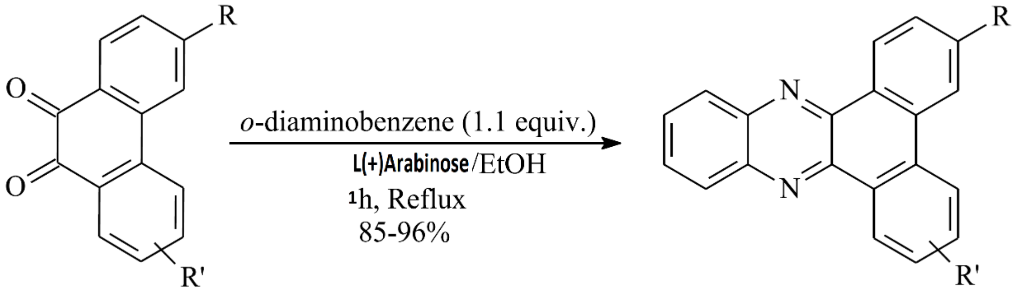
The dibenzo [a, c] phenazine core possesses a phenanthrene ring fused to pyrazine [1]. Phenanthrene derivatives (10a-d) were efficiently prepared in excellent yields and high purity via a one-step sequence [2, 3]. We investigated the possibility of formation dibenzo [a, c] phenazine via condensation of o-diaminobenzene with phenanthrenequinone in ethanol. This reaction is performed in the presence of L (+) Arabinose as a cheap and readily available catalyst at 70°C. A simple and highly efficient procedure for the synthesis of dibenzo [a, c] phenazine is reported (Scheme 1). This method offers the advantages of proceeding, neutral and mild conditions, environmental, lock of toxicity, short reaction time, giving high to excellent yields of the products and simple work-up.



10a-d

11a-d

Product	R	R'
11a	H	H
11b	3-CH_3	H
11c	3-Br	6-Br
11d	3-CO_2CH_3	8-CH_3

Scheme1: Synthesis dibenzo [a, c] phenazine in the presence of L (+) Arabinose as an effective catalyst

References

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Paper code: 498

Synthesis of pegilated and tetrazolo-functionalized mesoporous SiO_2/APTES nano particles as a novel nanocarrier for gene delivery application

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Gene therapy, as a promising therapeutics to treat genetic or acquired diseases, has achieved exciting development in the past two decades. In the main objective in gene therapy is successful in vivo transfer of the genetic materials to the targeted tissues. However, naked therapeutic genes are rapidly degraded by nucleases and show poor cellular uptake, so that the development of safe and efficient gene carriers is one of the prerequisites for the success of gene therapy. Non-viral vectors, such as cationic lipids and polymers, have been developed as gene carrier molecules[1]. The usage of theses nano carriers offer substantial advantages including the prevention of degradation, possibility of delivering high concentrations of gene into tumor tissues, specific targeting, and controlled release[2]. In this regard, the synthesis of a novel nanocarrier based on mesoporous nano silica was reported herein (Fig 1). At the first, SiO_2 nanopartciles were synthesized and then composite by 3-aminopropyl triethoxysilane. The synthesized silica composite was functionalized using glutaraldehyde and 5-aminotetrazole. At the end, the synthesized nanocarrier was stabilized using PEG. The synthesized nanocarrier has shown high application in gene transfection and protection.

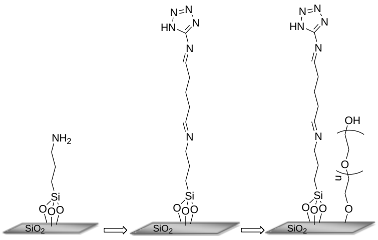

Fig. 1: Synthesis of the novel nanocarrier based on pegilated mesoporous functionalized silica.

References

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Paper code: 500

Synthesize and functionalize of the novel SiO_2/APTES derivatives for applications in enzyme stabilization

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Enzymes are large and fragile protein molecules that catalyze chemical reactions, so over the years, scientists and engineers have found it more difficult to immobilize enzyme catalysts on easily separable supports for use and re-use in a variety of technologies such as industry, medicine, and biotechnology [1]. The need to overcome these so as to take advantage of enzyme activity and specificity and other attractive aspects of enzyme technology has been a major incentive in development of the new biochemistry based on immobilization procedures. Silica-based porous materials, because of their high surface area and tunable pore diameter, are regarded as suitable hosts for large molecules such as proteins [2].

In this regard, the synthesis of a novel nanostabilizer based on mesoporous nano silica was reported herein (Fig 1). At the first, SiO_2 nanopartciles were synthesized and then composite by 3-aminopropyl triethoxysilane. The synthesized silica composite was functionalized using glutaraldehyde and ethylene diamine and was stabilized using chitosan biopolymer. The synthesized nanocomposite has shown well application in enzyme Uricase stabilization and immobilization.

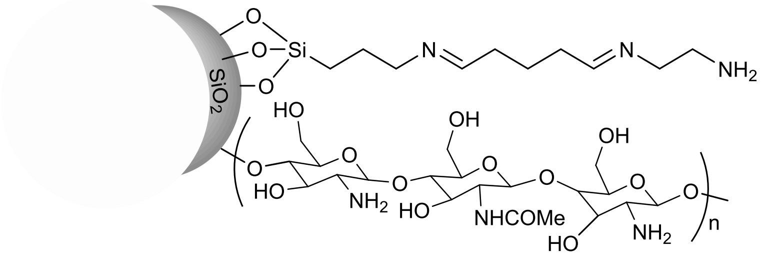

Fig. 1: Schematic structure of the navel nano SiO_2/APTS for immobilization of the enzyme Uricase.

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Paper code: 502

Synthesis and characterization of a new ferrocene-based calix[4]arene as electrochemical sensor

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The design and synthesis of receptors that have the ability to selectively bind and sense neutral and ionic species is a new emerging topical field of supramolecular chemistry. The importance of spatial pre-organization of the complexing groups has been recognized and calixarenes in particular have been developed as structures for the preparation of selective receptors [1]. The versatility of calixarenes has been extensively used as their scaffolds present a hydrophobic aromatic core that can be functionalized easily at both the upper and lower rims [2]. Such receptors are generally achieved through combining well-defined recognition centers with signaling moieties to enable detection of ion binding via optical and electrochemical methods [3].
We present here a ferrocene reporting unit that has been successfully incorporated onto the lower-rim of calix[4]arene through click chemistry. This novel redox-active receptor is expected to be used as an electrochemical sensor to recognize ions with a good selectivity. The new ferrocene-based calix[4]arene was characterized by ^{1}H and ^{13}C NMR spectra. The details of this procedure and characterization of receptor will be reported during the Seminar.

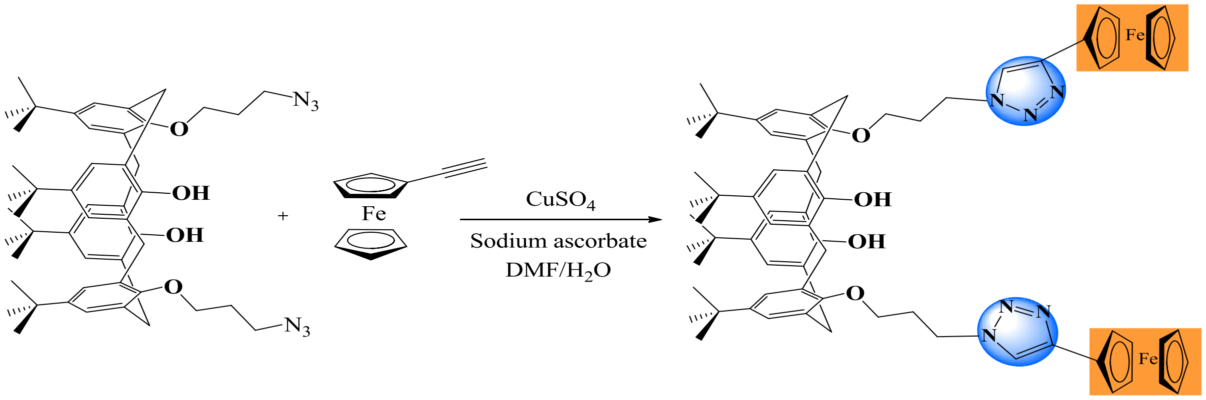

Fig. 1 A new ferrocene-based calix[4]arene as an electrochemical sensor

References

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Paper code: 503

A novel and practical method for the selective synthesis of sulfonyl chlorides and thiosulfonates from thiols using Triazo-Cl-H_2O_2 as well as direct conversion of sulfonyl chlorides to sulfonamides and sulfonates

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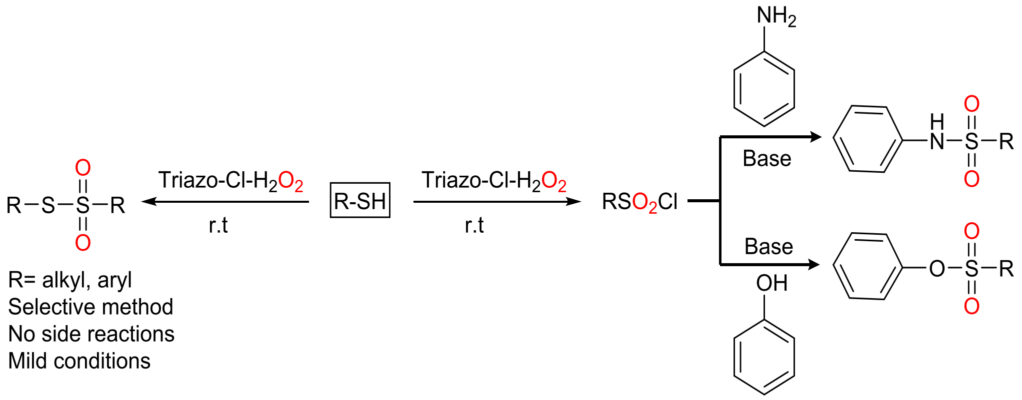
Developing versatile and eco-friendly methodologies that make easy the synthesis of biologically active organic compounds is in great demand. Organosulfur compounds have attracted remarkable attention in recent years [1].

The Triazo-Cl-H_2O_2 as an effective and chemoselective reagent is developed for direct conversion of thiols to sulfonyl chlorides as well as synthesis of sulfonamides and sulfonates. Furthermore, thiosulfonates obtained by changing the Triazo-Cl/H_2O_2 molar ratio. High yields of products, short reaction time, and excellent selectivity are some of advantages of this method.

In continuation to our reported works in this field [2] herein, we describe a new methodology for the oxidative chlorination of thiols using Triazo-Cl in the presence of H_2O_2 as a green oxidant at room temperature (Scheme 1).



Scheme 1: Synthesis of sulfonyl chlorides, sulfonamides, sulfonates and thiosulfonates from thiols

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Paper code: 504

Study on the *peri-* and *stereoselectivity* of cycloaddition reaction of disulfonyl diene with cyclopentadiene by computational methods

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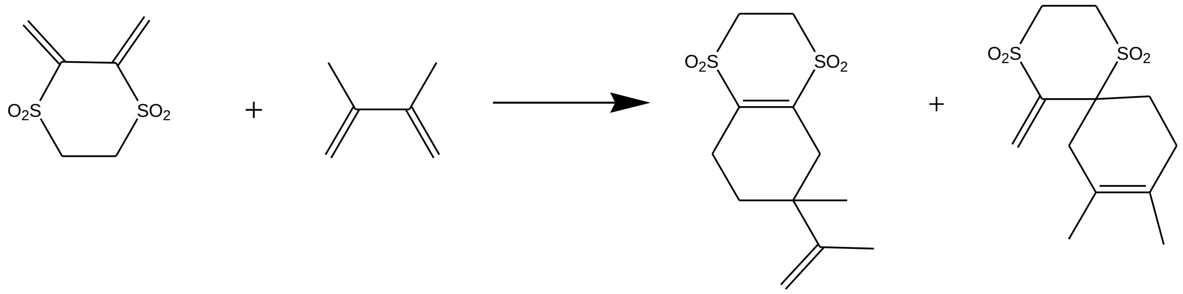
Synthesis and properties of sulfonylated 1,3-dienes have received considerable attention over the years [1]. One of the characteristic properties of these dienes is their dual behavior in [4+2] cycloaddition reactions. They can reacted undergo cycloaddition reactions with a variety of olefins ranging from electron-deficient to electron rich dienophiles [2]. 2,3-(ethylene disulfonyl)-1,3-butadiene (**1**) is a very reactive diene which can react with a number of alkenes in [4+2] cycloaddition reactions. It is important to note that **1** as electron-deficient, readily reacted with both electron-rich and electron-poor dienophiles. The aim of this work was to study the mechanism of *peri-* and *stereoselectivity* of the cycloaddition reactions of disulfone **1** with 2,3-dimethylbutadiene **2** by DFT method at different levels.

Theoretical calculations indicated two pathways for each reactions, *endo* and *exo* which *endo* paths are more reactive than *exo* ones. The disulfone **1** can reacts with 2,3-dimethylbutadiene **2** in [2+4] cycloaddition reaction with the lower energy barrier than [4+2] cycloaddition reaction. The dienophilic character of **1** is more pronounced than its dienic character in these DA reactions. Moreover, an analysis of the reactivity indices and Parr functions for the reactants allows us to provide an explanation of the periselectivity of these cycloaddition reactions.



1 **2** **3** **4**

Fig. 1 The possible regio- and stereoselectivity pathways for the cycloaddition reactions of 2,3-(ethylene disulfonyl)-1,3-butadiene **1** and 2,3-dimethylbutadiene **2.**

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Paper code: 505

DFT study on the mechanism of the cross Diels-Alder of monosulfonyl-1,3-dienes

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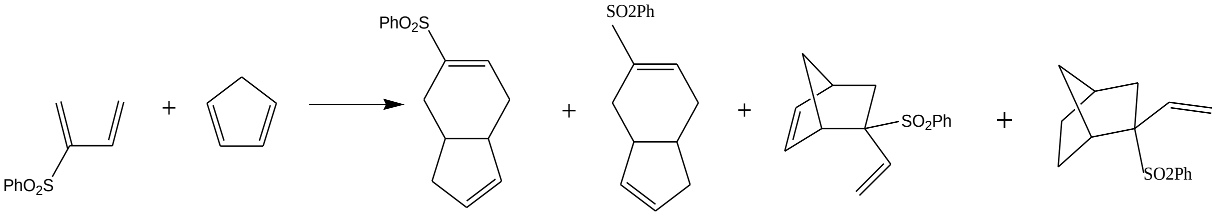
Although the Diels-Alder dimerization reactions of conjugated dienes are frequently observed; the cross Diels-Alder (CDA) reactions between two different conjugated dienes have not been systematically studied [1]. The CDA reactions usually produce mixtures of all possible structural stereoisomeric and regioisomeric cycloadducts [2]. The stereo- and regioselectivity of the CDA reactions can be controlled and only one of the products produced. Herein, the mechanistic details of these reactions, especially with respect to regio- and stereoselectivity, for the CDA reactions of 2-sulfonyl butadiene **1** with cylopentadiene **2** using the DFT method in the gas phase and in solvent were analyzed. Then, some possible cycloaddition reactions that are related to the participation of each reactant of 2π and 4π electrons were proposed.

The calculated energy results indicated that the studied cycloaddition reactions proceed through concerted reaction mechanism with the most asynchronicity. Also, an analysis of the relative energies which were associated with the different reaction pathways showed that the monoulfone **1** in the most stable cycloaddition reactions is reacting as the dienophilic part with the vinyl group on the *exo* face. The steric and secondary orbital orientation overlapping is the reason of this direction.

Moreover, analysis of the conceptual DFT reactivity indices allows the explanation of the reactivity, and the regioselectivity.



1 **2** **3** **4** **5** **6**

Fig. 1 The possible peri- and stereoselectivity pathways for the [2+4] and [4+2] cycloaddition reactions of 2,3-(ethylene disulfonyl)-1,3-butadiene **1** and cylopentadiene **2**

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Paper code: 512

Copper-catalyzed click synthesis of 1,2,3-triazole-linked benzimidazole

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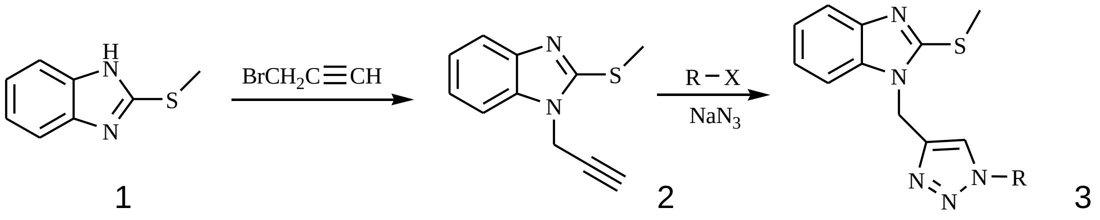
Copper-catalyzed azide-alkyne cycloaddition (CuAAC) reaction, also known as the “click reaction”, has become one of the most important reactions used for the preparation of 1,2,3-triazoles [1]. The 1,2,3-triazoles showed significant antiproliferative against a wide variety of human cancer cell lines, including those that are multidrug resistant [2]. The benzimidazole skeleton is an important class of nitrogen-containing heterocyclic compounds with a significant pharmacological efficiency including the anti-bacterial, and anti-viral properties [3]. On the other hand, when 1,2,3-triazoles and benzimidazole are linked by copper-catalyzed click reactions at the specific ring positions of bi- or tri-heterocyclic containing new molecules, interesting physiological proprieties are observed. Herein, we now wish to investigate a straightforward synthesis of new derivatives of the 1,2,3-triazole-linked benzimidazole *via* the copper-catalyzed click reactions (Scheme 1).



Scheme 1

A mixture of 2-(methylthio)-1H-benzo[d]imidazole (1), K_2CO_3, and propargyl bromide was stirred in DMF for 24h at room temperature. The solvent was evaporated to dryness, the product was washed with water. The resulting solid substance was filtered to afford 2-(methylthio)-1-(prop-2-ynyl)-1H-benzo[d]imidazole (2) in good yield. The click reaction of compound (2) with various alkyl halides, sodium azide, in the presence of 5 mol% of $Cu(OAc)_2$ and 10 mol% of sodium ascorbate at room temperature in ethanole, to afford the compound (3) were obtained in good-to-high yields.

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Paper code: 529

Tannic acid: An efficient catalyst for one-pot synthesis of xanthene derivatives under solvent-free conditions

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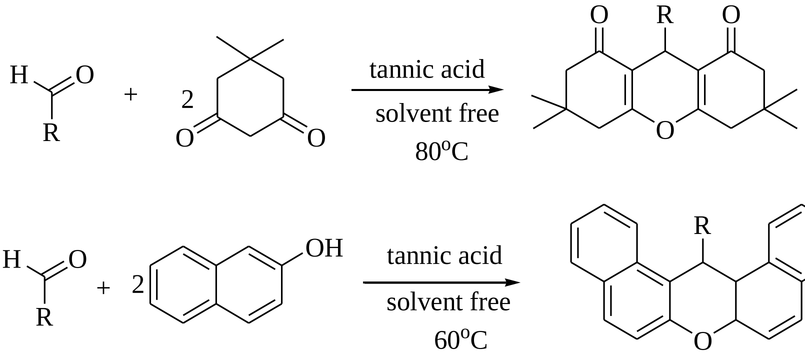
The synthesis of xanthenes is important in organic synthesis because of their wide range of biological and pharmaceutical properties, such as agricultural bactericide activity, anti-inflammatory and antiviral and antibacterial activity. They have also been used in laser technology, used as leuco-dye and fluorescent material for visualization of biomolecules and in laser technologies.[1-5] In recent year, Tannic acid has received considerable attention as an efficient catalyst for various organic transformations such as synthesis of imidazole derivatives, 1-amidoalkyl-2-naphthols and synthesis of benzodiepines derivatives.[6]

In continuation of our interest in the synthesis of heterocyclic compound[7] we report the simple and efficient procedure for one pot synthesis of xanthene derivatives using tannic acid as catalyst in a solvent free reaction (Scheme 1).



Scheme 1. Tannic acid as a catalyst for the synthesis of xanthene derivatives.

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Paper code: 532

Synthesis of poly functionalized pyridine derivatives from sulfonolketenimines, tetramethylguanidine and acetylenic esters

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Pyridines, especially the poly substituted pyridines are among the most prevalent heterocyclic structural units in pharmaceutical and agrochemical targets, as well as in materials science [1]. Ketenimines, as useful intermediates, have attracted much attention due to their diverse chemistry and relative reactivity [2]. Due to the activity of the central carbon atom of ketenimines towards various nucleophiles, they are applied in the construction of heterocycles [3]. Herein, we report a simple and efficient procedures for the synthesis of dimethyl 6-(dimethylamino)-4-(4-methylphenylsulfonamido)-5-phenylpyridine-2,3-dicarboxylate v*ia* the Cu-catalyzed four-component coupling reaction of acetylene dicarboxylates, 1,1,3,3-tetramethylguanidine, sulfonyl azides and terminal alkynes (Fig. 1). The structures of products were characterized by their IR, ^{1}H NMR, ^{13}C NMR and mass spectral data. Various advantages of these transformations will be presented and discussed.

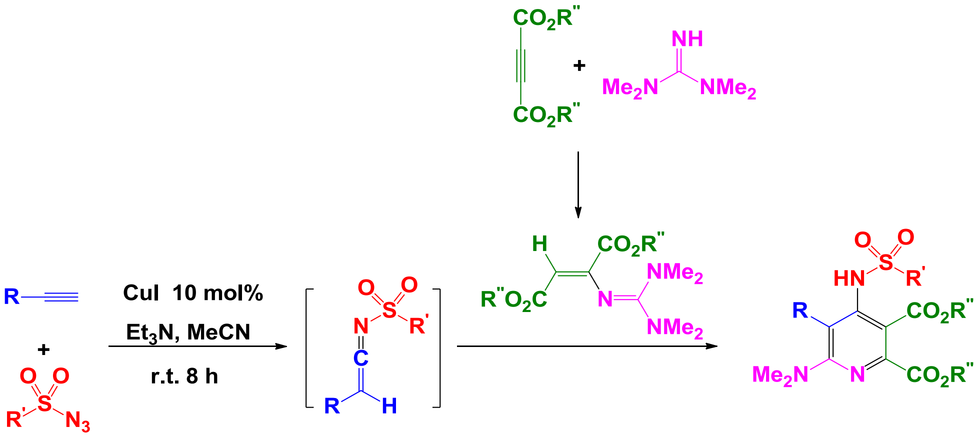

Fig. 1 Synthesis of poly functionalized pyridine

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Paper code: 533

Bronsted acidic ionic liquids: green, efficient and reusable catalyst for synthesis of dihydropyridines

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Sustainable chemistry unarguably is one of our main aims of the twenty first century. Chemists are at the forefront of research in this area, injecting *lots* of *attempts* and experiments to considerably decrease energy, matter costs, wastes and risks. As a consequence, various strategies have been envisioned to simplify elimination of wastes and recycling of catalyst. [1] Meanwhile, ionic liquids recently emerged in the literature as a new kind of green and environment friendly *solvents*. They have also been called to as designer solvents beacuse their properties can be modified by slight changes in the structure, such as the select of the organic cation, inorganic anion and alkyl chain attached to the organic cation. Bronsted acid ionic liquids have their inimitable acidic characters, containing high acid strength and manageable acid density, which have made them well documented. [2]

In this methodology, at the beginning, environmentally friendly Bronsted acidic ionic liquids (BILs) have been synthesised by direct reaction of nitrogen heterocyclic compounds with various acids. Then, syntheis of dihydropyrimidines were investigated through one-pot, three-component reaction between substituted aromatic aldehydes, ethyl acetoacetate and urea (thiourea), using these green solvents at different temperature without any catalyst. The best results were afforded when [MIMH]OAc was used at 100 °C for 5-10 min. *It is worthwhile to mention* that, the products were isolated and no further chromatographic purification was accomplished since no impurities were observed by NMR. Increasing the amount of catalyst, however, did not improve the yield significantly. Further investigation on the temperature effect indicated that high temperature did not reduce the reaction time.

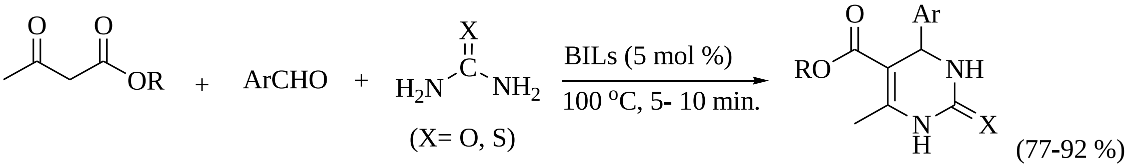

Fig. 1 One-pot, multicomponent synthesis of dihydropyridines in Bronsted acidic ionic liquids

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Paper code: 534

Graphene oxide: An efficient recyclable solid acid for the synthesis of 2-substituted benzimidazoles from aldehydes and diamines at ambient temperature

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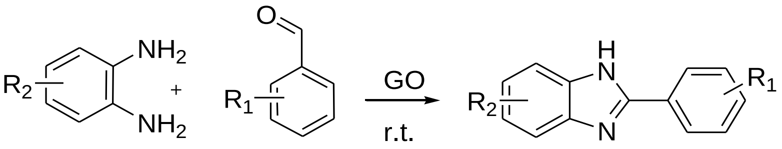
Benzimidazole skeletons are found in numerous pharmaceutical agents and in materials applications [1]. The synthesis of benzimidazoles generally requires the heating of *o*-phenylenediamine and carboxylic acids or their derivatives (nitriles, chlorides, or orthoesters), under strong acidic conditions, sometimes combined with very high temperatures using polyphosphoric acid or by microwave irradiation [2].

In a one neck flask, aryl aldehydes (1 mmol), diamines (1 mmol) and ethanol (5 ml) were mixed with graphene oxide (GO) at room temperature. After completion of the reaction monitored by TLC, GO was filtrated off and the product was appeared as a solid compound after evaporation of ethanol. The desired product was recrystallized by ethanol and identified by Perkin Elmer FT-IR spectrometer and ^{1}HNMR spectra on Bruker DRX- 300 MHZ NMR instrument.

Aromatic aldehydes and diamines were used in the synthesis of 2-substituted benzimidazoles in the presence of GO at room temperature (Scheme 1). High yields, simple and comfortable separate operation provided several special advantages this protocol.



Scheme1. Synthesis of 2-substituted benzimidazole derivatives

This method gives remarkable advantages such as simple work-up procedure, using of the green and inexpensive catalyst with excellent yields

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Paper code: 542

Substituent effects on thermodynamic parameters of new plumbylenes at DFT

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Plumbylenes are the heaviest members of group 14 of divalents whose discovery and characterizations are of great significance [1]. Here, fifty novel plumbylenes are introduced and characterized .A comparison is made between novel acyclic, cyclic-saturated and cyclic-unsaturated diaminoplumbylenes, at DFT B3LYP/6-311++G** level. Study Substituent effects (R) on thermodynamic parameters of new plumbylenes are showed, the nucleophilicity index (N) of all types our structure appear to be inversely proportional to Singlet-triplet energy gaps ($\Delta E_{S\text{-}T}$), and band gap ($\Delta E_{\text{HOMO-LUMO}}$). Our singlet state plumbylenes appear to be more stable than their corresponding triplet states. R effects on *N* of normal and abnormal plumbylenes for every normal acyclic plumbylenes appears more nucleophile than its corresponding abnormal isomer for steric and electronic substituent (R = NH_2, OH, SH, CN, NO_2, Ph, *i*-Pro, *t*-Bu, and Ad). Every abnormal cyclic saturated and cyclic unsaturated turns out more nucleophile than its corresponding normal isomer for R= CN, NO_2, Ph, *i*-Pro, *t*-Bu, and Ad, while every normal cyclic saturated and cyclic unsaturated turns out more nucleophile than its corresponding abnormal for R= NH_2, OH, SH. For all of types our normal plumbylenes, the maximum value of nucleophilicity is related to Function of R = NH2 > Ph > *i*-Pro > *t*-Bu > Ad.

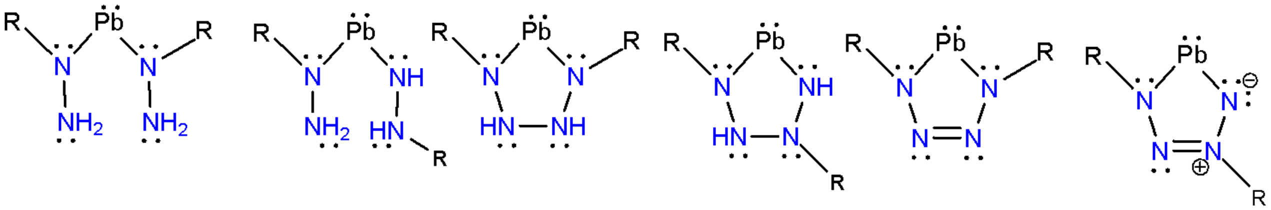

Fig.1 Scrutinized acyclic, cyclic-saturated, and cyclic-unsaturated diaminoplumbylenes, at DFT (R = OH, NH2, OMe, SH, Ph, CN, CF3, NO2, i-Pro, t-Bu, Ad).

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Paper code: 566

Synthesis of pyridine derivatives using a novel nanostructured molten salt catalyst *via* anomeric based oxidation

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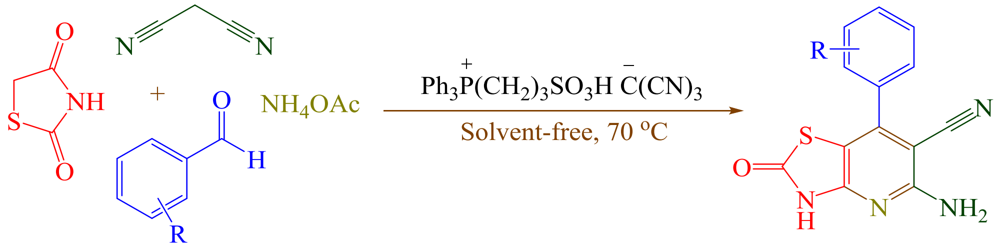
The pyridines, especially the polysubstituted pyridines are significant class of biologically active heterocycles. Most of these pyridines have potential for pharmaceutical activities and could be used as antimalarial, antitumor, antiepileptic, anesthetic, vasodilator, anticovulsant and agrochemicals. 2-Amino-3-cyano-pyridine derivatives were reported as potent inhibitor of HIV-1 integrase and A_{2A} adenosine receptor antagonists. 2-Amino-3-cyanopyridines are substantial and appropriate intermediates in producing a variety of heterocyclic compounds [1-3].

In this report in, in continuation of our recent studies on design and synthesis of ILs, MSs and MCRs, we elicit the synthesis of 5-amino-7-aryl-2-oxo-2,3-dihydrothiazolo[4,5-b]pyridine-6-carbonitriles through a one-pot four-component reaction via anomeric based oxidation (ABO) under solvent-free condition using a catalytic amount a nanostructured molten salt (Scheme 1). The scope and limitations of described methodology will be presented.



Scheme 1: Catalytic synthesis of pyridine derivatives via anomeric based oxidation process

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Paper code: 568

An efficient one-pot three-component synthesis of novel derivatives of pyrido[2,3-*d*]pyrimidines by using nanocatalyst [γ-Fe_2O_3@HAp-SO_3H]

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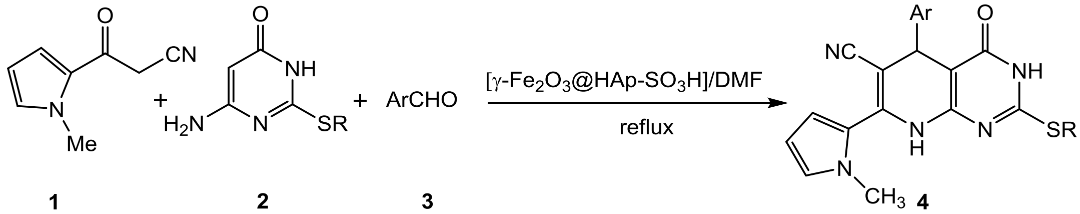
Pyrido[2,3-*d*]pyrimidine derivatives possess wide range of physiological properties, which include antibacterial, diuretic, analgesic, anti-inflammatory, antipyretic, antitumoral [1].

On the other hand 6-aminouracil and thiouracil derivatives find wide applications as starting materials for the synthesis of fused pyrimidines such as pyridopyrimidines. Based on our continued program in developing biologically important heterocycles [2,3]. we report here a convenient and practical method for the synthesis of new derivatives of pyrido[2,3-*d*]pyrimidines by using [γ-Fe_2O_3@HAp-SO_3H] as recyclable nanocatalyst. In this protocol the reaction of 3-(1-methyl-1*H*-pyrrol-2-yl)-3-oxopropanenitrile (1 mmol) (1), 6-amino-2-(alkylthio)pyrimidin-4(3*H*)-one (1 mmol) (2), arylaldehyde (1 mmol) (3) and [γ-Fe_2O_3@HAp-SO_3H] (0.01 g) in DMF (3 mL) was heated under reflux. The reaction furnished the desired products in reasonable reaction times (7-14 min) and high yields (84-90%) (Scheme 1). The structures of all the prtoducts were established by spectroscopic (IR, ^1H NMR, ^{13}C NMR) analysis.



Ar = 4-ClC_6H_4, 4-HOC_6H_4, 4-MeC_6H_4, 4-$CH_3OC_6H_4$, 3-HOC_6H_4, C_6H_5, 2,4-$Cl_2C_6H_3$, 2-$CH_3OC_6H_4$

R = Bu, Pr

Scheme 1. The synthesis of pyrido[2,3-*d*]pyrimidine derivatives

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Paper code: 571

Benzyl methyl morpholinium hydroxide [BMMorph][OH] as an ionic liquid media for efficient synthesis of carboacyclic nucleoside via Michael addition of purine and pyrimidine nucleobases with α,β-unsaturated carbonyl compounds

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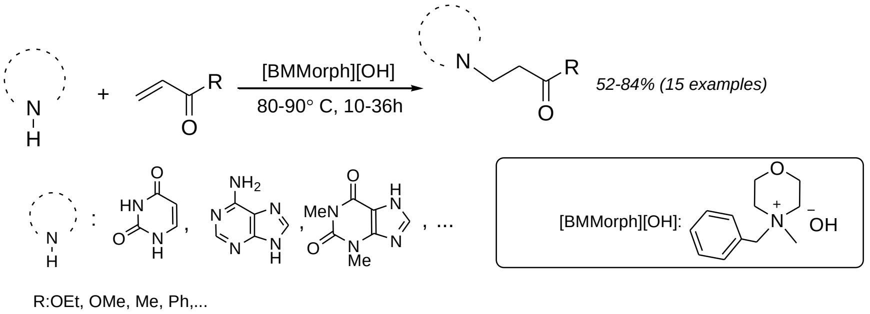
The reaction of nucleobases with α,β-unsaturated carbonyl compounds is significant as this reaction provide a straight and appealing route into carboacyclic nucleoside synthesis [1]. This class of compounds has found particular interest for a variety of biological studies. Moreover, it is demonstrated that some α,β-unsaturated ketones could be served as alkylating agent useful in cancer chemotherapy, as their reaction with electron-rich site of nucleobases by conjugated addition (Michael addition) inhibits DNA replication in tumor cells. One of the most significant aspects of green chemistry is the elimination of hazardous and toxic solvents in chemical synthesis to avoid the generation of waste. In this regard, ionic liquids have proved to be an alternative green reaction media, catalysts, and reagents owing to their unique properties such as extreme of polarity, inflammability, less volatility, high thermal stability, recyclability, negligible vapor pressure and ability to dissolve a wide range of materials. During the past decade, there has been a dramatic increase in employing the recyclable room-temperature ionic liquids (RTILs) as solvent for organic synthesis [2]. In this connection, we have described the synthesis of benzyl methyl morpholinium hydroxide [BMMorph][OH] and its application in Michael-type addition of purine and pyrimidine nucleobases with α,β-unsaturated esters or ketones in good to excellent yields (Scheme 1)



Scheme 1: The Michael addition of nucleobases with α,β-unsaturated esters or ketones in [BMMorph][OH] media.

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Paper code: 572

Benzyl methyl morpholinium ascorbate [BMMorph][Ascorb] as an efficient catalyst and media for 'Click' synthesis of 1,2,3-triazolyl based carboacyclic nucleoside

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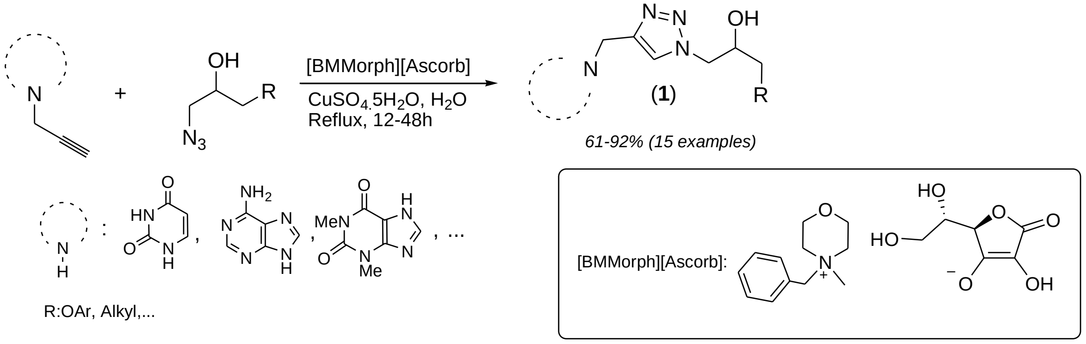
1,2,3-Triazoles are an important class of heterocyclic compounds, that interest in their synthesis stems from their wide range of applications in pharmaceuticals, agro chemicals, dyes, photographic materials, corrosion inhibition, etc. and biological activities such as antiviral, antiepileptic, antiallergic, anticancer, anti-HIV, antimicrobial activities against gram positive bacteria and β3-adrenergic receptor agonist. Due to such multifarious applications different methods have been exploited for their synthesis and amongst them Huisgen 1,3-dipolar cycloaddition of azides with alkynes is the most popular method for the construction of 1,2,3-triazole framework. The incorporation of 1*H*-1,2,3-triazolyl group into a molecular scaffold is an interesting task, since the 1*H*-1,2,3-triazolyl moiety involves remarkable biological activities, as well as recognition by enzymes and receptors in the cell . Moreover, 1*H*-1,2,3- triazolyl cores are known as the non-classical isostere of amide because of having considerable topological and electronic similarities. Given the biological importance of 1*H*-1,2,3-triazolyl cores, they have been extensively used in the design of new nucleosides as surrogate moieties in different fragments of the nucleosides. Hereby, we have described the synthesis of benzyl methyl morpholinium ascorbate [BMMorph][Ascorb] and its application in 'Click' synthesis of 1,2,3-triazolyl based carboacyclic nucleoside (**1**) in good to excellent yields (Scheme 1). In this reaction, [BMMorph][Ascorb] was used to catalyze the cycloaddition reaction of some *N*-propargyl nucleobases or heterocyclic compounds with β-azidoalcohols in the presence of $CuSO_4.5H_2O$ in aqueous media at reflux condition [1].



Scheme 1: [BMMorph][Ascorb] mediated Huisgen's azide-alkyne cycloaddition reaction

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Paper code: 573

Synthesis and characterization of Pd(II) tetradentate Schiff base complex as an efficient catalyst for the oxidative coupling of thiols to disulfides using *tert*-BuOOH

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Conversion of thiols to the corresponding disulfides under mild reaction conditions plays crucial roles in organic synthetic chemistry and biochemistry. On the other hand, disulfides have many industrial applications and are important reagent in organic synthesis [1]. Although, various reagents for the preparation of disulfides from thiols have been reported, however, these procedures have some drawbacks such as low yields, long reaction times and harsh reaction conditions. To improve mentioned problems, various catalytic methods have been developed for the oxidative coupling of thiols to their corresponding disulfides. In this regard, the Schiff base transition metel complexes are attractive catalysts due to their easy synthesis and their thermal and chemical stability [2].

In this work, the tetradentate Schiff base ligand was prepared according to published method [2] and metallated with $PdCl_2$ by the standard procedure of refluxing ethanolic solutions of Schiff base ligand and metal salt in 1:1 molar ratio to obtain complex **1**. The prepared complex **1** was characterized by FT-IR, UV-vis and ^{1}HNMR spectroscopic techniques and elemental analysis (CHN). The synthesized complex **1** successfully applied as a new homogeneous catalyst for oxidative coupling of thiols with *tert*-BuOOH (TBHP) at room temperature (Fig. 1). In order to elucidate the role of the palladium complex as catalyst, the reaction was carried out in the absence of the Pd(II) complex, and a trace amount of the product was obtained. Good yields of the products, mild reaction conditions and no by-products can be mentioned as advantages of this method for the preparation of disulfides.

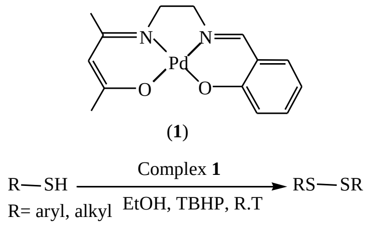

Fig. 1 Oxidative coupling of thiols to disulfides catalyzed by complex **1**

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Paper code: 580

One-pot synthesis of *N*-alkyl 9*H*-carbazole derivatives from alcohols using 1-tosylimidazole (TsIm)

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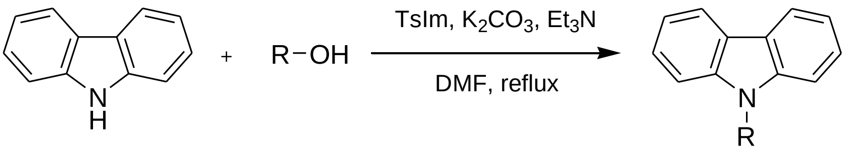
Carbazole and its derivatives are an important type of heterocyclic compounds that are widespread in nature [1]. Carbazoles especially *N*-alkyl derivatives are well known for their biological activities such as anti-inflammatory, anticonvulsant, antimicrobial, antiviral, antitumor, antidiabetic and analgesic activities [1]. In addition, some carbazole derivatives are useful in optoelectronic materials, conducting polymers, and synthetic dyes [2]. The *N*-alkylation of carbazole is usually achieved using alkyl halides, alkyl tosylates, Michael acceptors, and epoxides. Due to the advantageous and attractive strategy of the direct synthesis of carbazole derivatives from alcohols, some limited methods have been developed. Along this line, methods based on Mitsunobu conditions are widely applied [3]. However, this method is accompanied by several drawbacks including: utilizing toxic, expensive, and explosive reagents such as diethyl azodicarboxylate (DEAD) and diisopropyl azodicarboxylate (DIAD); the presence of unreacted PPh_3 and formation of $O=PPh_3$ which requires a tedious work up and cumbersome separation process. To overcome these drawbacks, we wish to report 1-tosylimidazole (TsIm) as an efficient and appropriate reagent for the one-pot synthesis of *N*-alkyl 9*H*-carbazole derivatives using alcohols in the presence of K_2CO_3/triethylamine mixture in anhydrous DMF at reflux condition (Scheme 1). The full optimization of the reaction condition including solvent type, base, and temperature are discussed. This method affords the corresponding *N*-alkyl 9*H*-carbazole derivatives in reasonable to good yields.



R= alkyl, benzyl,allyl, ...

Scheme 1 synthesis of *N*-alkyl 9*H*-carbazole derivatives from alcohols using TsIm.

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Paper code: 586

Factors affecting on the acidic site of prunasin in gas phase, water and DMSO

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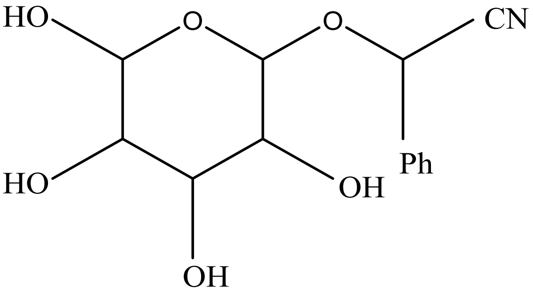
Prunasin (figuer 1) generats in hydrolysis of amygdalin and it has anti caner activity and drug effects [1,2]. Evedently, the p*K*a of a compound directly influences its pharmaceutical profile [3]. This work investigates effects of hydrogen bonding on p*K*a of prunasin in gas phase, DMSO and H_2O. The M06 and B3LYP functional and a suitable basis set, AIM and NBO analyses will be employing also confirm the role of long rang hydrogen bond effect on the acidity of prunasin. p*K*a process with Second-order perturbation stabilization energies ($E^{(2)}$), charge transfer values and relative energy of bond for the intramolecular hydrogen bonding interactions in conjugate bases of acids calculated at the M06 level of theory process was adepted.



figuer 1: Prunasin

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Paper code: 587

Design and synthesis of a gelatin base ion imprinted polymer for selective extraction of Lead ion

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Water pollution by heavy metals is a global environmental issue that has increased through activities such as mine exploitation, industrialization and urbanization all over the planet [1]. Lead has a severe toxicity and is considered one of the most dangerous metals due to brain damage and damage to the nervous system of the kidney and the digestive tract, especially in children. For this reason, the release of heavy metals into the environment is a serious threat to human health and ecosystems [2].

The molecular imprinted polymers represent a new category of artificially produced materials with proprietary identification sites. Since their discovery in 1972, imprinted polymers have attracted the attention of many scientists [3].

In this work, a new Pb(II)-ion imprinted polymer (Pb(II)-IIPs) based on gelatin was synthesized and applied for the selective extraction and preconcentration of Pb(II) ions from aqueous solution. Gelatin and vinyl pyridine as a chelating ligand, methylene bisacrylamide (MBA) as a crosslinking agent and ammonium peroxydisulfate (APS) as an initiator was used. The resulted product, (vinyl pyridine-gelatin/Pb(II)) was characterized successfully. After removing the template Pb(II) ions from polymeric networks, the Pb(II)-IIPs have been achieved (Fig 1).

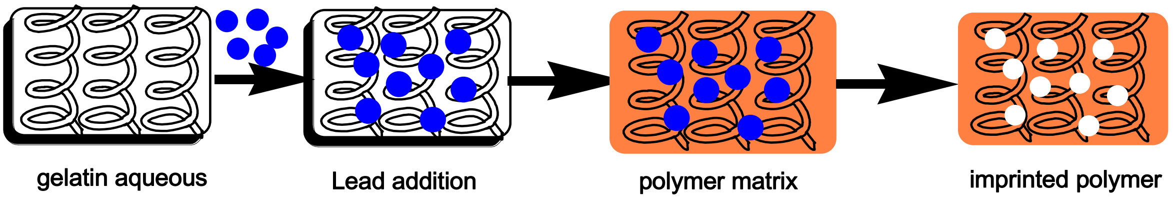

Fig. 1 One pot synthesis of lead (II) imprinted polymer.

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Paper code: 594

Synthesis of dihydropyrimidone-4-one derivatives from amines, phenyl cyanides and acetylenedicarboxylate

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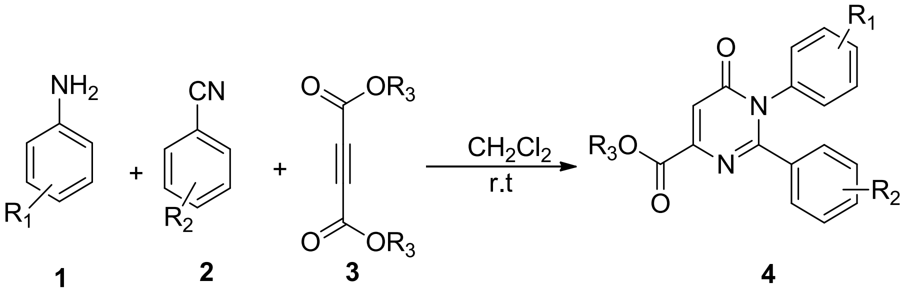
The pyrimidone skeletons exist in the core structure of several biologically active compounds, such as calcium receptor (CaR) antagonist, methaqualone, GnRH receptor antagonist and angiotensin II (A II) receptor antagonist. Evodiamine, amajor quinazolinocarbolin alkaloid isolated from the fruit of Evodia rutaecarpa Bentham, has been reported exhibiting vasorelaxant and cardiotonic effects [1,2]. Although several methods for synthesis of pyrimidone fused pyrimidones derivatives have been developed [3]. Most of these protocols suffer from tedious procedures, poor precursor scopes, and/or low efficiency. Therefore the development of the facile methodologies for the generation of highly functionalized pyrimidone derivatives library is still challenging in organic synthetic chemistry and medicinal chemistry. Here we wish to report the result of our study on the reaction of amines **1**, phenyl cyanides **2** and acetylenedicarboxylate **3** lead to dihydropyrimidone-4-one derivatives **4**. The structures of this products were proved by ^{1}H-NMR, ^{13}C-NMR and IR spectral data.



R_1= 4-OCH$_3$, 4-M, 2-F, 4-F
R_2= 4-H, 2-Cl, 2-Br
R_3=OMe, OEt

Scheme 1: Preparation of alkyl 6-oxo-1,2-aryl-1,6-dihydropyrimidine-4-carboxylate derivatives.

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Paper code: 596

One pot, two-step synthesis of pyrimidine derivatives via arylamins, benzonitriles, benzaldehydes and Meldrum's acid

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Pyrimidines and their derivatives, a type of important N-containing heteroaromatic compounds, were found in a large number of pharmacologically active compounds and natural products such as alkaloids and pharmaceutical drugs, anticancer, anti-inflammatory, antimalarial, antiviral agents [1], [2]. Herein, we describe efficient method to the synthesis of pyrimidine derivatives via appropriate arylamine **1** and benzonitrile **2** and the mixture was stirred at 120 °C for 1h under solvent-free conditions. Then a mixture of appropriate benzaldehyde derivatives **3** and meldrum's acid **4** was stirred in acetonitrile at reflux conditions for 24 h. After completion of the reaction, determined by TLC, the solvent was removed under reduced pressure, and the viscous residue was purified by thin-layer chromatography using n-hexane–ethylacetaat as eluent to give **5** products (Fig 1). All the synthesized compounds were known by ^{1}H and ^{13}C NMR, IR and melting points.

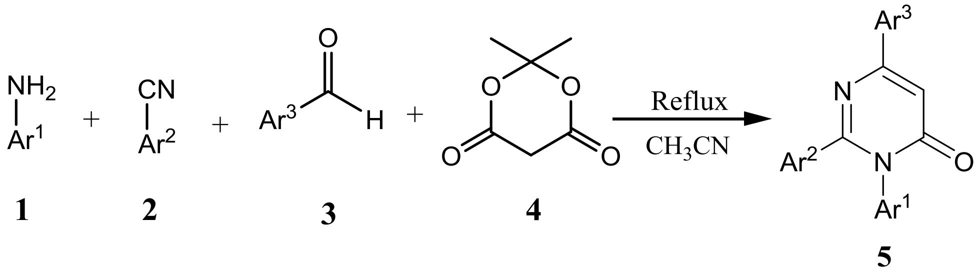

Fig. 1 Synthesis of pyrimidine derivatives

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Paper code: 604

Synthesis and Antibacterial activity evaluation of two 2-Aminothiophene derivatives

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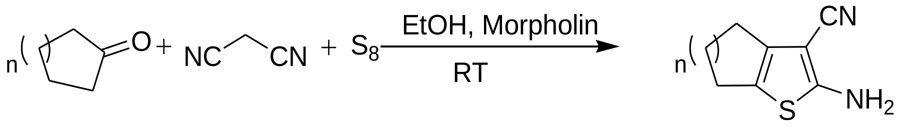
Thiophene derivatives are an important class of heterocyclic compounds, Because of their potential applications in various aspects such as pharmaceuticals, dyes, and agrochemicals. In additions, they are used as antibacterials, antifungal, antioxidant, antitumor, and anticoagulant agents. 2-Aminothiophene derivatives occupy a special position as important intermediates in synthesis because they are found in natural products as novel conducting polymers, and as isosteric replacement for phenyl groups in medicinal chemistry [1,2,3,4]. In this study, first, 2-Aminothiophene derivatives were synthesis using Gewald reaction and then their antibacterial activity was evaluated against three microorganisms using minimum inhibitory concentration (MIC) Method. The structures of the compounds were approved by FT-IR and NMR spectroscopy. According to the results which are shown in the table 1, the synthetic compounds prevented the growth of the all selected bacteria. The highest activity was observed against the Gram-negative bacterium of *P. aeruginosa* with a concentration of 125 µg/mL which is more than that of ampicillin as a common antibiotic.



1a n= 1
1b n=2

2a n= 1
2b n=2

Fig.4 Synthesis of 2- aminothiophene derivatives

Table 1 minimum inhibitory concentration results of 2-aminothiphene derivative

Microorganism	**2a**	**2b**	Ampicillin
Klebsiella pneumoniae	1000^a	1000	250
Escherichia coli	250	250	250
Pseudomonas aeruginosa	125	125	250
Staphylococcus aureus	1000	1000	250

a: Concentration in term of µg/mL

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Paper code: 608

Fe3O4@nano-cellulose/TiCl as an efficient and magnetically nano-catalyst for the synthesis of indenopyrido[2,3-d]pyrimidine derivatives

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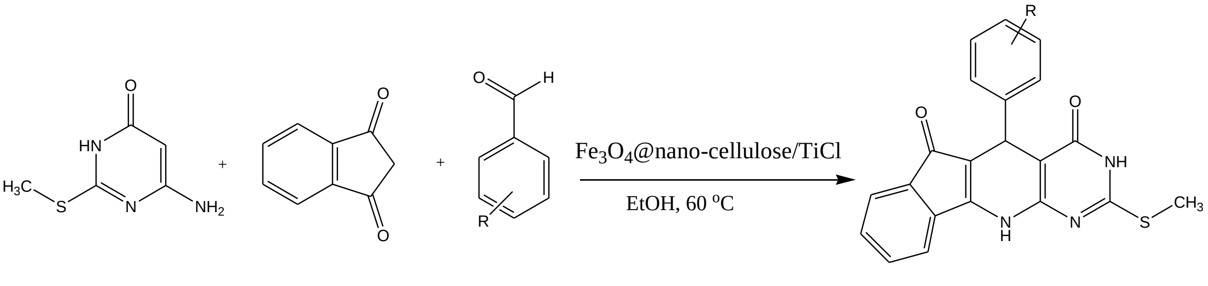
Magnetic core-shell nanoparticles, Fe_3O_4@nano-cellulose, are prepared through in situ co-precipitation of Fe^{3+} and Fe^{2+} ions *via* NH_4OH in an aqueous solution of nano-cellulose [1-2]. Treatment of Fe_3O_4@nanocellulose with $TiCl_4$ leads to the formation of Fe_3O_4@nano-cellulose/TiCl as a novel recyclable catalyst. This catalyst was characterized by FT-IR, FESEM, TEM, XRF, VSM, EDX and XRD. Pyridopyrimidines are nitrogen-bearing heterocyclic compounds which have various pharmaceutical applications. In particular, pyrido[2,3-d]pyrimidine derivatives show variable biological activities such as anticancer agents inhibiting dihydrofolate reductases, antiviral, antihistaminic and anti-inflammatory [3].

In this research, the synthesis of indenopyrido [2,3-d] pyrimidine derivatives has developed via a three component reaction of aldehyde, 1,3- indanedione and 6-amino-2-(methylthio) pyrimidin-4(3H)-one using Fe_3O_4@nano-cellulose/TiCl in ethanol at 60°C (Scheme 1). After completion of the reaction, the catalyst was separated by an external magnet and reused for the next experiment. For more purification of product, solid was recrystallized by ethanol. Several advantages of this protocol are good yields, environmentally benign, easy work-up and moderate reusability of the catalyst. The structures of the products were confirmed by elemental analyses, IR, ^{1}H, and ^{13}C NMR spectra.



Scheme 1. Synthesis of indenopyrido[2,3-d]pyrimidine derivatives in the presence of catalyst

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Paper code: 618

Preparation of Polystyrene Containing Photochromic Functional Group

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The photochromic supramolecular systems based on photochromism have been extensively investigated in recent years. Owing to their excellent stimuli-response properties, photochromic benzospiropyrans are of the most popular dyes, are currently paid notable attention. Spiropyrans have been widely studied for use in data storages, chemical sensors, smart materials, also biological imaging [1]. Because of polystyrene (PS) is a transparent, colorless polymer, it is used extensively for low-cost applications. Polystyrene is a commercially available and versatile polymer, which is used for many purposes such as packaging, consuming goods, and etc [2].

In this work, synthesis of polystyrene, having photochromic properties is studied. To this purpose, polystyrene was functionalized with 5-(Chloromethyl)salicylaldehyde by friedel crafts reaction firstly. The product was obtained by reaction between 1,3,3-Trimethyl-2-methyleneindoline and salicylaldehyde on the polystyrene (scheme 1). The product was characterized by IR and ^{1}HNMR spectroscopy methods, as well as elemental analysis. The photochromic properties of the resulting photochromic functionalized polystyrene were studied by UV-Vis spectroscopy.

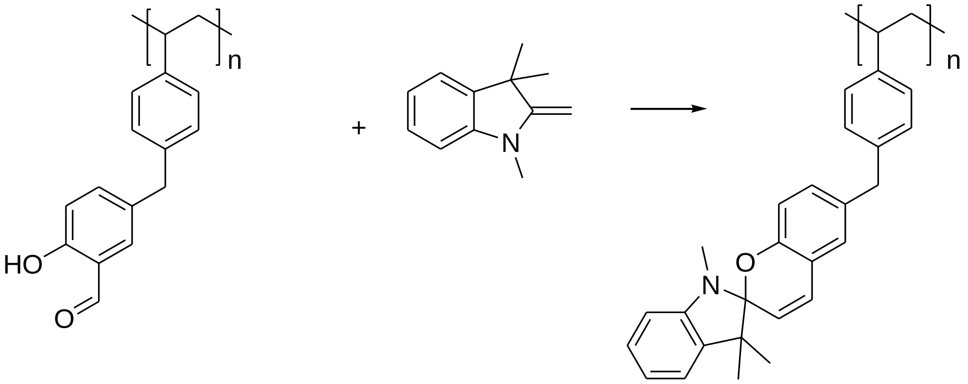

Fig. 1 preparation of photochromic polystyrene.

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Paper code: 621

Preparation of Photochromic polyvinyl chloride

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The spirobenzopyran family constitutes one of the most widely studied photochromic systems owing to their facility of synthesis and potential applications in optical information storage and processing, memory devices, molecular switching, and other emerging technologies [1]. The photochromism of spirobenzopyran is related with a reversible color change between the closed-ring (colorless) spiropyran (SP) structure and the open-ring (highly colored) merocyanine (MC) form [2,3].

Polyvinyl chloride (PVC) was N_3-functionalized firstly. The product was obtained by click reaction of functionalized polymer and photochromic compound (fig 1). The product was characterized by IR and ^{1}HNMR spectroscopy methods, as well as elemental analysis. The photochromic properties of the resulting photochromic functionalized polystyrene were studied by UV-Vis spectroscopy.

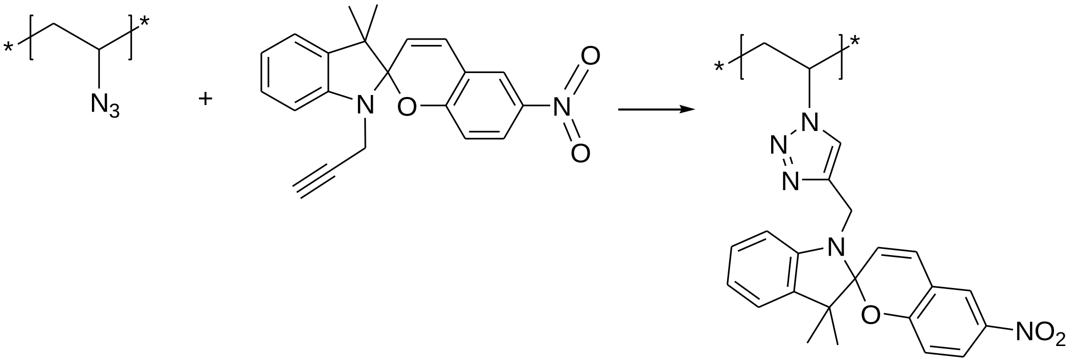

Fig. 1 preparation of photochromic PVC.

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Paper code: 624

Aqua three-component synthesis of new isoxazole-5(4*H*)-ones catalyzed by sodium malonate

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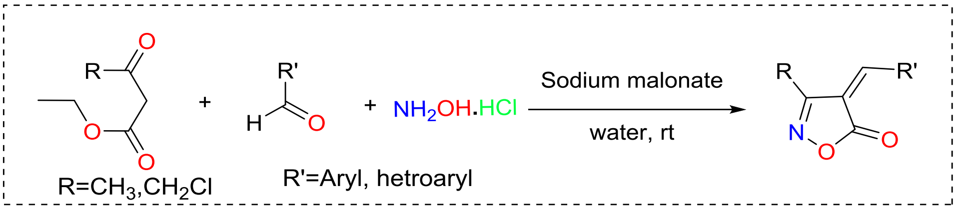
Isoxazoles are known to possess many chemical, biological, and medicinal applications because of their versatile biological activities, including antifungal, antimicrobial, anticancer, anti-inflammatory, and antioxidant. Isoxazoles act as dyes, high-temperature lubricants, light-conversion molecular devices and pesticides. In addition, the isoxazole rings show the power of masked 1,3-dicarbonyl equivalents. These heterocycles are also considered as valuable synthetic intermediates in organic and total synthesis [1-3].

In this work, new derivatives of isoxazole-5(4*H*)-ones were successfully synthesized *v*ia three-component reaction (3-CR) according to Scheme 1. The target heterocyclic compounds were obtained *v*ia this efficient method and green reaction conditions. The structures of the synthesized heterocycles were elucidated by spectral (IR, ^{1}H NMR, and ^{13}C NMR spectra) analysis. Some of the obvious features of this 3-CR is: the use of commercially available catalyst, easy purification processes by a simple filtration, and relatively shorter reaction times.



Scheme 1. The three-component synthesis of new isoxazole-5(4*H*)-ones catalyzed by sodium malonate in water at room temperature (rt).

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Paper code: 630

Highly dispersed Palladium nanoparticle-loaded magnetic catalyst for Suzuki reaction in water

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It is well-known that palladium-catalyzed coupling reactions are very important and powerful methodologies in the synthetic organic chemistry [1]. Among them, the Suzuki reaction is one of the most versatile methods for the synthesis of a variety of biaryls and alkenes via C-C bond formation. Our aim has been to investigate designing of the efficient catalytic system with high activity for Suzuki cross-coupling reaction with minimum by-products in green media. Herein, we report our work on impregnating Pd nanoparticles into epichlorohydrin and aminoguanidine-functionalized Silica coated Fe_3O_4 magnetic nanoparticles as an efficient catalyst for Suzuki reaction in water. Magnetic nanoparticles coated by aminoguanidine were used for selective adsorption of acid dyes from aqueous solution which was reported previously [2]. However, to the best of our knowledge, there has been no report about the heterogeneous magnetic Pd/epichlorohydrin-aminoguanidine (EP-AG) catalyst for Suzuki cross coupling reaction. The FeS-EP-AG-Pd nanocatalyst was prepared in 4 steps: in the first step the Fe_3O_4@SiO_2 magnetic nanoparticles was prepared by Stöber method, in step 2, EP-AG linker as novel designed ligand bonded on the surface of FeS nanoparticles. In step 3, $Pd(OAc)_2$ was complexed to this ligand. Finally, Pd nanoparticles were generated via $NaBH_4$ reduction procedure. A schematic pathway of FeS@EP-AG-Pd catalyzed Suzuki cross-coupling reaction is shown in Fig. 1.

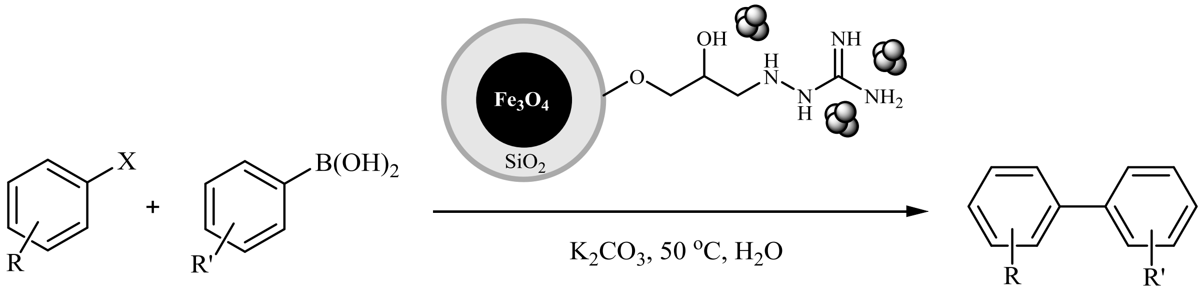

Fig. 1 Studied pathways of Suzuki coupling.

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Paper code: 633

Metal-Free Assembly of Four C-N and Two C-C Bonds: Diestereoselctive Synthesis of Pyrido [1,2-*a*] pyrimidines *via* a FiveComponent Reaction

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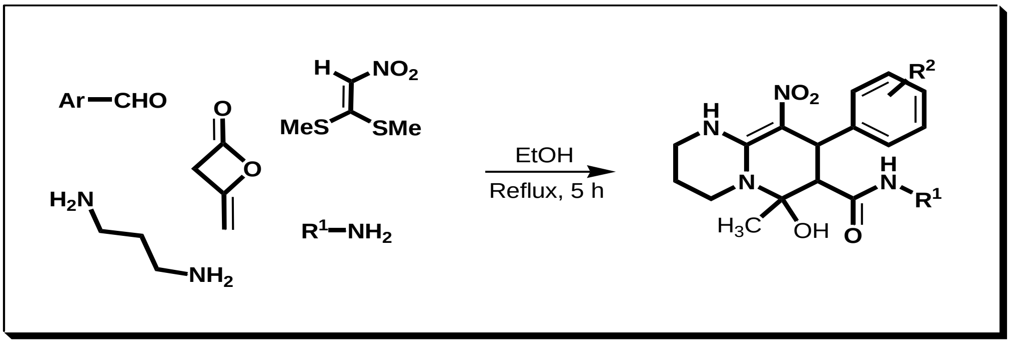
A highly convergent heteroannulation protocol for the synthesis of *N*-fused, pyrido[1,2-*a*]pyrimidines was successfully achieved *via* a one-pot, sequential five-component reaction, utilizing primary amines, diketene, differently substituted aromatic aldehydes, nitro ketene dithioacetal and propanediamine in ethanol at 70ºC. This new efficient domino protocol generates two rings by the concomitant formation of C–N (four) and C–C (two) multiple bonds presumably via a sequential reaction involving, ring-opening/ Knoevenagel condensation, /nucleophilic substitution (SN)/ Michael addition followed by imine-enamine tautomerization and final *N*-cyclization. The merit of this protocol is highlighted by its easily available or readily accessible starting materials, operational simplicity, atom economy, clean reaction profile, and tolerance towards to a wide variety of functional groups. The products were isolated by just decantation of the solvent and for the purification column chromatography was non-required.

Pyridopyrimidines, display a broad spectrum of pharmaceutical applications such as anti-inflammatory, antioxidant, anticancer, antimicrobial, and antiviral and constitute the backbones of several prescribed drugs[1]. In this important line pyrido[1,2-a]pyrimidine structural unit is present in some prescribed and market purchasable drugs, such as the tranquilizer, pirenperone[2], antiasthmatic agent, pemirolast[3], barmastine, and antiulcerative agent.



Scheme1. One-pot domino synthesis of pyrido[1,2-a]pyrimidines

References

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Paper code: 635

Synthesis of MgO nanoparticles supported on ionic liquid-based periodic mesoporous organosilica as a nanocatalyst for the synthesis of novel spirooxindole-furan derivatives

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The catalytic application of a novel MgO containing periodic mesoporous organo silica with ionic liquid framework (MgO@PMO-IL) is described as a highly efficient and recoverable catalyst for the synthesis of novel spirooxindole-furan derivatives via the three-component reaction of 1,3-dicarbonyl compounds, N-phenacyl pyridinium salts and isatin derivatives. The MgO@PMO-IL was prepared and charactrized by diffuse reflectance infrared fourier transform spectroscopy (DRIFT), N_2 adsorption/desorption analysis, transmission electron microscopy (TEM) and thermogravimetric analysis (TGA). The nanocatalyst was recoverd by simple filtration process and successfully reused seven times without any significant decrease in its efficiency. Spirooxindole-furan derivatives were achieved in high to excellent yields with a simple work-up procedure and short reaction times.

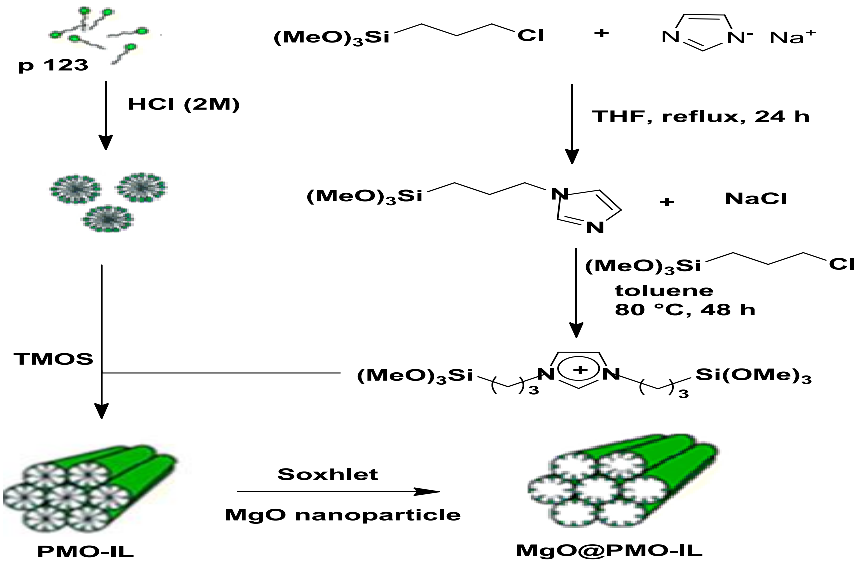

Fig. 1: preparation of the MgO@PMO-IL nanocatalyst

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Paper code: 638

Green synthesis and characterization of Betti bases derivatives by NS-PCS and FHS as the catalyst via Mannich reaction

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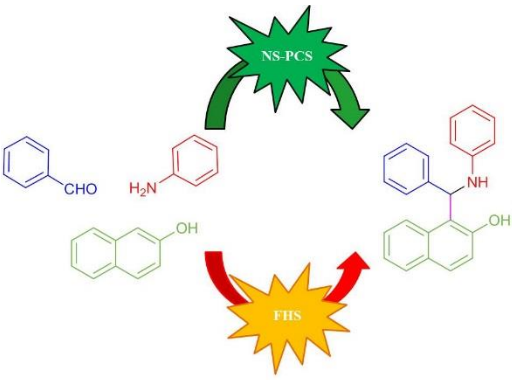
In the current world, issues that pertain to our environment are of especial importance. One of these issues is the pollution caused by chemical compounds during their production process. As a result, finding chemical synthesis methods that are consistent with environmental protocols are also important. Multicomponent reactions (MCRs) are one of the best ways of developing green chemistry. In recent years MCRs have become a vigorous tool for synthesis of complex building blocks of prodrugs[1]. The catalytic performance of the α-aminoalkyl-β-naphthol derivative material, in water as a green solvent has been examined in the synthesis via MCR Mannich reaction of aldehydes, β-naphthol, and amines by porous carbon spheres which doped by Nitrogen and Sulfur (NS-PCS)[2] and Ferric Hydrogen Sulfate (FHS)[3]. The catalysts were easily separated from the reaction mixture and reused for several consecutive runs without significant loss of their catalytic efficiency.



Schem1. Synthesis of Betti base.

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Paper code: 646

The effect of magnetized solvent on rate of oxidation reaction of phenols and aromatic amines compounds by horseradish peroxidase

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For the first time, the rate of oxidation reaction of some phenolic derivatives and aromatic amines in the presence of hydrogen peroxide as oxidant in pure and magnetized water,investigated, by enzyme horseradish peroxidase (HRP). Therefore Pyrogallol, Catechol, Resorcinol, Ortho-phenylenediamine, Para-phenylendiamine (PPD), Ortho aminophenol (OAP), Meta-aminophenol (MAP) and Para-aminophenol (PAP) selected for enzymatic oxidation processes. The reaction performed in the presence and absence of magnetized water under identical conditions completely. It was found that the magnetized water decreases enzyme activity due to the change in its structure. The change of enzyme structure and activity were studied through UV-Vis and fluorsence spectroscopy. The dissolved hydrogen peroxide in magnetized water, as enzyme substrate, reduced enzyme activity toward pure water.

The results indicate that magnetized water affects on the initial rate of oxidation reaction of selective derivative in through the strength change of hydrogen bonds. The initial rate of Pyrogallol, Resorcinol, OAP, MAP and PAP increased and catechol decreased due to getting weaker intermolecular and stronger intramolecular hydrogen bond [1]. The initial rate of OPD and PPD decreased due to hindrance steric and less exposed to the enzyme's active site because of enhancement of molecules level and the average number of hydrogen bonds in each molecule in magnetized water [2]. It is worth mentioning that hydrogen radical is removed from the amine group for radical formation and the initiation of reaction in enzymatic oxidation prcesses of aromatic amines [3].

Table. 1 Initial rate of phenols and aromatic amine derivatives oxidation reaction in pure and magnetized solvents

Initial rate/ substrate	Pyrogallol	Catechol	Resorcinol	OPD	PPD	OAP	MAP	PAP
$V_{0\ \text{pure solvent}}$	20.0×10^{-6}	9.38×10^{-6}	13.70×10^{-6}	3.10×10^{-6}	10.90×10^{-6}	4.01×10^{-6}	2.98×10^{-6}	14.00×10^{-6}
$V_{0\ \text{magnetized solvent}}$	21.40×10^{-6}	6.40×10^{-6}	17.00×10^{-6}	2.17×10^{-6}	8.02×10^{-6}	4.45×10^{-6}	5.20×10^{-6}	25.50×10^{-6}

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Paper code: 658

Reactions of chlorinated pyridines at 4-position: synthesis, structure and reactivity of a variety of tetrachloropyridyl niterene

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Heterocyclic chemistry is, of course, of central importance to the pharmaceutical industry and many commercially important life-science products contain at least one heterocyclic sub-unit within their structures [1]. The chemistry of pentachloropyridine is dominated by nucleophilic aromatic substitution reactions [2]. Pentachloropyridine reacts with nucleophiles in both the 4- and 2- positions. The general rule seems to be that bulky nucleophiles are more likely to attack the less hindered 2- position, whilst small nucleophiles substitute the 4- position in another hand solvent effects is important too [3]. Herein we wish to report the reactivity of aldehydes toward perchloroaryazide (4-azido-2, 3, 5, 6-tetrachloropyridine that was synthesis with sodium azide and pentachloropyridine [7]) in the presence of N,N-dimethyltiourea and DMSO as solvent (fig-1). The structures of compounds were confirmed with ^{1}H-NMR, ^{13}C-NMR and IR spectroscopy.

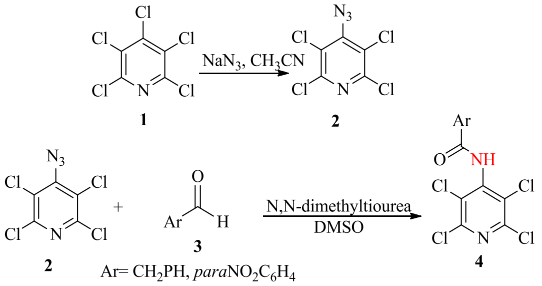

Fig 1-Reaction of Aldehydes with 4-Azido-2, 3, 5, 6-Tetrachloropyridine

In conclusion, we have shown that some N-(perchloropyridin-4-yl) benzamide derivatives could be synthesized from insertion of nitrene result of 4-azido-2, 3, 5, 6-tetrachloropyridine into C-H band of aldehydes. Moreover, **2** may be an excellent starting compound for the synthesis of highly reactive monomeric tetrachloropyridyl derivatives which could not be further identified.

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Paper code: 659

Synthesis of 2-(1-(4-((2-hydroxyarylidene)amino)phenyl)ethylidene) anils

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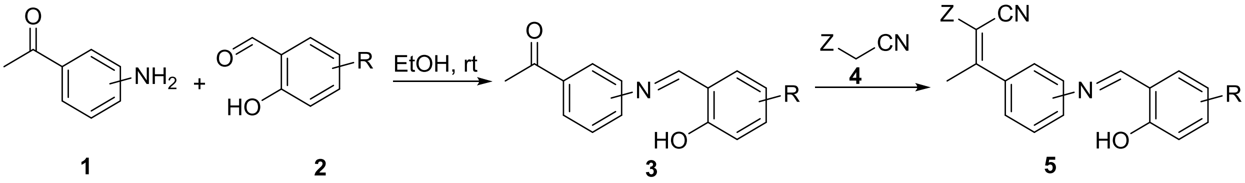
Organic photo- and thermochromic compounds have received particular attention of chemists, due to their potential applications as materials for optical data processing, electronic display systems, optical switching devices, ophthalmic glasses, molecular motors, the second order nonlinear optical (NLO) materials, and biomedical applications [1]. N-Salicylideneanilines (anils, SAs) are among the most attractive photo- and thermochromic compounds because they are used as sensors, optical data storage, and display devices [2]. Also, SAs and their derivatives exhibit solvatochromic and liquid-crystalline properties. In 1909, Senier and Shepheard discovered that SAs exhibited photochromism both in solution and in the solid state [3]. After this discovery, and especially from 1939 onwards, these compounds, which are sensitive to light and heat, have been considered for several reasons, including they are relatively straightforward to synthesize, easy to handle and use in the solid state, resistant to fatigue, and their ability to switch between three different forms (enol, cis-keto, and trans-keto forms). The photochromic and thermocromic process in SAs consists of a reversible tautomerization between enol-form and cis-keto form followed by *cis*-keto to *trans*-keto pedal motion [4]. In this work, the synthesis was successfully achieved *via* two steps according to Scheme 1. In the first step, 1-(4-((2-hydroxyarylidene)amino)phenyl)ethan-1-ones (**3**) were obtained by condensation of aminoacetophenones (**1**) with salicylaldehydes (**2**) in ethanol at room temperature (rt). Then, anils (**3**) were treated with active nitrile compounds (**4**) in the presence of ammonium acetate to afford 2-(1-(4-((2-hydroxyarylidene)amino)phenyl)ethylidene) derivatives (anil-nitriles) (**5**) in good yields.



Scheme 1. The synthesis of anil-nitrile compounds.

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Paper code: 660

A mild Synthesis of Pyrophthalone Derivatives Catalysed by ZnO Nanoparticles under Solvent-free Conditions

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Pyrophthalone derivatives have been proposed as photo semiconductors for the preparation of electrophotographic materails [1]. A study of the electro physical properties of pyrophthalones in thin-film systems [2] showed that pyrophthalone, tetra chlorophyrophthalone, and γ-pyrophthalone have considerable photosensitivity.

Some pyrophthalone derivatives display considerable anticoagulant activity and low toxicity. Antiphlogistic and analgesic action has been found for these compounds [3]. The complexation properties of some pyrophthalone derivatives, imino-pyriphthalone and quinophthalone towards some transition metal ions have been studied.

According to this research we were prompted to develop a general and efficient method for the synthesis of pyrophthalone derivatives starting from phthalic anhydride and pyridine derivatives under solvent-free conditions in the presence of ZnO nanoparticles as catalyst (Fig 1).

We have demonstrated a ZnO nanoparticles-catalysed synthesis of Pyrophthalone derivatives. The cheap ZnO NPs catalysis promoted the condensation reaction in good to excellent yields with broad substrate scope, which provides a promising method for the synthesis of pharmacologically significant Pyrophthalone derivatives.

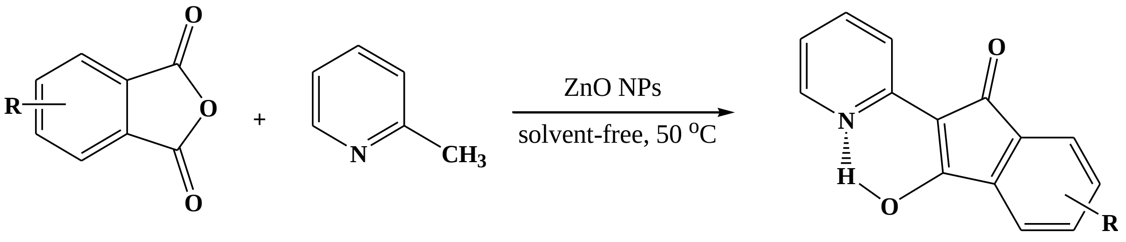

Fig. 1 ZnO nanoparticles catalyzed synthesis of Pyrophthalone derivatives

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Paper code: 661

Survey reactivity of enaminones derivatives with pentafluoro(chloro)pyridine

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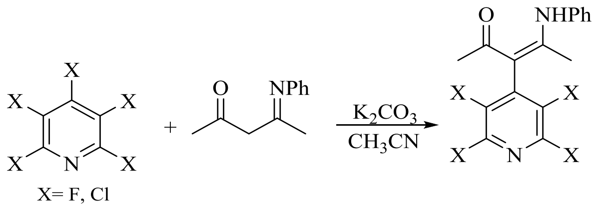
Heterocyclic chemistry occupies an important place in organic chemistry research and ability to vary the properties of heterocyclic [1]. perhalogenated aromatic compounds are a class of heterocyclic that has drawn much attention due to their potentially in organic chemistry, as a building block for the synthesis of other heterocyclic, agrochemical and veterinary products [2], and possess biological and pharmaceutical activities [3]. Here in we tired the optimize reaction condition, while a one pot reaction of pentafluoro(chloro)pyridine and enaminones is achieved. The structures of all the compounds were confirmed by IR, ^{1}H NMR ^{19}F NMR and ^{13}C NMR spectroscopy as well as elemental analysis.



Turning to our attention, synthesis of new substituted pyridine would be planned; proposed mechanism showed EA mechanism, initial attack occurs through carbon atom of enaminones attack to para position of perhalogenated heteroaromatic as electrophile, followed with Meisenheimer intermediates, and products can obtain in good yield.

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Paper code: 664

Cholinesulfuric acid drivatives as an efficient catalyst for reaction of aryl aldehydes, cyclic 1,3-diketones and malononitrile

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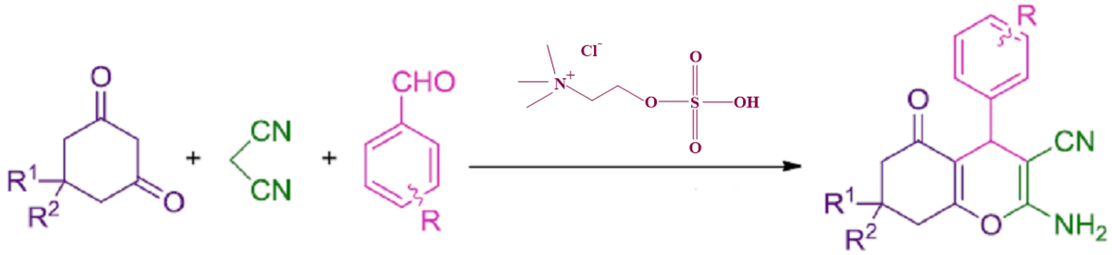
Choline sulfate is a naturally-occurring osmolyte that is synthesized by plants, lichens, algae, fungi, and several bacterial species [1-2]. Cholinesulfuric acid is a biocompatible choline sulfate-based acidic ionic liquid that can be used in organic transformations [3].

Herein we report an efficient and environmentally friendly method for the synthesis of tetrahydrobenzo[*b*]pyrans as important pharmaceutical compounds has been developed using Cholinesulfuric acid as a cheap and readily available catalyst. A mixture of an aromatic aldehyde, malononitrile and cyclic 1,3-dicarbonyl compounds in the presence of the cholinesulfuric acid ionic liquid in H_2O/EtOH resulted in excellent yields of the corresponding products. This new methodology is of interest due to use of aqueous media as a green solvent system, reusability of the acidic ionic liquid catalyst, its short reaction time, high yields and no further purification.



Scheme 1. Three-component reaction for the synthesis of tetrahydrobenzo[*b*]pyrans.

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Paper code: 665

γ-Fe2O3–activated carbon: an efficient nano-catalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-ones under solvent free conditions

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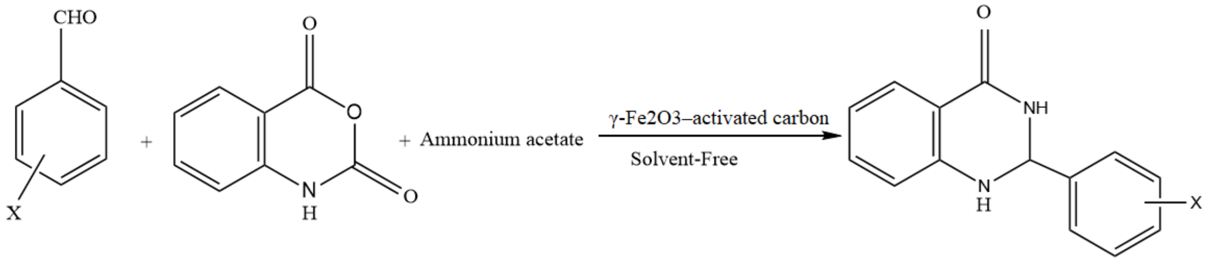
2,3-Dihydroquinazolin-4(1H)-ones are an important class of heterocycles with a wide range of pharmacological and biological activities. A number of synthetic methods to prepare these compounds have been described in the past few years[1-2].
Herein we report an efficient and environmentally friendly method for the synthesis of 2,3-dihydroquinazoline-4(1H)-one derivatives using . γ-Fe2O3–activated carbon as a nanocomposite catalyst. 2,3-dihydroquinazolin-4(1H)-one derivatives can obtained from condensation of isatoic anhydride, aromatic aldehydes and ammonium acetate in good yields. The catalyst can be reused without losing its activity. The reaction completed at 105 °C within 10-40 min with yields of 76-88%. Shorter reaction times and higher yields were chieved under under solvent-free conditions.



Scheme 1. One-pot synthesis of quinazolin-4(3H)-ones catalyzed by nanocomposite

References

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Paper code: 693

Synthesis of new derivatives of pyrazole using three component reactions

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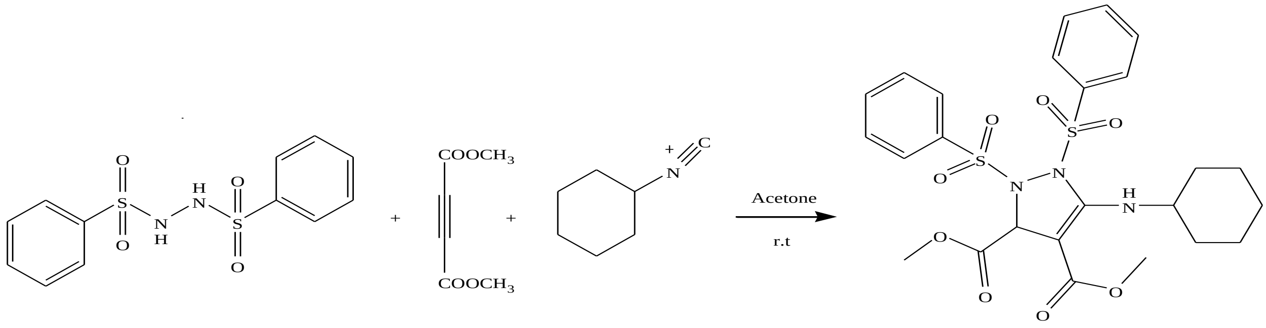
Pyrazole is a five membered and two-nitrogen containing heterocyclic ring. These

structures have been investigated in the development of novel compounds with hypoglycemic, analgesic, anti-inflammatory, antimicrobial, anticonvulsant, antidepressant, antimycobacterial, antioxidant, antiviral, insecticidal and antitumor activities. Therefore, these compounds have been synthesized as target structures by many researchers and were evaluated for their biological activities. It is believed that the bioactivity of pyrazole derivatives will be beneficial for the rational design of new generation of small molecule drugs [1]. Although pyrazoles have been intensely studied for over a century, there is still great demand for novel derivatives with enhanced or unusual medicinal activities to combat various diseases and pathophysiological conditions [2].

In the present study we wish to introduce an efficient three components reaction protocol for the catalyst free synthesis of pyrazole and derivatives by the reaction of 1,2-disulfonylhydrazides **1**, dialkyl acetylenedicarboxylates **2** and isocyanides **3** at the room temperature (Scheme 1).



1 **2** **3**

Scheme 1. Catalyst free synthesis of 1,2- disulfonylhydrazides

References

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Paper code: 703

Magnetically Recyclable CoFe2O4@SiO2/Co (III) Salen complex as a Heterogeneous Nanocatalyst for the synthesis of di-indolyloxindole.

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Di-indolyloxindoles are heterocyclic compounds with biological properties such as anti-inflammatory, antibacterial and laxative effects [1]. From economic and environmental viewpoints, developing novel, efficient and inexpensive catalytic system for the synthesis of heterocyclic compounds specially di-indolyloxindoles is still an important goal in chemistry. Heterogeneous catalysts have been extensively studied as a powerful and extremely versatile synthetic tool to afford selectively heterocyclic compounds [2].

In this study, $CoFe_2O_4@SiO_2$/Co (III) Salen complex was synthesized and used for the synthesis of di-indolyloxindoles in water at 80 ℃. The results showed that the corresponding products were syntrhesized in good to excellent yields**.** This catalyst exhibits good reusability, efficiency, and complies with the concept of “green” chemistry.

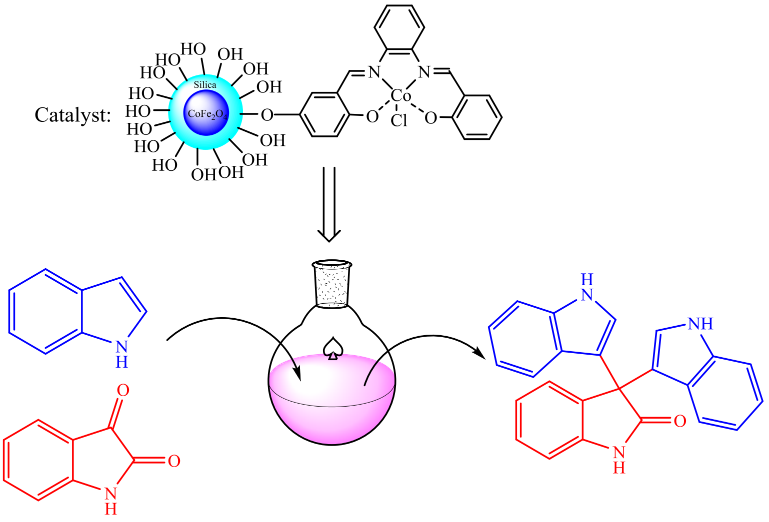

Fig. 1 The synthesis of di-indolyloxindole in the presence of $CoFe_2O_4@SiO_2$/Co(III) salen complex.

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Paper code: 708

Three-component reaction of malononitrile, aldehydes and *β*-naphthol in the presence of Co-salen complex.

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Chromenes compounds are an important class of oxygen—containing heterocycles and medicinal scaffolds which are widely used in the medicinal industries. 2-Amino-4*H*-chromenes have a wide range of biological activities including antimicrobial antiviral, mutagenicity,antitumor, antiproliferative, cancer therapy, antitumor and Central nervous system activity [1]. In a past decade, the synthesis of 2-Amino-4*H*-chromene derivatives is still the subject of extensive research. Many catalyst including homogeneous and heterogeneous catalysts have been applied for the synthesis of these compounds. Metal salen complexes with good catalytic activity can be a good candidate for the synthesis of heterocyclic compounds [2]. Herein, we synthesized Co (III) salen complex anchored onto the surface of $CoFe_2O_4/SiO_2$ nanoparticles. The heterogeneous Co (III) salen nanocatalyst was used in the multicomponent synthesis of aromatic aldehydes, malononitrile and *β*-naphthol in solvent free conditions to give 2-Amino-4*H*-chromene The results showed that the heterogeneous catalysts has excellent catalytic activity and the desired products were synthesized in good to excellent yields.

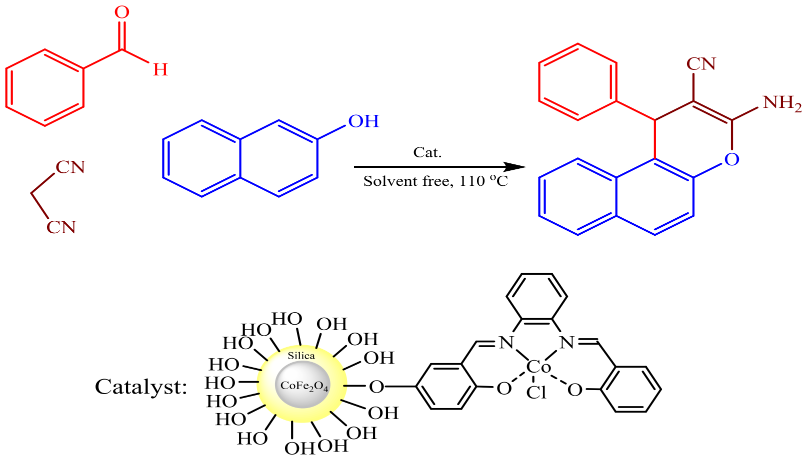

Fig. 1 Three-component synthesis of 2-Amino-4*H*-chromenes.

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Paper code: 717

Synthesis of a novel pyridine-2,6-dicarboxamide as a fluorescent chemosensors for recognition of ions

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Molecular receptors have attracted particular attention during the last decades due to high importance of metal cations and anions complexation in many scopes, e.g. industrial activities, environmental conservation, biochemistry and many others [1]. Ions are essential in nature, but a large amount of them can be harmful to health and environment. Thus molecular receptors (sensors), allowing rapid and selective ion recognition, are highly required. Among molecular receptors, fluorescence sensors appeared so useful for this purpose. To design a fluorescent sensor, a general way is to incorporate a fluorophore and a receptor together. Once the target metal ions bind with the receptors, the electronic structures or the molecular structures of the fluorophores will alter to result in an obvious change in the intensity or wavelength of the emission spectroscopy accordingly [2].

Pyridine-2,6-dicarboxamide-based scaffolds have been extensively used for coordinating varied metal ions. It's believed that the presence of a chelating cavity gives such scaffolds towards metal binding [3]. However, if the chelating cavity could also incorporate with a suitable fluorophore; then scaffolds may offer significant sensing possibilities.

In this work, we present pyridine-2,6-dicarboxamide-based fluorescent probe, offering a chelating cavity that is incorporated with fluorenyl moieties as fluorophores (Fig 1). The synthesis of desired fluorescent chemosensor will be reported in details and their structures will be characterized by melting point, ^{1}H NMR, and ^{13}C NMR spectroscopy.

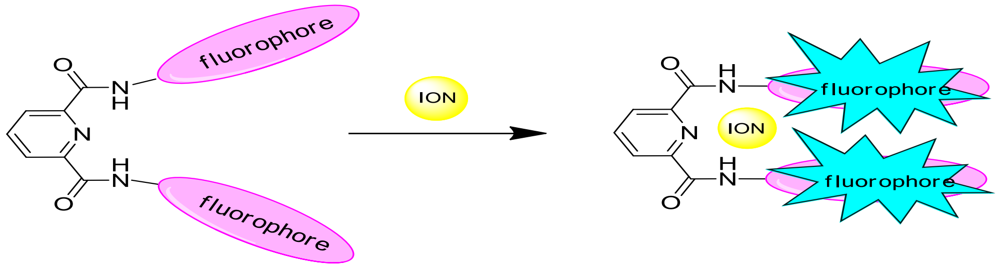

Fig. 1 Pyridine-2,6-dicarboxamide chemosensors

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Paper code: 727

Pd Immobilized on a Nano Worm-like Silica Network Catalyzed Coupling reactions

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Palladium-catalyzed cross-coupling reactions are one of the most important tools for the C-X (X: N, S, O, ...) bond formation. The point of Pd catalysis was highlighted by the award of the 2010 Nobel Prize to Heck, Negishi and Suzuki for their remarkable work in this field [1]. Several challenges like the limited availability and high price and environmental attention make it vital to improve Pd catalysts with the notable properties including the highly active site with excellent recyclability and little metal leaching to reduce the costs and pollutions [2]. Herein, a highly active and stable Pd nano-catalyst was prepared and characterized. Initially, a novel nano worm-like silica network was successfully prepared by a simple sol-gel protocol, then was functionalized by designed ligands and finally palladium immobilized on acceptor bed by a simple method for the first time. The nano-catalyst showed great activities in C-S bond formation reaction. Extraordinary simplicity, mild reaction condition, excellent yields were some advantages of this protocol. More importantly, this catalytic system is capable to use for the gram-scale synthesis of the desired products (figure 1).

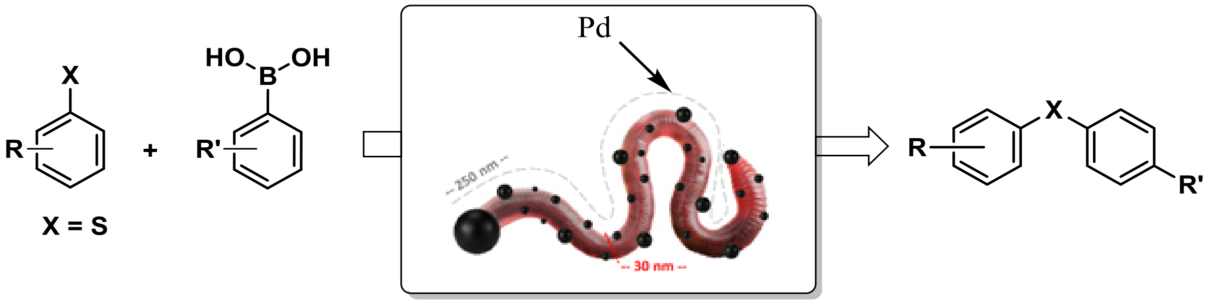

Figure 1. The reactions of aryl halides with arylboronic acids in the presence of the catalyst

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Paper code: 732

Metal modified beta-cyclodextrin (MMC) exhibits high reactivity for synthesis of fused pyrimidines

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In one hand, Cyclodextrins, particularly beta ones, are broadly used in the pharmaceutical field for their ability to increase the solubility and the stability of drugs and small organic molecules by the complex formation at the reaction [1]. Chemistry of Cyclodextrin is quickly becoming one of the major fields of supramolecular chemistry and catalyst. On the other hand, benzo- and hetero-fused pyrimidines are famous because of their interesting properties such as antiviral, antibacterial, anti-AIDS, and antinociceptive activities and there are some methods for preparation of this kind of compounds. However, most of the described methods suffer from disadvantages like long reaction times, poor yields, harsh conditions, the use of expensive reagents, the use of multi-step and cumbersome procedures, and no agreement with the green chemistry protocols. Therefore, development of an efficient, one-step and environmentally procedure for the preparation of fused pyrimidines is desirable [2]. Considering the above facts, in continuation of our investigations on the application of cyclodextrins in organic transformations, we design a novel cyclodextrin catalyst and report a highly efficient and simple method for the synthesis of fused pyrimidines under solvent-free condition.

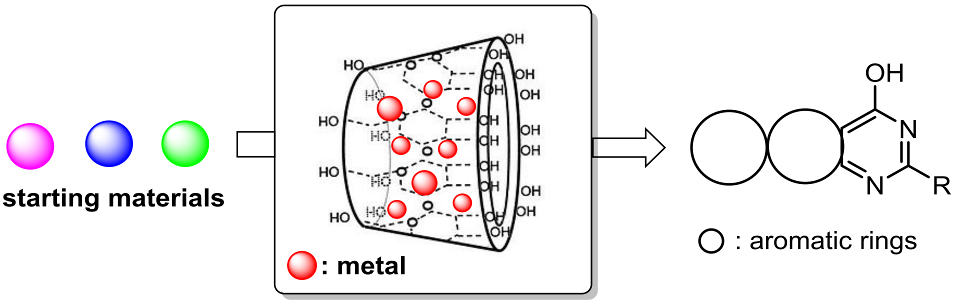

Figure 1. The synthesis of fused pyrimidines with Metal modified beta-cyclodextrin (MMC)

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Paper code: 735

Preparation of an agar-trapped ionic liquid using as catalyst in the synthesis of xanthene derivatives

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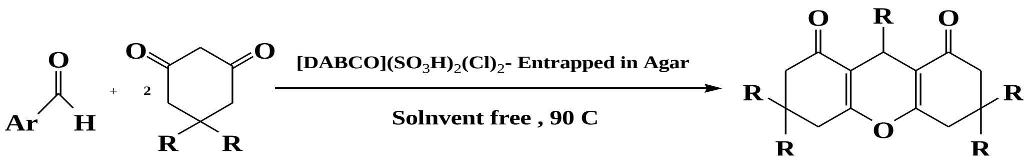
Xanthens are one of the important class of organic compounds that are useful intermediates in organic syntheses. Xanthene derivatives are commonly referred to compounds which are used as a class of dyes which includes fluorescein. Using of ionic liquids to catalyze the synthesis of xanthene derivatives lead to cost-saving procedures which minimize the environmental impacts.

The concept of gel entrapped base catalysts combines the advantages of alkali and organic bases with those of heterogeneous supports. These are prepared by immobilization of alkali or organic bases by entrapping them in an aqueous gel matrix of agar-agar which is a polymer composed of repeating agarobiose units alternating between 3-linked *β-D*-galactopyranosyl and 4-linked 3,6-anhydro-*α-L*-galactopyranosyle units. Their use helps to reduce the amount of bases used and affords facile separation of products from the catalyst. The gel entrapped base catalysts do not absorb moisture on exposure to air and remain intact. Their use in organic syntheses also provides excellent opportunity of recyclability and reusability [1, 2].

In this study the preparation of an agar-trapped ionic liquid was investigated. With entrapping the ionic liquid, we try to decrease the moisturize absorption in the catalyst. After preparation, the agar-trapped ionic liquid was employed as novel catalyst in the synthesis of xanthene derivatives in a straightforward procedure under solvent-free conditions (Scheme 1).



Scheme 1. Synthesis of xanthene derivatives in agar-entrapped sulfonated DABCO

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Paper code: 736

Catalytic Trimethylsilylation of alcohols and phenols by tribromoisocyanuric acid (TBCA) under mild and solvent free conditions

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Protection step of active protic functional groups are frequently required in the synthesis of multifunctional compounds. The replacement of polar O–H bonds in alcohols and phenols with the O–Si linkage is of great importance across the chemical sciences. The silylation of hydroxyl groups to their corresponding trimethylsilyl ethers is a useful methodology in organic synthesis and materials science [1]. Among the various protecting groups used for hydroxyl function, the trimethylsilyl group is one of the popular methods. Several methods have become available for trimethylsilylation of the hydroxy functional group using a variety of silylating agents.1,1,1,3,3,3-Hexamethyldisilazane (HMDS) as a cheap, stable and commercially available material is one of the reagents that is used for the silylation of alcohols [2,3]. In continuation of our studies on catalytic application of N-halo compounds as organocatalyst in organic chemistry, we decided to report the catalytic application of tribromoisocyanuric acid (TBCA) as a new source of Br^+ for the efficient silylation of a wide range of hydroxyl compounds under mild and solvent-free conditions (Figure 1).

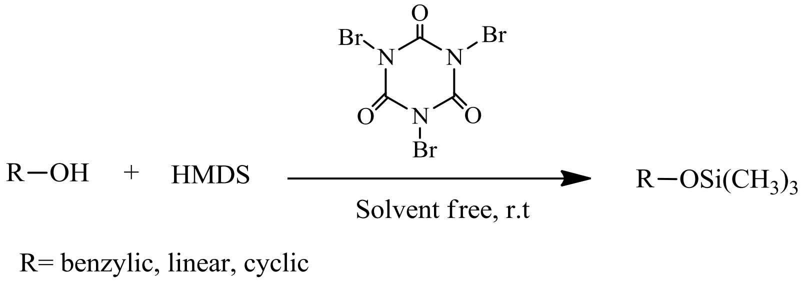

Fig. 1 Trimethylsilylation of alcohols and phenols by HMDS in the presence catalytic amount of TBCA

In order to show selectivity of this catalytic system, we tried several competitive reactions under similar conditions. The result shows that, the primary alcohol was completely converted to the corresponding trimethylsilyl ether, while 0% conversion was observed for the tertiary alcohol. Excellent selectivity was also observed for secondary alcohols in the presence of a tertiary alcohol. Similarly, this method showed excellent selectivity for the trimethylsilylation of phenol in the presence of aniline or thiophenol.

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Paper code: 739

Introducing an efficient method for preparation of 2,8-bis(methylthio)-5-propyl-5,10-dihydropyrido[2,3-d:6,5-d']dipyrimidine-4,6-diol (L)

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Hetero-fused pyrimidines are famous because of their interesting properties such as antiviral, antibacterial, anti-AIDS, and antinociceptive activities [1]. Folate metabolism has long been known as a target for cancer chemotherapy because of the essential function of fused pyrimidine antifolates as antitumor agents [2]. A number of cardiocirculatory disorders were observed by atherothrombotic coronary artery diseases, such as unstable angina (UA), myocardial infarction (MI), or acute stroke associated with deep vein thrombosis (DVT), is one of the most major causes of death worldwide. The significance of fused pyrimidines as antiplatelet and antithrombotic drugs has been strongly built by clinical trials. Thus, additional investigation of pyrimidine chemistry looks to be worthwhile. In the present study, we report the synthesis of fused pyrimidines L with propyl side chain.

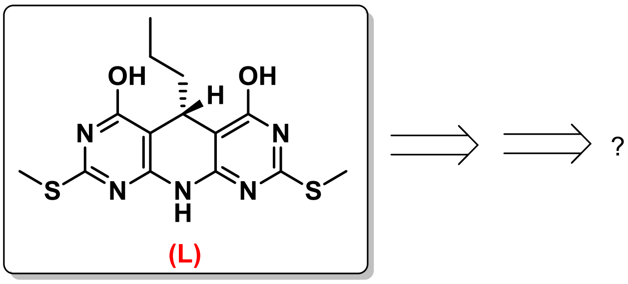

Figure 1. Preparation of L

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Paper code: 741

Ultrasound promoted synthesis of spirocyclohexanones catalyzed by *proline*

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Spirocyclic compounds have surprised synthetic chemists for *more than* a half-*century*. These compounds have significant conformational features and structural implications for biologically important natural products [1].

The Michael addition reaction is one of the most *powerful method* for C-C bond formation in current synthetic organic chemistry specifically intermolecular double-Michael reactions are the most useful tool for *constructing* spirocyclic products from the noncyclic substances [2]. *There have been an increasing number of reports* on the *synthesis of* organic compounds in the presence of ultrasonic waves with higher yields, shorter reaction times, and milder conditions than the classical methods. It has also been found that the separation of the product in the ultrasonic technique is more easier and efficient than conventional methods [3].

Hence, as mentioned above, herein, synthesis of various spirocyclohexanones from arylidine acetons, which were prepared by aldol condensation between one equivalent acetone and two equivalent arylaldehydes , and (thio) barbituric acid in different conditions were investigated. The results showed that the highest yields (88%) were obtained in the presence of catalytic amount of proline (25%) in EtOH, as a green solvent, at 70 °C under ultrasonic irradiation. Changing the catalyst to lower or higher amounts led to sharp decreases in the reaction results. The reaction is diastereoselective and only *cis* isomers were achieved in high yields. Finally, the products were purified by washing with water and EtOH. So, using ultrasound not only allows rapid and clean conversion but also simplifies experimental setup and workup leading to rapid generation of spirocyclohexanone without chromatography and even recrystallization.

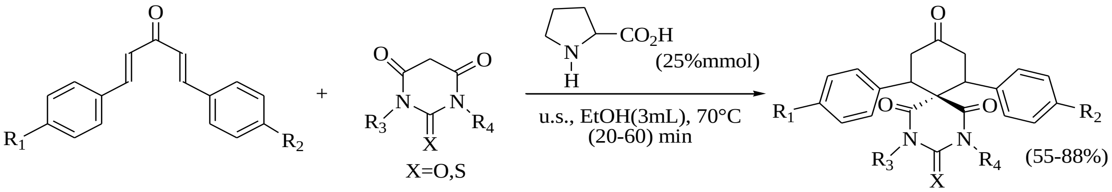

Fig. 1 Synthesis of Spiro Cyclohexanone Rings Under Ultrasound irradiation

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Paper code: 764

The preparation and characterization of BNPs-SO_3H: a highly efficient and reusable nanocatalyst for the preparation of 5-substituted 1*H*-tetrazoles

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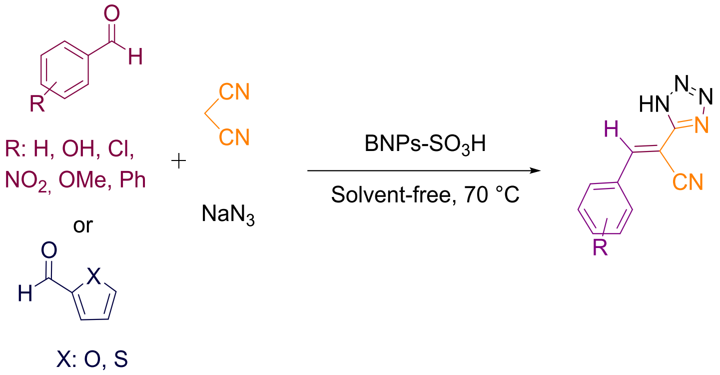
Today, development of nano-chemistry allows to preparation of nanocatalysts which include the benefits of both groups of heterogenous and homogeneous catalysts. [1] On the one hand, nano-catalysts are similar to those of heterogeneous catalysts, easily separated from the reaction mixture and on the other hand, they have the same activity and selectivity as homogenous catalysts. [1] Boehmite is an oxyhydroxide (AlO(OH)) particles, which has an orthorhombic structure and its surface is covered by hydroxyl groups. Thermal and mechanical stability, high surface area, ease of handling and the low costs of the required materials, are benefits of boehmite nanocatalyst. [2] Tetrazole derivatives having one carbon and four nitrogen atoms and these compounds are not found in nature.[2] Tetrazole derivatives show various biological properties such as antimicrobial, anti-inflammatory, anticancer,…[3]
Here, we introduced BNPs-SO_3H as a highly effective nanocatalyst for the synthesis of 5-substituted 1*H*-tetrazoles using sodium azide, malononitrile and various aldehydes (Scheme 1).



Scheme 1. Synthesis of 5-substituted 1*H*-tetrazoles with BNPs-SO_3H

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Paper code: 778

Desulfurization by Metal Oxide/Graphene Composites

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increasing attention is being paid to the chemistry of diesel fuel processing. However, refineries are challenged by the harmful sulfur oxides releases into the air from the combustion of high sulfur content fossil fuels [1]. Oxidative desulfurization is an innovative technology that can be used to reduce the cost of producing ultra-low sulfur diesel (ULSD) [2]. Adsorptive desulfurization is based on the ability of a solid adsorbent to selectively adsorb organic sulfur compounds from liquid transportation fuels. Since these fuels consist of various thiophenic [3].

In this work, surface of the graphene oxide (GO) was modified and then magnetic graphene oxide (MGO) was synthesized following by modification of surface of MGO with Zn. Varying concentration of *Dibenzothiophene (DBT) solutions were tested with different amount of synthesized adsorbents.* Concentration of each solution before and after filtration was determined by UV spectrometer. Purpose of magnetization was to ease separation of used adsorbents.

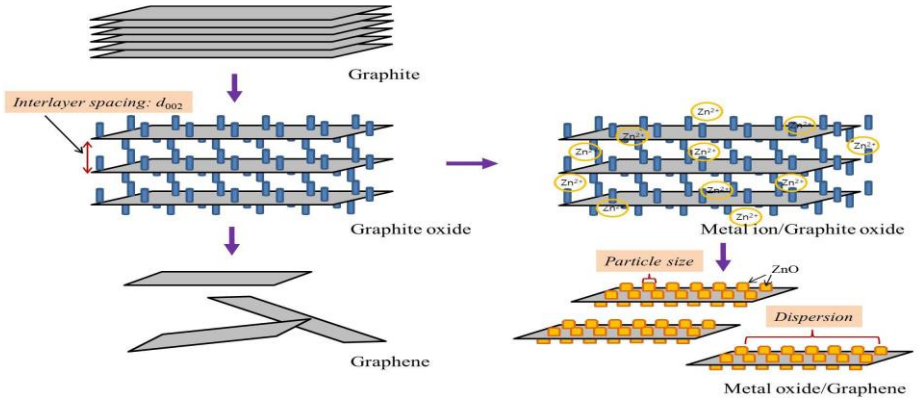

Figure 1. Illustration of the synthesis of metal oxide/rGO composite

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Paper code: 790

Cetyltrimethylamonium hydrogensulfate catalyzed synthesis of quinoxalines in aqueous media at room temperature

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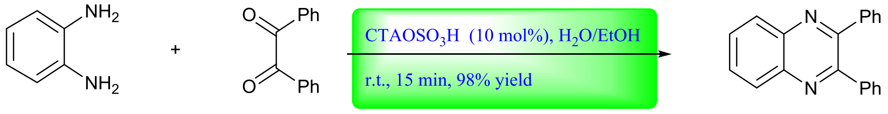
The aim of this study is to provide quinoxaline derivatives as useful compounds in pharmaceutical chemistry that have a wide range of biological activities such as antiviral, antibacterial, anti-inflammatory, anti-tumor, and depression, as well as efficacy in the industry[1]. Therefore, several methods for the synthesis of quinoxalines have been reported in the literature[2]. However, some of these reported methods are associated with one or more disadvantages such as harsh reaction conditions, use of expensive reagents, use of environmentally toxic reagents and use of large amount solid supports, which result in the generation of a large amount of toxic waste. Thus, several previous methods have been excluded from practical applications due to environmental and economic considerations. Hence, there is still a need to develop efficient methods for the synthesis of quinoxaline derivatives. Herein, we disclose a green process for efficient condensation of 1, 2-diketone with 1, 2-diamine catalyzed by Cetyltrimethylamonium hydrogensulfate (CTAHS), a Brønsted acid surfactant, in aqueous media at room temperature (Scheme). The solid quinoxaline product was precipitated as reaction proceed and was achieved in high to excellent yield by addition water to reaction mixture and a simple filtration.



Scheme

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Paper code: 792

Copper acetate/sulfadiazine complex as a highly active catalyst for 1,2,3-triazoles synthesis in aqueous polyethylene glycol media at room temperature

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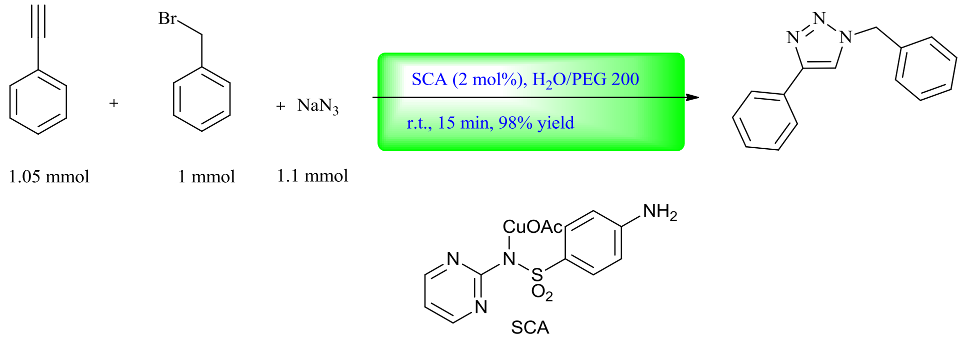
The 1,2,3-triazole moiety, a key structural element of many natural products, pharmaceuticals and synthetic agents, has increasingly attracted the synthetic pursuit of chemists because of its important biological properties [1]. So far, numerous synthetic methods have been developed and reported in literature [2-3]. One of the most popular protocol for the preparation of these compounds is 1,3-dipolar "Huisgen" cycloaddition reaction which is catalyzed by Cu(I) and ruthenium(II). Development of new methods and catalysts for the synthesis of the aforementioned target molecules under cleaner and milder reaction conditions is of demands. Herein, we report preparation of a novel $Cu(OAc)_2$/sulfadiazine complex (SCA) and used as a successfully catalyst for the synthesis of 1,2,3- triazole derivatives *via* a three-component condensation of terminal alkynes, benzyl halides and sodium azide under mild conditions (Scheme). The advantages of this method are using aqueous PEG 200 as a green solvent, low loadings Cupper catalyst, high yields, excellent regioselectivity, and clean reactions.



Scheme

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Paper code: 798

Synthesis of Pyrimidine-4-thiones and Thiazoles from TMG Adducts and Isothiocyanates

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Heterocyclic compounds, such as pyrimidines play an important role in the field of drugs, agrochemicals, and biological processes. In recent years, pyrimidines and pyrimidinethiones have been the subject of numerous pharmacological studies [1]. Thiazole is a well-known five-membered heterocycle that is present in many natural and synthetic products with a broad range of biological activities such as antimicrobial, antipyretic, antiparasitic, antihistaminic, and antiviral properties [2]. Herein, we report a simple procedure for the synthesis of alkyl 2-(dimethylamino)-1,4-diphenyl-6-thioxo-1,6-dihydropyrimidine-5-carboxylates **4** and 2-(dimethylamino)thiazoles **5** *via* the three-component reaction of tetramethylguanidine (TMG, **1**), ethyl phenylpropiolate **2**, and aryl isothiocyanates **3**. The reactions proceed smoothly and the products are obtained in moderate to good yields. Various features of these reactions are presented and discussed.

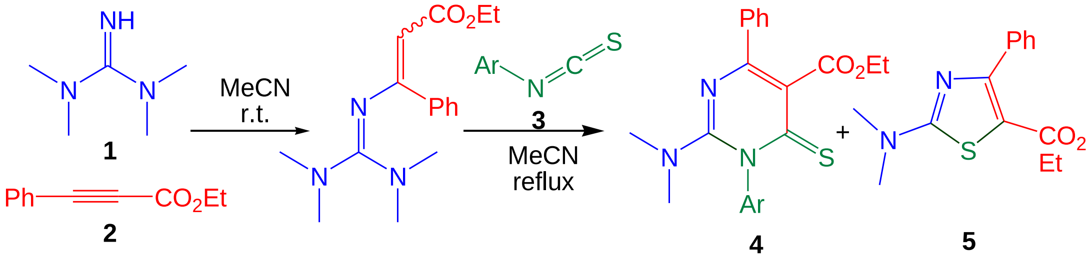

Fig. 1 Synthesis of Thiazoles and Pyrimidine-4(3*H*)-thiones.

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Paper code: 806

Fe_3O_4@C-SO_3H: Synthesis, Characterization and Its application on benzo[4, 5]imidazo[1, 2-a]-pyrimidines synthesis

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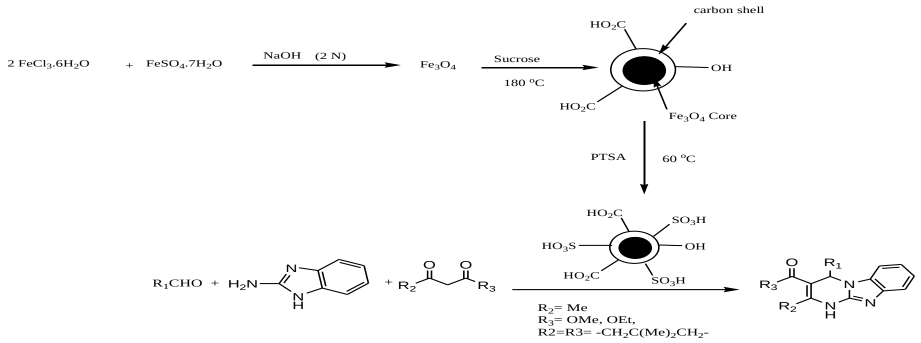
The magnetic Fe_3O_4@C-SO_3H nanoparticle (MNPs) was widely studied and showed high catalytic activities in many chemical reactions [1-4]. In this report, a sulfonic acid-functionalized magnetic nanoparticle (Fe_3O_4@C-SO_3H) was successfully prepared using Sucrose via a solvothermal process. The sulfonic acid-functionalized Fe_3O_4@C-SO_3H magnetic nanoparticle was obtained by grafting the sulfonic groups on the surface of Fe_3O_4@C nanoparticles in the presence of p-Toluenesulfonic. The magnetic Fe_3O_4@C-SO_3H nanoparticle was used as an efficient and new catalyst for the one-pot synthesis of benzo[4, 5]imidazo[1, 2-a]-pyrimidine derivatives through the condensation of aldehyde, β-dicarbonyl compounds and 2-aminobenzimidazole under solvent-free conditions in excellent yields. High catalytic activity and easy magnetically separation from reaction media are two important factors for evaluating the performance of Fe_3O_4@C-SO_3H nanoparticles in the preparation of pyrimidine derivatives. (Scheme).



Scheme

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Paper code: 819

A highly efficient method for the synthesis of polyhydroquinoline by carbon-based solid acid catalyst

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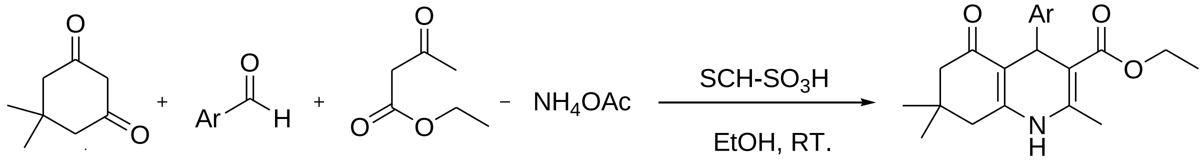
Much attention has been focused on Heterogeneous catalysts, since these catalysts can be recovered and reused several times after the reaction without loss of activity. Among the heterogeneous solid acid catalyst in organic synthesis, Carbon base solid acids (CBSAs), are important materials with many practical and research applications [1-2]. In continuation of our research on the synthesis of heterogeneous acid catalyst [3-5], in this report the synthesis of sulfonated carbon-based solid acid nanocatalyst (SCH-SO_3H) has been investigated through the one-step hydrothermal reaction of Starch, sodium 2-Hydroxyethansulfonat as sulfonating agent in the presence of citric acid and HCl (Scheme). The structures and morphology of the prepared nanocatalyst were studied with SEM, IR, XRD, CHNS analysis. Also acidity of nanocatalyst was determined by acid-base titration. The application of SCH-SO_3H was investigated in the one-pot synthesis of polyhydroquinoline through the reaction between dimedone, benzaldehyde, ethylacetoacetat and ammonium acetatein EtOH as green solventat room temperature. A variety of aldehydes were used to afford the corresponding products in good to high yields.



Scheme

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Paper code: 820

A Facile Synthesis of quinoxalines and dicyano pyrazines using $Ca(IO_3)_2$ as efficient and recycling catalyst

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Quinoxaline derivatives are an important class of nitrogen containing heterocycles and have been widely used in dyes pharmaceuticals and electrical/photochemical materials. Also, quinoxaline ring moiety is a part of various antibiotics such as Echinomycin, Levomycin, and Actinoleutin that are known to inhibit growth of gram positive bacteria, and are active against various transplantable tumors [1]. Also, dicyanopyrazine derivatives have been synthesized and are valuable in a broad range of chemistry fields due to their applications as functional dyes, nonlinear optical materials, *etc.* [2]. Because of their importance, up to now, several methods have been reported for the synthesis of these compounds including the condensational reaction of an aryl 1,2-diamine with a 1,2-dicarbonyl compound in refluxing or in the presence of an acid catalyst under various reaction conditions [3].

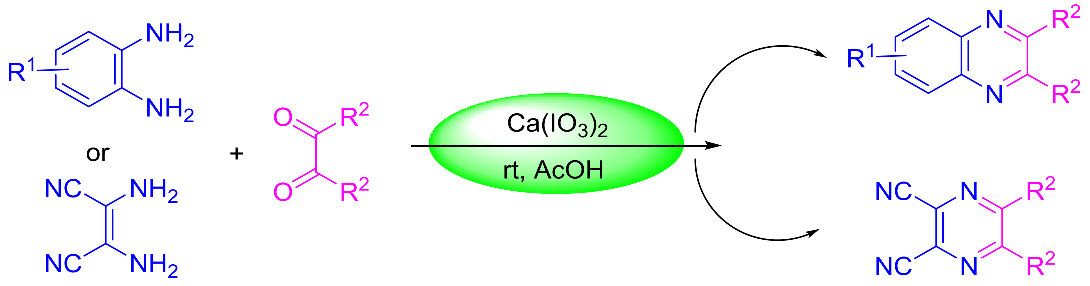

Fig. 1 The synthetic pathway for preparation of quinoxaline and dicyanopyrazine derivatives

Looking at the above facts, in this study, we report use of $Ca(IO_3)_2$ as an efficient heterogeneous catalyst for the preparation of 2,3-diaryl quinoxaline and dicyano pyrazine derivatives by reaction of *o*-arylenediamine or diaminomaleonitrile and 1,2-dicarbonyl compounds. The attractive features of this procedure are its good conversions, easy workup, and short reaction times, safely and recyclable catalyst, making it a useful practical method for the synthesis of the title compounds.

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Paper code: 825

Five-component synthesis of dihydropyridines based on diketene

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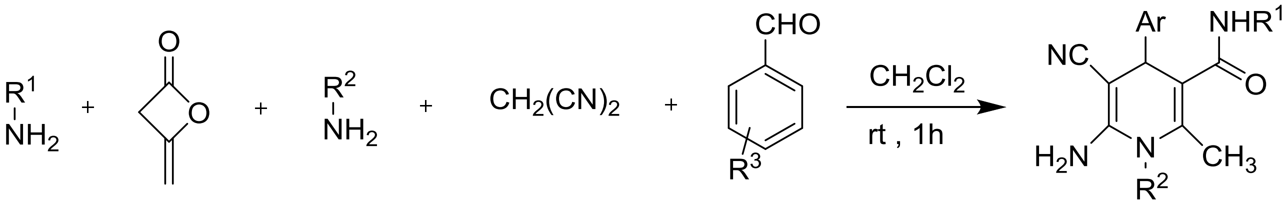
The 1,4-dihydropyridine (1,4-DHP) skeleton is one of the most versatile heterocyclic pharmacophores since it has been found as the central fragment in many clinical pharmaceuticals.[1] The most notable examples are the series of 1,4-DHP-based calcium channel blocker drugs such as nifedipine, felodipine, and nicardipine, which are still widely prescribed for the treatment of hypertension and related cardiovascular diseases.[1,2] In addition, the results obtained from a study with 1,4-DHPs as an a1aadrenoceptorselective antagonist discloses their promising potential in treating benign prostatic hyperplasia.[3]

A novel five-component strategy involving commercially available diketene, primary amines, malononitrile and various benzaldehydes for the synthesis of densely functionalized 1,4-dihydropyridines in good yields was achieved. The reaction pathway involves a sequential ring-opening of diketene/enamine formation/Knoevenagel-condensation/Michael addition and 6-exo-tet cyclization, resulting in multiple bond-formation events including two C-C and three C-N bonds ultimately leading to the formation of the respective 1,4-dihydropyridines.



Scheme 1. One-pot procedure for the synthesis1,4-dihydropyridine

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Paper code: 838

A multicomponent synthesis of 2-amino-3-cyanopyridine derivatives by carbon-based solid acid catalyst

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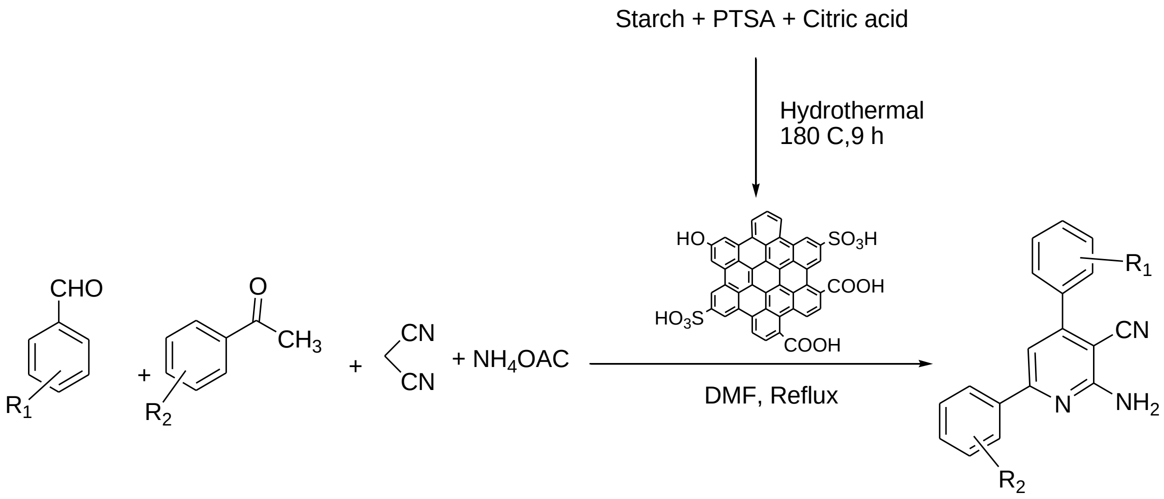
The interesting biological properties of pyridines derivatives have promoted a great deal of research effort toward development of new synthetic methodologies for 2-amino-3-cyanopyridines and their derivatives [1, 2]. In continuation of our research on solid acid synthesis [3], here we wish to report a simple and efficient method for the one-pot synthesis of 2-amino-3-cyanopyridines in excellent yields using a catalytic amount of starch-derived carbon based solid acid. The synthesis of sulfonated carbon-based solid acid nanocatalyst (SCP-SO_3H) has been investigated through the one-step hydrothermal reaction of Starch as carbohydrate source and p-toluenesulfonic acid as sulfonating in the presence of citric acid (Scheme).

The application of SCP-SO_3H was investigated in the synthesis of 2-amino-3-cyanopyridines via the condensation of aldehydes, acetophenone, malononitrile and ammonium acetate. A variety of ketones and aldehydes was used to afford the corresponding products in good to excellent yields.



Scheme

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Paper code: 844

The Synthesis of Epoxy Polyuretheane -Silica Nanocomposites

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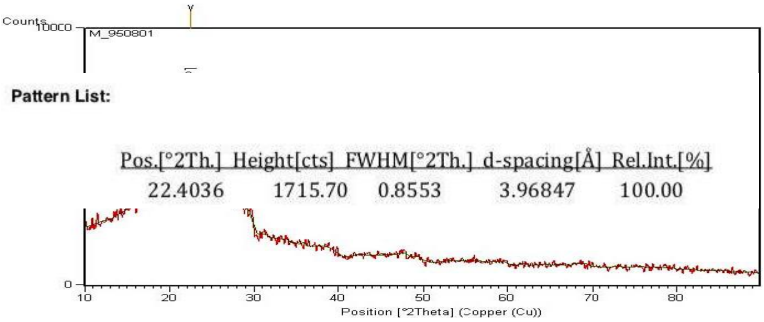
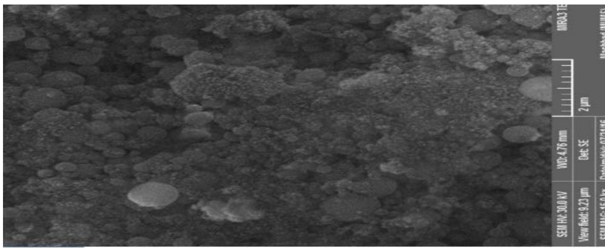
Nanoparticles are mixed with polymers and create nanocomposites which have new properties. In order to disperse nanoparticles in the polymer, first, their surface is stabilized by silane coupling factor. This prevents nanoparticles agglomeration and improves the compatibility between nanoparticles and polymer which enhances many of their properties. In this research, the epoxy polyurethane-nanosilica nanocomposite is synthesized in situ. To synthesize this nanocomposite, SiO2 nanocomposites are prepared in N,N-dimethylformamid (DMF) through Stober method and then their surface is modified by 3-Methacryloxypropyl triethoxysilane (MPS) and they were characterized by Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscope (SEM). Novolac epoxy resin (EP) was prepared by the reaction of epichlorohydrin and Novolac in the presence of soda (NaOH) and epoxy acrylate resin (EA) was synthesized based on the ring opening reaction of Novolac epoxy resin and methyl methacrylate acid was synthesized in the presence of tetrabutylamonium bromide (TBAB) catalysis and characterized by FT-IR spectroscopy and HNMR. Then, mps-SiO2 modified nanoparticles were exposed to electrosonic waves in DMF solvent and monomers of acrylate (styrene, butyl acrylate and synthesized acrylate epoxy) + initiator of azobis isobutyro nitrile (AIBN) were added to the nanoparticle uniformly and dropwisely and in situ polymerization occurred. Now, the nanoparticle is in a polymer capsule which is known as the core-shell structure. 1 and 3 percent of core-shell nanoparticles were added to the polyurethane base. Thermal properties of synthesized nanoparticles were studied by thermogravimetric analysis (TGA) and characterized by FT-IR spectroscopy and scanning electron microscopy (SEM). Results showed that adding core-shell nanoparticles up to 3 percent led to the improvement of thermal resistance of polyurethane [1].



Pattern List:

Pos.[°2Th.]	Height[cts]	FWHM[°2Th.]	d-spacing[Å]	Rel.Int.[%]
22.4036	1715.70	0.8553	3.96847	100.00



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Paper code: 845

A synthesis of (arylthio-ethylidene)indolin-2-ones *via* S-arylation of oxoindolin-ethanethiolates with aryl halides

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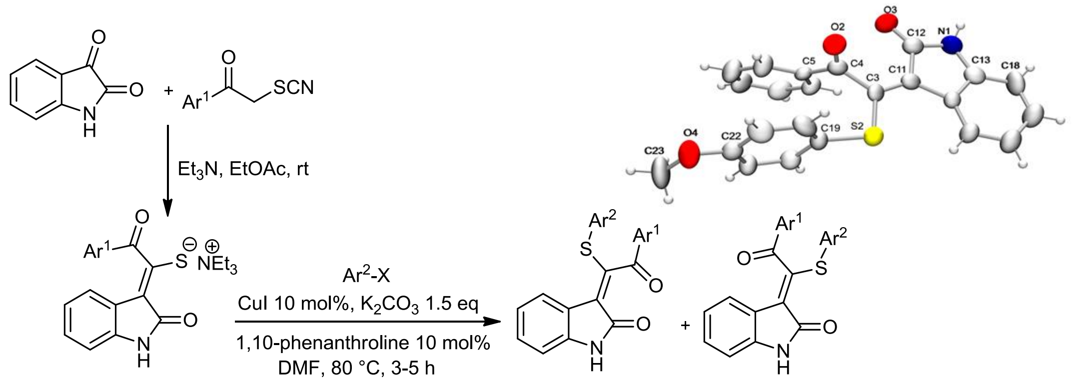
In recent years, Ullmann-type reactions have grown into a versatile tool for access to C−X (X = C, N, O, S, etc.) bonds [1]. Although several palladium, nickel, and cobalt catalysts have proven to be highly effective in such coupling processes [2], copper reagents are favorable catalytic systems for C-X bond-forming reactions. [3]. Among various cross-coupling reactions, S-arylation is comparatively less studied.Herein, we report a novel protocol for the synthesis of (*Z*/*E*)-3-[2-oxo-2-aryl-1-(arylthio)ethylidene]indolin-2-ones by a one-pot reaction of 1-aryl-2-thiocyanatoethan-1-ones, isatin, and aryl halides in DMF. (Fig. 1). The structures of products were characterized by their IR, ^{1}H NMR, ^{13}C NMR and mass spectral data. Various advantages of these transformations will be presented and discussed.



Ar^1 = Ph, *p*-Tolyl, 4-$MeOC_6H_4$, 4-BrC_6H_4, 4-ClC_6H_4

Ar^2 = Ph, *p*-Tolyl, 4-$MeOC_6H_4$, 2-$O_2NC_6H_4$, 4-$O_2NC_6H_4$

Fig. 1 Synthesis of (arylthio-ethylidene)indolin-2-ones.

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Paper code: 846

κ-Carrageenan: An efficient, green and reusable catalyst for the one-pot synthesis of 3, 4-dihydropyrimidin-2(1H)-ones and their corresponding 2(1H)thione

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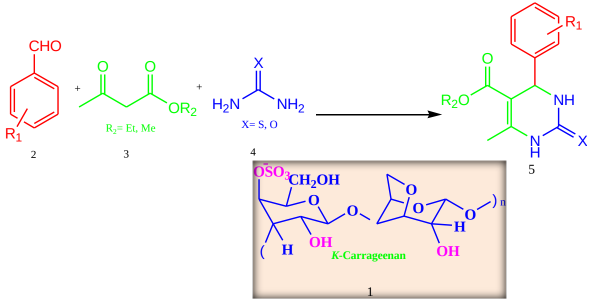
The disclosure of Biginelli reaction by the chemist Pietro Biginelli, functionalized 3,4-dihydropyrimidin-2(1H)-ones/thiones (DHPMs) have emerged as prototypes for the design of compounds with a broad variety of biological activities such as antiviral, antitumor, cardiovascular antibacterial, anti-inflammatory and antioxidant properties.[1] A simple, green, nontoxic and efficient method was found to be for the synthesis of 3,4-dihydropyrimidin-2(1H)-ones and -thiones through one-pot three-component reaction of ethyl acetoacetate (methyl acetoacetate), an aromatic aldehyde and urea or thiourea under solvent-free conditions using Kappa Carrageenan as an efficient, heterogeneous, economical, biocompatible and green catalyst.[2, 3] Compared with classical Biginelli reaction conditions, the new method has several advantages such as good yields, relatively short reaction times, mild reaction conditions and a the nontoxic catalyst with a very easy work up.[4]



Scheme 1. Biginelli Reaction: reaction of ethyl acetoacetate (methyl acetoacetate) (3a, b), an aromatic aldehydes (2a-h) and urea or thiourea (4a, b)

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Paper code: 850

Light-induced switching of azo-imidazoles on gold nanoparticles

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In the past decade, a large number of photochromic compounds with different photoresponsive units have been synthesized and their properties have been investigated [1,2]. Recently photochromic compounds have attracted considerable attention due to their extensive applications in display and anti-counterfeiting systems, optical storage and memory devices, and optical molecular switches. The self-assembly of functional photochromic molecules as ligands on the surface of metal nanoparticles is a promising strategy for the fabrication of nanoscale devices with potential applications in clinical diagnostics, optical storage and photo-switchable surface wettability [3].

In the present study, gold nanoparticles (AuNPs) were immobilized with sulfur-modified photochromic azo-imidazole derivatives and their photochromic performance was studied. In this class of photochromic compounds, a reversible switching reaction occurred between the trans-enol photoisomer into cis-keto and/or quinone-hydrazone photoisomers and vice versa under UV irradiation.

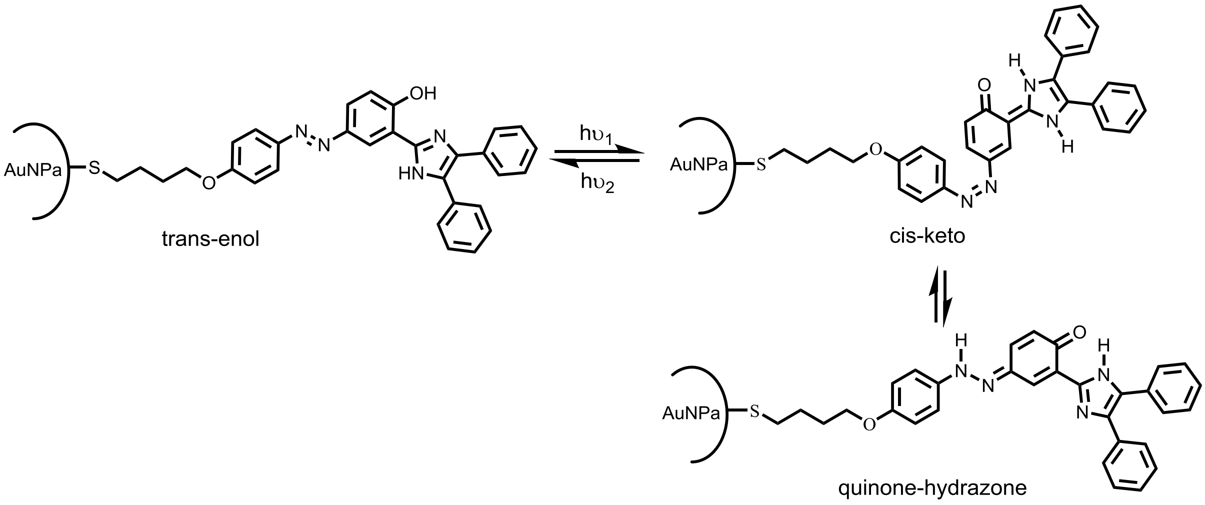

Fig. 1 photoisomerization of azo-imidazole@Au

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Paper code: 855

Synthesis of functionalized trifluoro methylated ketenimines and 1-azabuta dienes via isocyanide based multicomponent reactions

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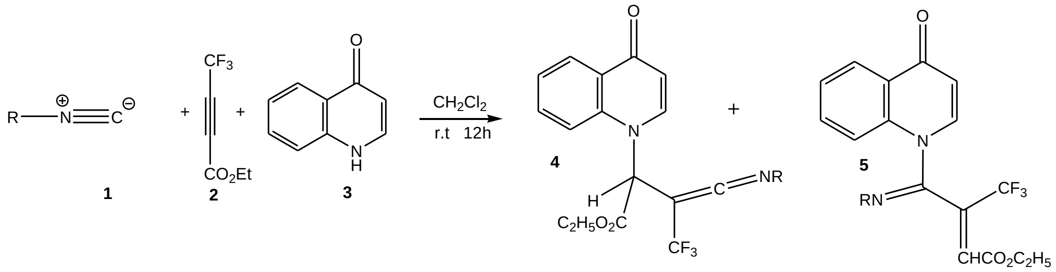
Trifluoromethylated compounds play a significant role in life sciences which have many remarkable functions and numerous properties such as agrochemicals and pharmaceuticals activities [1, 2]. On the other hand, multi-component reactions are a one of the best method for synthesis of highly functionalized fluoranitated and stable ketenimines and aza-butadiens derivatives and they have many applications such as: nucleophilic additions, radical additions, cycloaddition reactions [3].In this research a series of novel trifluoromethylated ketenimines and 1-aza butadiene derivatives were synthesized via a one-pot multicomponent reactions of alkyl isocyanides, ethyl 4, 4, 4-trifluoro butynoate and quinolin-4(1H)-one in good yields (scheme 1).



1	R
a	*t*-But
b	*1, 1, 3, 3-tetramethyl* Butyl
c	*c*-Hexyl

4	R	yield of **4** (%)
a	*t*-But	70
b	*1, 1, 3, 3-tetramethyl* Butyl	75

5	R	yield of **5** (%)
a	*c*-Hexyl	73

Scheme 1. Typical procedure for synthesis **4** and **5**

The structures of all products were clearly established by IR, NMR (^{1}H, ^{13}C and ^{19}F) and mass spectroscopy. The present method carries the advantage that not only the reaction is performed under neutral conditions, but also the starting materials and reagents can be mixed without any activation or modification.

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Paper code: 860

Synthesis of novel amino and pyrrolyl acridine 1, 8-dione derivatives

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A new series of amino substituted tetrahydroacridine 1, 8-diones were synthesized by multi-component reaction of dimedone, *p*-phenylene diamine and benzaldehyde derivatives. The synthesized amino acridines then were reacted with 2, 5-dimethoxy tetrahydrofurane in acetic acid to give pyrrolyl acridine 1, 8-diones [1], [2]. Acridine-1, 8-diones are important compounds due to their various pharmacological properties, such as cytotoxic, anticancer, antimicrobial, antifangal. Pyrrole nucleus is an essential structural motif in various groups of biologically active and natural molecules. (Fig.1)

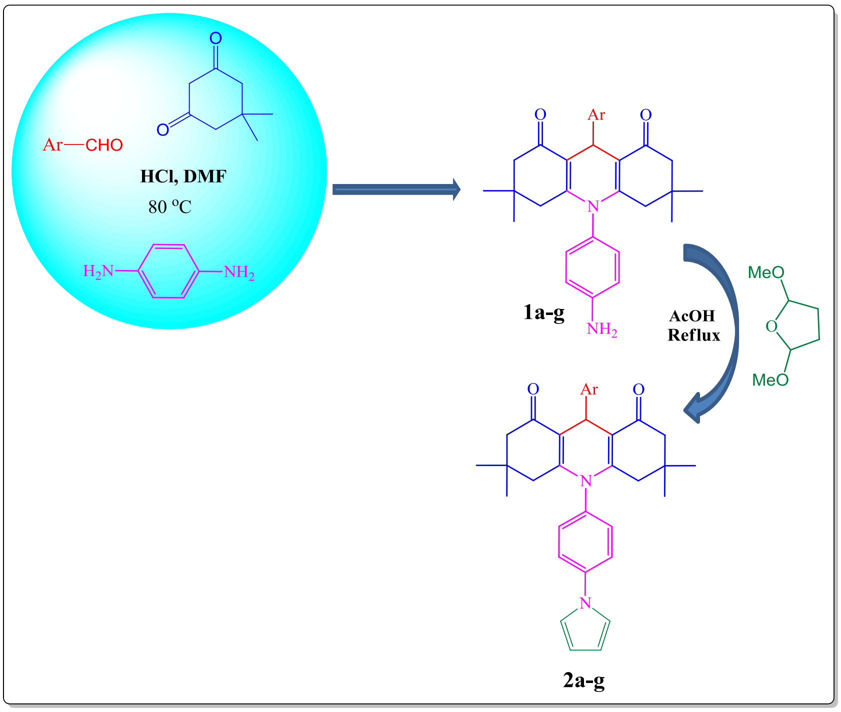

Fig 1: 1 Synthesis of pyrrolyl acridine 1, 8-diones from amino acridine 1, 8-diones.

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Paper code: 866

Preparation of doxorubicin, gold and magnetic NPs loaded on Albumin NPs as well as in vitro treatment of MCF-7 breast cancer cells

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Among different diseases, cancer is the main cause of death all over the world. It is treated by chemotherapy, radiotherapy, surgery or a combination of these protocols. However, the main hurdles in treatment of cancer are the nonspecific absorption of chemotherapeutic drugs by healthy cells as well as drug resistance at tumor sites. Nowadays, through design of drug delivery systems, scientists overcome these limitations by increasing the drug solubility, specificity, maximum tolerance dosage and decreasing drug toxicity. Doxorubicin is one of the famous and common agent for treating various types of cancers such as soft-tissue sarcoma and has so many adverse side effects such as cardiotoxicity, myelosuppression, typhlitis, nausea, vomiting, and alopecia [1]. So there is a serious need to design a biocampatible and controllable nanocarrier with minimum adverse effects for doxorubicin delivery to the cancer cells.

The aim of this work is to study the preparation and characterization of a new, biodegradable and controllable doxorubicin, gold and magnetic nanoparticles loaded on albumin nanoparticles (Dox/GNPs/MNPs-BSA-NPs) as well as considering its capability for in vitro treatment of MCF-7 human breast cancer cells. Monodisperse citrate-stabilized Au NPs and Fe_3O_4 NPs were synthesized using Bastus et al. [2] and modified coprecipitation method [3], respectively, while doxorubicin, AuNPs and MNPs loaded albumin nanoparticles (Dox/GNPs/MNPs-BSA-NPs) were prepared by desolvation-crosslinking method. Drug loading capacity of the designed system was determined by uv-visible spectrophotometer and found to be about 59.37 mg Dox/g albumin. Furthermore, about %65.6 of the encapsulated drug release during 192 hours through a mild diffusion. The anti-tumor effect on MCF-7 human cancer cells treated in vitro with Dox/GNPs/MNPs-BSA-NPs was evaluated by MTT assay. The experimental results revealed that Dox/GNPs/MNPs-BSA-NPs significantly inhibit the proliferation of MCF-7 cells while the coating of albumin helps reduction the toxicity of GNPs and MNPs. The prepared nanoparticles composed of mixed doxorubicin, MNPs and GNPs is a promising design for control and targeted delivery of anticancer drugs to the MCF-7 cells.

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Paper code: 867

Sodium Formaldehyde Solfoxylate, Synthesis, Optimization and Performance Evaluation

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Reducing agents in various industries have different applications. Rongalite or sodium formaldehyde sulfoxylate (SFS) is a compound that is used as industrial bleaching agent and reducing agent. Due to the wide range of sodium formaldehyde sulfoxylate applications, such as reducing agent for redox-catalyzed polymerization, stripping and discharge agent for textiles, reducing agent in vat dying, bleaching agent for molasses, antioxidant in pharmaceuticals and green reagent in organic synthesis, research activities have been done on the synthesis of this material. [1], [2], [3], [4]. We which to report synthesis of this substance was selected and optimized with industrial approach and synthesized in two steps. In the first step, Zinc dithionite was synthesized as an intermediate and in the second step, sodium formaldehyde sulfoxylate was obtained. Optimization of temperature, solvent has also been studied.

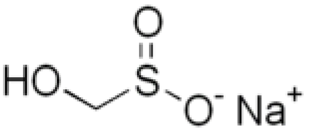

Fig. 1 The Structure of Sodium Formaldehyde Sulfoxylate (SFS).

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Paper code: 868

One-pot, three-component synthesis of isoxazol-5(4*H*)ones using $NH_4H_2PO_4$ in aqueous medium

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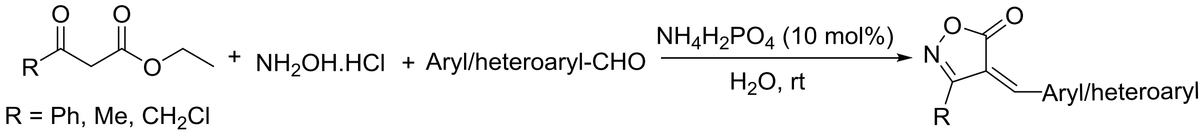
The isoxazol-5(4*H*)one unit is found in many molecules, including naturally occurring bioactive compounds, pharmaceutical drugs, and agrichemicals. Derivatives of isoxazol-5(4*H*)ones are possess biological properties such as antibacterial, anti-inflammatory, antifungal, anticancer, analgesic, anticonvulsive, anti-diabetic, anti-androgenic, hypoglycemic, inhibitory against PTP1B and the tumor necrosis factor-alpha, herbicidal, and insecticidal activities [1]. Also, the isoxazol-5(4*H*)ones can be found in various synthetic intermediates for the synthesis of many heterocyclic compounds and other functional organic molecules [2]. It has long been known that the multicomponent reactions (MCRs) are powerful means of synthesizing high-value chemicals in a single reaction flask. Simpler procedures and equipment, time and energy savings, as well as environmental friendliness have all led to a sizable effort to design and implement MCRs in both academia and industry [3]. In this MCR, the use of ammonium dihydrogen phosphate catalyst allows cyclocondensation to be carried out in a single-step, three-component reaction of structurally diverse aldehydes with various *β*-oxo esters and hydroxylamine hydrochloride without isolation of intermediates to give the corresponding various isoxazol-5(4*H*)ones in aqueous medium at room temperature. The salient feature of this method includes mild conditions, relatively short reaction time, good to high yields, easy separation of products, and simple procedure.



Scheme. 1 Three-component synthesis of isoxazol-5(4*H*)ones in water at room temperature.

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Paper code: 871

Nanocrystalline silica-H_2SO_4 as an efficient Heterogeneous catalyst for the synthesis of $2^{/}$-aminobenzothiazolo-arylmethyl-2-naphthols under solvent-free conditions

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With the development of green chemistry, solid acid catalysts have received much attention for green catalytic procedures with advantages of no pollution, easy separation and reusability. However, compare with the catalytic activities of traditional protonic acids such as H_2SO_4 etc, that of the solid acid catalysts were always not good enough mostly because of the lower acid density and strength. For decades' researchers in this field around the world has been committed to improve the acid density and strength as well as the stability of solid acids. In addition, there is a several interest in heterogeneous system because of its importance in industry and in developing technologies [1-3]. In this paper, nanocrystalline silica-H_2SO_4, as a newly reported catalyst, has been used as an efficient and reusable catalyst for the synthesis of $2^{/}$-aminobenzothiazolo-arylmethyl-2-naphthols with using benzothiazol-2-amine, 2-naphthol, aromatic aldehydes [4]. In practice, this method is a combination of a satisfactory synthesis and more significantly easy product isolation and purification. A simple, high yielding in the presence of nanocrystalline silica-H_2SO_4 as a catalyst is described. The catalyst could be used at least five times without any change in the activity. Full characterization of the catalyst was performed by XRD, IR, TGA spectra and also by FE-SEM images.

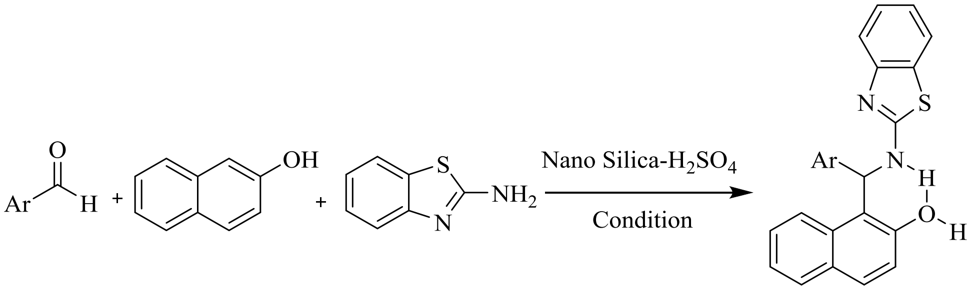

Fig. 1 nano-silica-H_2SO_4 catalyzed synthesis of $2^{/}$-aminobenzothiazolo-arylmethyl-2-naphthols

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Paper code: 874

Condensation reaction between 3-acetylcumarine and arylaldehydes in the presence of L-proline

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Coumarins are one of the most important group of natural compounds which contain anti-HIV, anti tomour ,anti hypertension, anti osteoporosis, anti allergic, pain killer and preventive of growth and proliferation of microbes .

In this research, it is applied a new method for synthesis of coumarin ingredients by using two steps and aldol reaction, which is contain synthesis 3-acetyle coumarin as a primary substance by using a mixture of ethyl acetoacetate and salicylaldehyde and a few drops of ethyl amin and in next step it is containes reaction of 3-acetyle coumarin and benzenaldehyde derivatives in presence of L-proline as a adaptable catalysis by enviroment in alcohol in reflex condition, in this study will be evaluated.

The purpose of this research is representing a adaptable synthesis method with enviroment and also the synthesis of coumarin elements by using of L-proline catalysis.

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Paper code: 882

Phenanthroline-SO_3H as a novel nano-molten salt catalyst: Application in multicomponent synthesis

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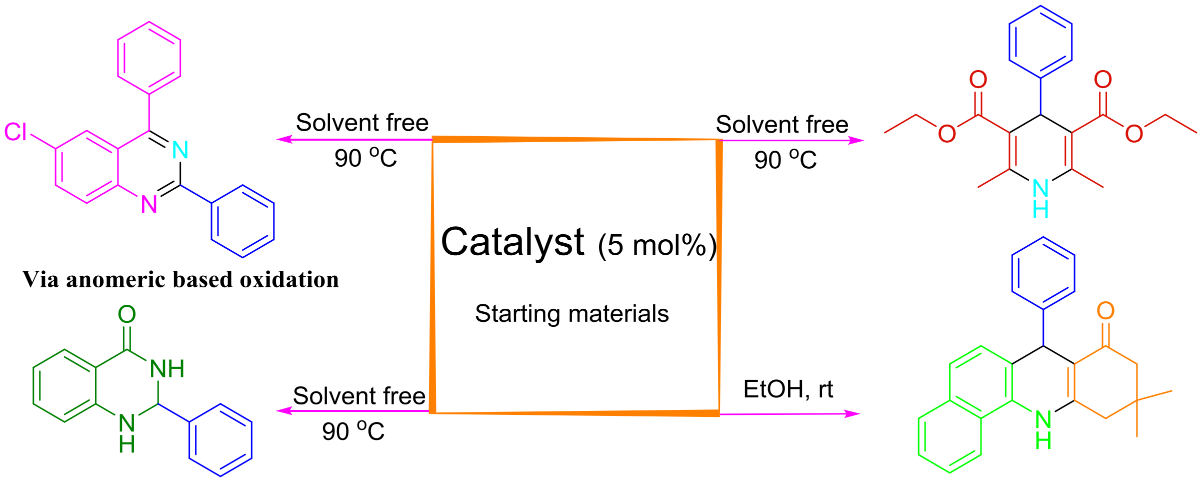
Nano molten salts as eco-friendly and green catalysts play an important role in the chemical processes. Easy recovery and reusability of these catalysts have led to their extensive use in the synthesis of a wide range of compounds [1, 2]. Multicomponent reactions (MCRs) have become a paramount important route in organic chemistry because most of the atoms of starting materials contribute to the final product. Therefore, this type of reactions have been widely used in the synthesis of complex pharmaceutically active heterocyclic compounds, especially nitrogen-containing derivatives due to the biological activity [3]. In this work, we wish to reported a clean method for synthesis of good range of heterocyclic compounds at room temperature using phenanthroline-SO_3H (5 mol%) as an efficient nano catalyst (**Scheme 1**).



Scheme 1: Synthesis of various heterocyclic compounds using phenanthroline-SO_3H (5 mol%) in ethanol at room temperature

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Paper code: 884

Phenanthroline based ionic liquids as a catalyst in the synthesis of 2-amino-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile in water

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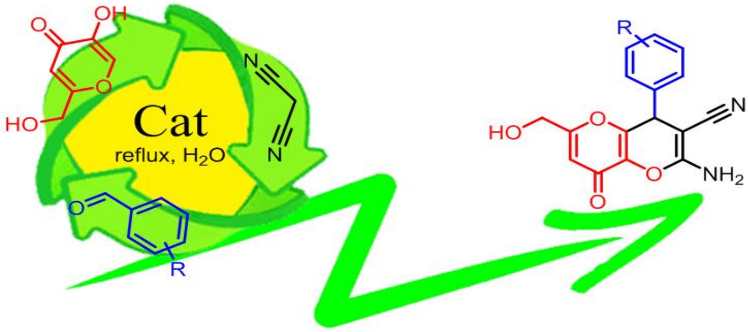
Phosphoric acid as a non-toxic acid is extensively using in the chemical industry such as: food industry, medicine, soldering, cleaning agents and the printing industry [1]. Due to the properties and use of phosphoric acid, the synthesis of a new catalyst based on this acid is great of demand [2]. One of the most important heterocyclic rings, which are presenting in a wide range of compounds, due to thier properties such as anticancer, anti-HIV, antimicrobial, anti-inflammatory and calcium channel antagonist activity [3, 4]. In the present work, we wish to report an efficient and eco-friendly three-component reaction condensation protocol in refluxing water and neutral media using ionic liquid with dihydrogen phosphate anions (5 mol%) as catalyst (**Scheme 1**).



Scheme 1: Synthesis of 2-amino-8-oxo-4,8-dihydropyrano[3,2-b]pyran-3-carbonitrile with novel nano molten salt of phosphoric acid in water.

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Paper code: 888

Application of novel quinoxaline–based nano molten salts in the synthesis of *N*-amino-2-pyridones and 1,4-dihydropyrano [2,3-c] pyrazoles

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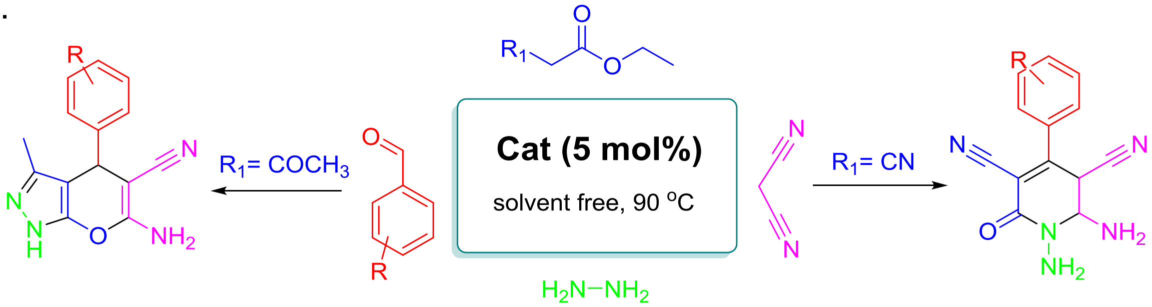
Modern investigation leads to nano scale science and technology for various purposes. Molten salts (MSs), ionic liquids (ILs) and room temperature ionic liquids (RTILs) are produced by decreasing symmetric via combination of suitable cations and anions. Typically, ionic liquids (ILs) and molten salts (MSs), refer to organic onium salts which molten below and above 100 °C respectively. MSs are a noteworthy class of liquids because of their unique ionic interactions and their broad number of scientific uses. [1-2]. *N*-amino-2-pyridones and 1,4-dihydropyrano [2,3-c]pyrazoles have been applied to the treatment of rheumatoid arthritis, psoriasis, cancer, Parkinson's disease, Huntington's disease, Alzheimer's disease, Down's syndrome, AIDS, schizophrenia, and myoclonus, as well as demonstrating biological properties such as antiviral, , pheromonal, and central nervous system activity [3-4]. In this work, we have designed and synthesized a novel nano molten salts with the ability to synthesize specific elongates in the reaction of four components under solvent-free conditions (Scheme 1).



Scheme 1: Synthesis *N*-amino-2-pyridones and 1,4-dihydropyrano [2,3-c]pyrazoles with novel nano molten salt of phosphoric acid in water.

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Paper code: 889

Application of novel phosphonium based ionic liquid at the synthesis amidoalkyl naphthols under mild and solvent free conditions

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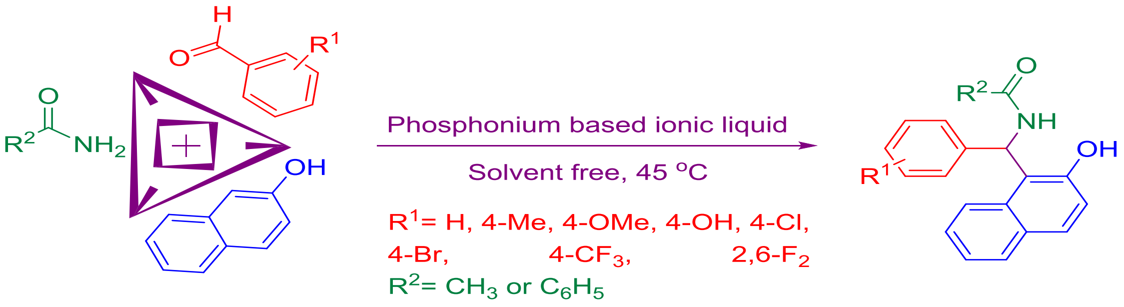
Multicomponent reactions (MCRs) as an elegant tool for the preparation of pharmaceutical active molecules and/or drug candidates are great demand. This protocol represents varied merits including atom and step economy so that preparation of complex structures in single synthetic protocol with high efficiency is performed. On the other hands, ionic liquids have found their influential position in different fields of chemistry and they can be used as catalyst, solvent or reagent for organic functional group transformation [1-3].

In this study, we combined the multicomponent reaction strategy and promising features of ionic liquids to present a powerful method for the preparation of amidoalkyl naphthol derivatives as versatile biological active structures from the reaction of different arylaldehydes, 2-naphthol and acetamide or benzamide under mild reaction conditions. All reaction performed smoothly in short reaction times with high to excellent operational yields.



Scheme 1: Catalytic synthesis of amidoalkyl naphthol derivatives

References

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Paper code: 890

A novel magnetic nanoparticle with morpholine tags as a multi-rule catalyst for synthesis of hexahydroquinolines

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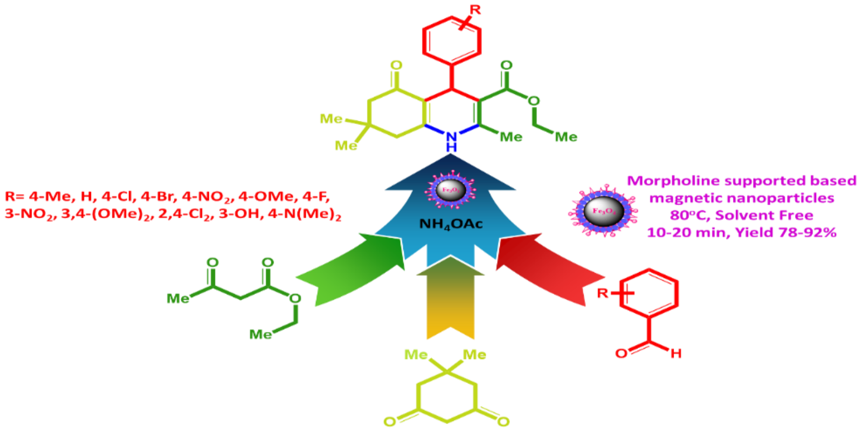
Hexahydroquinoline derivatives are ubiquitous in the nature due to their wide variety of pharmaceutical and biological applications as they can be applied as Ca^{2+} channel blockers. Therefore, in the recent times much attention has been focused on the topic of the synthesis of these privileged structural motifs. Also, hexahydroquinoline derivatives can be used as bronchodilators, hepatoprotective, vasodilators, anti-atherosclerotic, anti-diabetic, anti-tumor agents for the treatment of cardiovascular diseases such as hypertension [1-3].

In this exploration, we investigated the design, synthesis, characterization and catalytic performance of a novel morpholine supported based magnetic nanoparticle at the synthesis of biological active hexahydroquinoline derivatives through a four components reaction between aryl aldehydes, dimedone, ethylacetoacetate and ammonium acetate as nitrogen source (Scheme 1).



Scheme1 Catalytic preparation of hexahydroquinoline derivatives under mild reaction conditions

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Paper code: 897

Catalytic application of a novel oxyammonium based nano ionic liquid at the preparation of pyrano[4,3-*b*]pyrans and tetrahydrobenzo[*b*]pyrans

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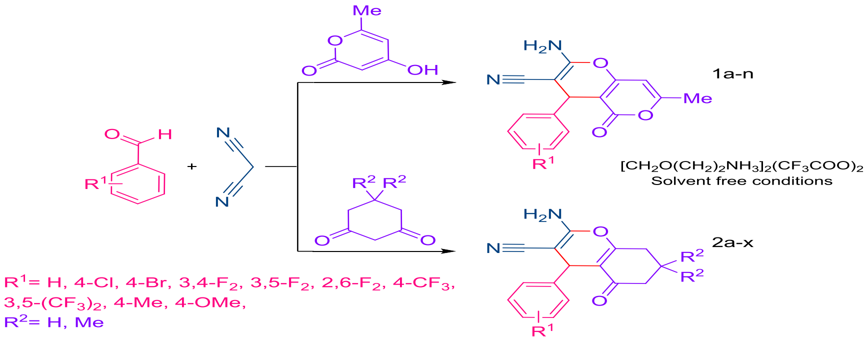
Due to the presence of bulky and asymmetric ions within the structure of ionic liquids, compare with classical inorganic salts, they cannot form a crystalline structure and therefore, melt at temperatures lower than 100 °C. At the present time, due to remarkable typical characteristics such as minor vapor pressure, large temperature window of molten state, excellent solvation properties, high chemical and thermal stability, lack of inflammability, wide electrochemical window, and respectable ion conductivity, ionic liquids emerged as an interdisciplinary area and found a critical place in various fields of science [1].

Fused 4*H*-pyran derivatives such as pyrano[4,3-*b*]pyrans and tetrahydrobenzo[b]pyran derivatives widely occur in various molecules exhibiting a broad range of pharmacological applications such as antiviral, anticonvulsant and antimicrobial, antileishmanial, antiproliferative, anticancer, anti-HIV, antituberculosis and anti-fungal agents. Therefore, it is expected that the preparation of these versatile compounds being exposed to chemists [2-3]. Herein we wish to present a mild and clean procedure for synthesis of pyrano[4,3-*b*]pyrans and tetrahydrobenzo[b]pyrans in the presence a suitable ionic liquid. The scope and limitations of described methodology will be discussed.



$[CH_2O(CH_2)_2NH_3]_2(CF_3COO)_2$
Solvent free conditions

R^1= H, 4-Cl, 4-Br, 3,4-F_2, 3,5-F_2, 2,6-F_2, 4-CF_3, 3,5-$(CF_3)_2$, 4-Me, 4-OMe,
R^2= H, Me

Scheme 1: Catalytic synthesis of pyran derivatives

References

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Paper code: 899

A novel ionically tagged magnetic nanoparticles as a reusable catalyst for synthesis of pyridines via anomeric based oxidation mechanism

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N-heteroaromatic structures particularly pyridine ring systems are ubiquitous in pharmaceutical active molecules and natural products. Among the *N*-heteroaromatic molecules, 2-amino-3-cyano pyridine scaffolds represent fascinating biological characteristics. These compounds can apply as A_{2A} adenosine receptor antagonists, IKK-β inhibitors, inhibitors of HIV-1 integrase, anti-microbial, anti-tumour, analgesic, anti-inflammatory and antipyretic agents[1-3].

Herein, we designed a novel, green and reusable nanomagnetic catalyst, which was synthesized and the catalytic application of the titled catalyst was examined at the synthesis of pyridine derivatives *via* a four-component reaction (Figue 1). Resulting experimental data suggest that the final step of the plausible mechanism proceed *via* an anomeric based oxidation mechanism. The presented catalyst shows excellent potential of recycling and reusing at the described multicomponent reaction. The suggested mechanism for the above mentioned reaction will be presented.

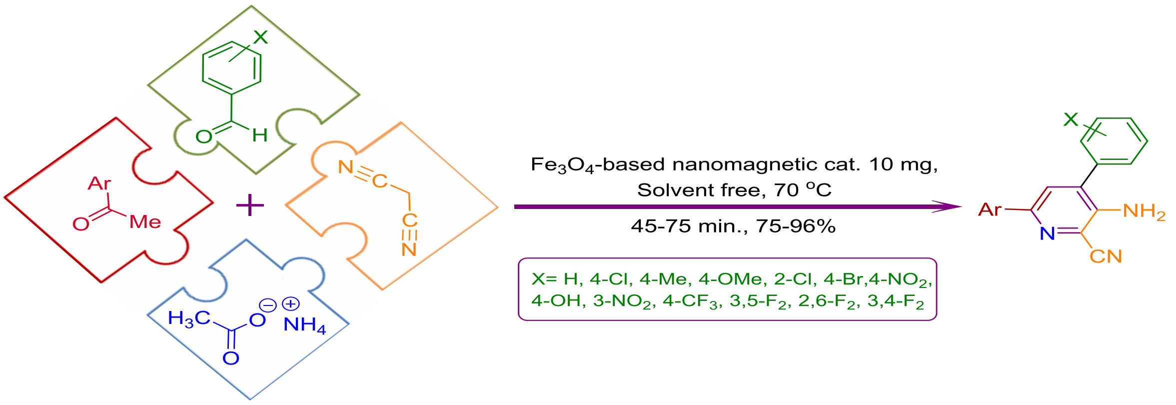

Fig. 1 Synthesis of pyridine derivatives in the presence of nanomagnetic catalyst.

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Paper code: 901

Formic acid catalyzed One-pot synthesis of α- aminophosphonates: an efficient, inexpensive and environmentally friendly organocatalyst

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α-aminophosphonates have always been in the center of attention among the organophosphouros compounds. α-Aminophosphonates are structural analogues of the corresponding α-amino acids in which a carboxylic motif is replaced by phosphonic acid or related groups.

Aqueous formic acid is used for the synthesis of α-aminophosphonates through Kabachnik–Fields reaction applying aromatic amine, phosphite, and carbonyl compounds. Using formic acid as an efficient and low-cost organocatalyst provides environmentally friendly, high yields, low reaction time and mild reaction condition.

Aqueous formic acid has been demonstrated to be a green, effective, inexpensive, insensitive to moisture and more accessible catalyst for synthesis of α- aminophosphonates through Kabachnik–Fields reaction in high yield and mild condition. To conclude, easy work up, low cost of catalyst and high efficiency make our method to be efficient and practical for synthesis of α- aminophosphonates. Further works need to be done to establish whether formic acid can be used in other acid catalyzed, nucleophilic addition and multi-component reactions in catalyst-free conditions.[1],[2]

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Paper code: 902

Hydroxy ethyl methyl morpholinium azide [HEMMorph][N_3] as a novel and highly efficient ionic liquid for three components Click Huisgen cycloaddition reaction.

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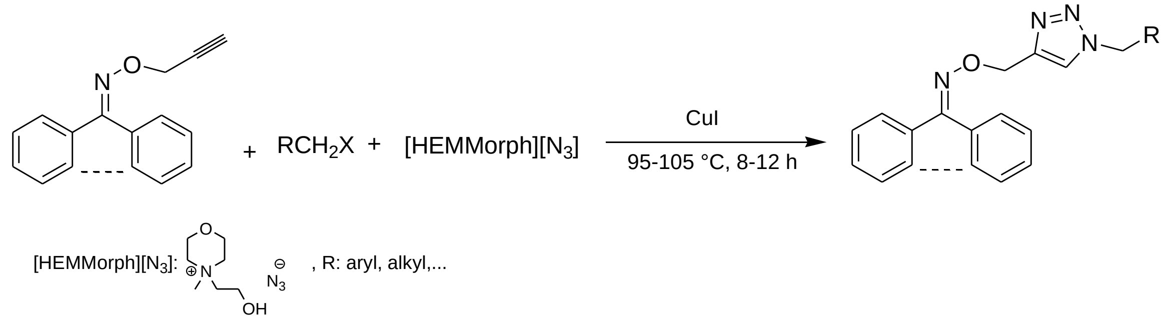
1,2,3-Triazoles are a significant group of azole derivatives with certain pharmaceutical properties. 1,2,3-Triazoles have indeed shown interesting biological activities, for instance, anti-allergic, anti-bacterial, anti-HIV and etc. 1,3-dipolar cycloaddition reaction between alkynes and azids was conducted by Huisgen cycloaddition reaction, which traditionally requires harsh reaction conditions like high temperature, non-regioselectivity and also long reaction times. The use of cupper (I) catalysts extensively accelerate the reaction's rate up to 10^7, which is known as Click cycloaddition reaction [1]. The elaboration of organic solvents can remarkably damage the environment. In this regard to eliminate these hazardous materials, ionic liquids (ILs) are suggested to be utilized as environmental benign solvents.

The molecular structures of ILs can be consisted or modified by diverse anions and cations. ILs are usually known as liquid compounds or can be liquefied below 100 °C, and capable to be recycled and reused [2].To exploit the benefits of ILs in organic synthesis, hereby we have explained the synthesis of novel hydroxyethyl methyl morpholonium azide [HEMMorph][N_3] as a highly efficient ionic liquid media and apply it in synthesis of new 1,2,3-triazolyl derivatives via three components Click Huisgen cycloaddition reaction.



Scheme 1: Synthesis of new 1,2,3-triazolyl derivatives using [HEMMorph][N_3]

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Paper code: 904

Synthesis of titanomagnetite nanoparticles functionalized with sulfamic acid groups and applications for the synthesis of quinazolin derivatives.

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2,3-Dihydroquinazolin-4(1H)-ones are an essential class of heterocyclic compounds. In this research, an efficient and eco-friendly method has been developed for the synthesis of quinazolin by silica- coated titanomagnetite nanoparticles functionalized with sulfamic acid groups and their applications as new catalyst . The catalyst can be separated from the reaction mixture and used again as a catalyst. The compounds of quinazolines have many medicinal and biological properties. Their most important Preparation of mono- and disubstituted 2,3-dihydroquinazoline (H1)-ones. To a solution of isatoic anhydride (1 mmol), 4-cl aniline(1 mmol) and aldehyde (1 mmol) under solvent-free conditions. The reaction mixture was stirred at 100°C for an appropriate time. Once the reaction was completed, as monitored by TLC, the mixture was cooled to room temperature, diluted with 10 ml of ethanol and stirred for 10 min. Then, an external magnetic field was applied to separate the catalyst, and the remaining solution was evaporated. The precipitated solid product was recrystallized from ethanol to yield pure product.[1,2].

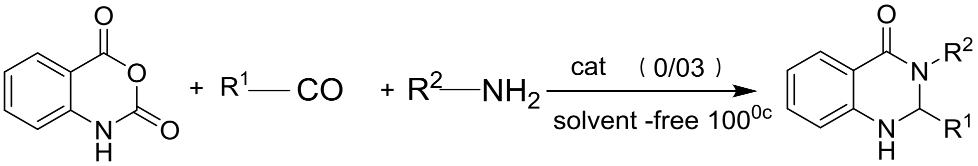

Fig. 1

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Paper code: 909

Application of [mim]C_6F_5O as a novel nano catalyst for synthesis of *β*-azido alcohols under mild and green conditions

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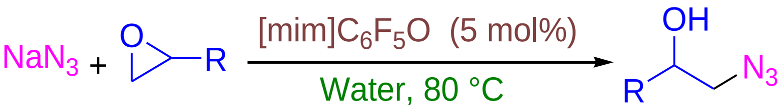
Activity, recovery and task-specific action should be considered, for designing of any novel catalyst. Homogenous catalysts have high activity but their recovery and separation from reaction mixture is difficult so that heterogeneous catalysts can be easily separated and reused but their activity is low [1]. Utilizing the nano catalysts can improve the efficiency of heterogeneous catalysis due to their high surface to volume ratio [2]. Increasing the catalyst's surface will increase the contact between catalyst and reactant. Thus improvement of the activity of the catalyst will be occurred [3]. In continuation of our studies on the knowledge-based development of nano catalysts and ring opening of epoxides, herein we wish to report 1-methyl-1*H*-imidazol-3-ium 2,3,4,5,6-pentafluorophenolate [mim]C_6F_5O as a novel hydrophilic and reusable nano catalyst for synthesis of *β*-azido alcohols from the corresponding epoxides in water at 80 °C (Scheme 1).



Scheme 1: The regioselective ring opening of epoxides using [mim]C_6F_5O as a novel nano catalyst.

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Paper code: 910

Synthesis of 1-amidoalkyl-2-phenols using a novel nanomagnetic catalyst with Cl[DABCO-NO_2]C(NO_2)$_3$ tags under mild conditions

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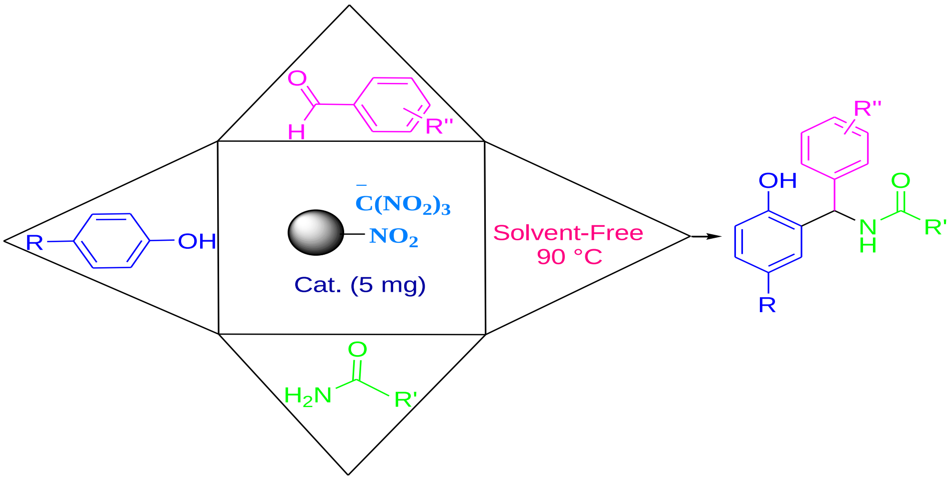
1-Amidoalkyl-2-naphthols are paramount important organic compounds as they can be easily converted to 1-aminoalkyl-2-naphthols via hydrolysis, which are biologically important compounds. 1-Aminoalkyl-2-naphthols have been used as Brady cardiac and hypotensive agents [1]. Moreover, 1-amidoalkyl-2-naphthols can be converted to 1,3-oxazine derivatives [2]. 1,3-Oxazine derivatives have pharmaceutical and biological properties such as anti-tumor, anticonvulsant, antimalarial, analgesic, antibiotic, antianginal, antirheumatic and antihypertensive [3]. So, improvement in 1-amidoalkyl-2-naphtols synthesis methodology is important. Herein, we introduce Fe_2O_3@SiO_2(CH_2)$_3$-Cl[DABCO-NO_2]C(NO_2)$_3$ as a novel nanomagnetic catalyst and use it as an efficient and reusable catalyst in the synthesis of 1-amidophenol-2-naphtols under solvent-free condition.



Scheme 1: The synthesis of 1-amidoalkyl-2-phenol derivatives using Fe_2O_3@SiO_2(CH_2)$_3$-Cl[DABCO-NO_2]C(NO_2)$_3$ as a novel nanomagnetic catalyst.

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Paper code: 911

Synthesis of a novel biological-based glycoluril with phosphorous acid tags: Application for synthesis henna-based compounds

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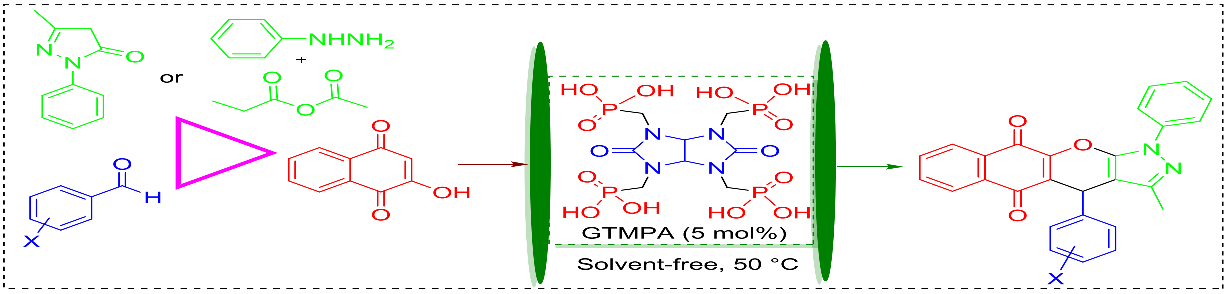
In recent years, there is a great interest in the design and synthesis of easy and safe chemicals and chemical processes [1-2]. Especially the design of new catalysts and catalytic systems from the viewpoint of green chemistry disciplines are more demand. Among of catalysts, heterogeneous solid catalysts are promising materials widely used when trying to develop simple catalytic and eco-friendly processes due to their easy recyclability by a simple filtration and/or centrifugation, and the potential for reusing as the most important issues [3-5]. In recent years, researchers are interested in nano-catalysts because of their high specific surface area and hence the high activity and selectivity usually shown by these materials. In this work the synthesis and characterization of a new glycoluril tetrakis(methylene phosphorous acid) (GTMPA)-derived solid acid nano-catalyst will be presented. Also, we wish to present an efficient and green catalyzed MCR towards the synthesis of 3-methyl-1,4-diphenyl-1,4-dihydrobenzo[6,7]chromeno[2,3-*c*]pyrazole-5,10-dione derivatives (**Scheme 1**).



Scheme 1: Synthesis of 3-methyl-1,4-diphenyl-1,4-dihydrobenzo[6,7]chromeno[2,3-*c*]pyrazole-5,10-dione using glycoluril tetrakis(methylene phosphorous acid) (GTMPA)

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Paper code: 912

Novel crabby biological-based glycoluril with sulfonic acid tags: Application for synthesis of new mono and bis-spiropyrans

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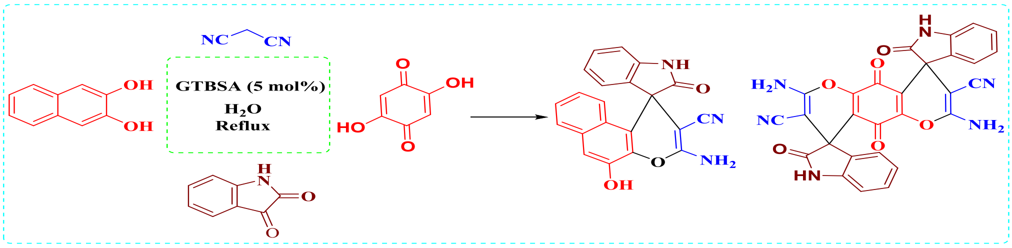
Organic and biological based solid acids are one of the most applicable compounds which have been used for acid-promoted processes and chemical methodologies. Solid acids have received great attention as a general material for a variety of chemical processes because of their reasonable properties such as nonmetallic, nontoxic, with no generated hazardous waste, reusability and high turnover [1-3]. These compounds have great attention for the past decades due to their advantages such as (i) commercial availability, (ii) identical acidic sites, (iii) water stability, (iv) low cost (v) substrate and functional group selectivity, (vi) recycle and reusability and (vii) easy separation from the reaction mixture [4]. In this work, synthesis and characterization of a new glycoluril tetrakis(butane-1-sulfonic acid) (GTBSA), as a novel nanostructure catalyst with alkane sulfonic acid pending groups will be reported. Also, we present an efficient and green catalyzed MCR towards the synthesis of mono and bis-spiropyrans via one-pot condensation of isatine and other components in refluxing water (**Scheme 1**).



Scheme 1: Synthesis of mono and bis-spiropyrans using GTBSA.

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Paper code: 918

synthesis of 1,8-dioxo-octahydroxanthene derivatives catalyzed by sulfacetamide

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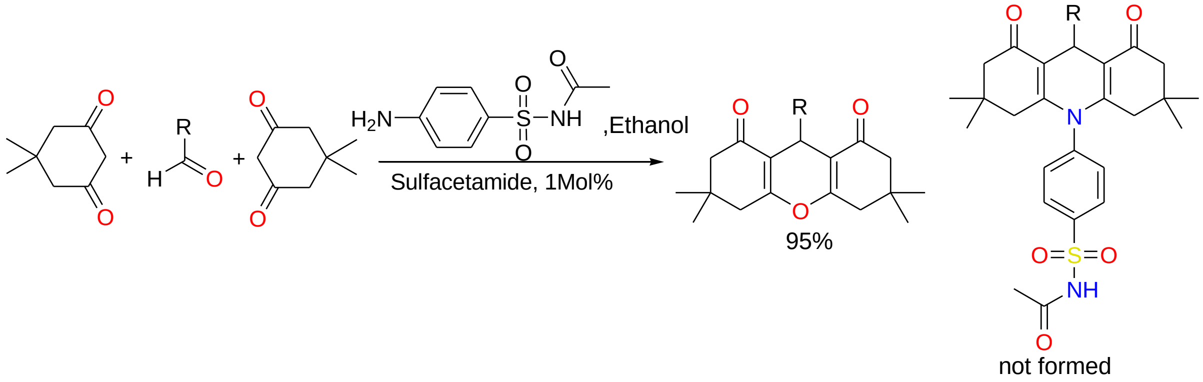
1,8-Dioxo-octahydroxanthenes and their derivatives have been used as additives in pH-sensitive fluorescent materials for visualization of biomolecules, dyes compounds in laser technologies for photodynamic therapy, antagonists for the paralyzing action of zoxazolamine, luminescent sensors, and chiroptical molecular switches [1]. Agricultural bactericide activity, anti-inflammatory effect, anticancer activity, antiviral activity as well as anti-depressant and anti-malarial effects have been reported for several functionalized 1,8-dioxo-octahydroxanthene derivatives. They are also important organic intermediates for the synthesis of a plethora of valuable organic molecules on account of the intrinsic reactivity of the 4*H*-pyran ring in them [2-4]. In the present work, ۱۳ derivatives of 1,8-dioxo-octahydroxanthene was successfully synthesized *via* three-component reaction of dimedone and various aryl aldehydes in the presence of sulfacetamide as the commercially available catalyst. The structures of the final synthesized heterocyclic compounds were characterized using spectral data (IR, ^{1}H NMR, and ^{13}C NMR) analysis.



Scheme 1. The synthesis of 1,8-dioxo-octahydroxanthene catalyzed by sulfacetamide.

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Paper code: 923

Application of Lanthanum Ferrite nano particle in the synthesis of diindolyl-oxindoles

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This study focuses on nano-$LaFeO_3$ particles as nanocatalyst for the synthesis of diindolyl-oxindoles,an important class of potentially bioactive compounds.The oxindole derivatives were prepared by the condensation of indole and isatin compounds in water, an excellent solvent in terms of environmental impact and reduction waste production [1]. The vast majority of catalysts used in modern chemical industry are based on mixed metal oxides including perovskite oxides ABO_3, where A is a rare-earth element, B is 3d transition metal remain prominent Also, perovskite oxides crystals can have broad applications in advanced technologies such as solid oxide fuel cells, catalysts and chemical sensors, magnetic materials, electrode materials, etc [2]. One of most common perovskite oxides, $LaFeO_3$ nanocrystal is a very known material and thus has received intensive investigations over years [3]. In the among tested temperature and the amount of catalyst, the condensation of indole and isatin was best catalyzed by 0.008 gr of Nano $LaFeO_3$ at 90 ℃ as the reaction was completed within a high yield (93-98%).

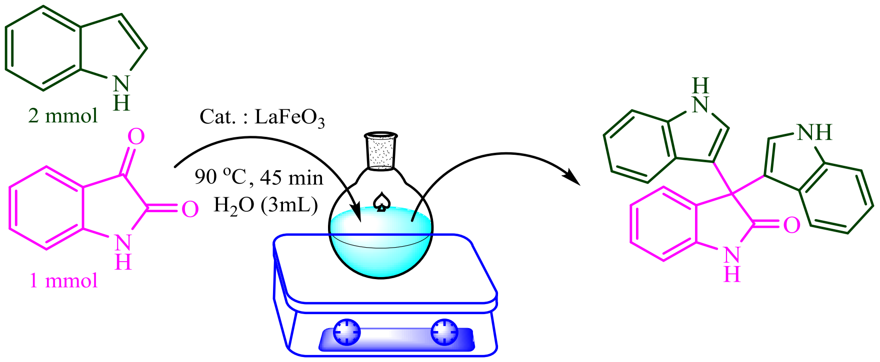

Fig. 1 Three-component synthesis of diindolyl-oxindoles.

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Paper code: 940

Inorganic–organic hybrid nano magnetic as a novel, efficient and reuseable nanocomposite for the synthesis of biphenyl compounds

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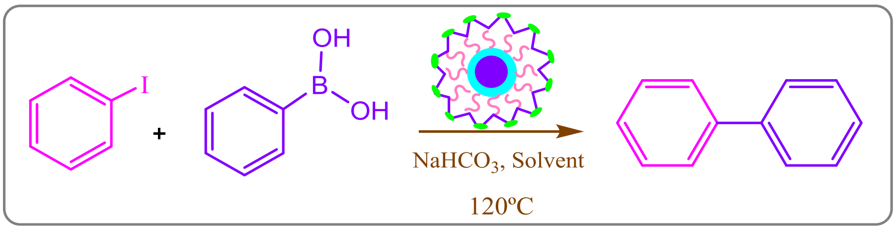
The transition metals-catalyzed Suzuki-Miyaura reaction including the arylboronic acids and aryl halides gives a very significant and clean approach for the formation of a biaryl compound, which creates a partial structure in many of the industrially significant syntheses involving functional polymers, fine chemicals and pharmaceuticals [1-3], because of its demonstrated reliability, its functional group compatibility, and the low cost and ease of handling of a wide variety of commercially available boron-based reagents. It is also the premier cross-coupling process and has been widely applied in organic [2], medicinal and materials chemistry. Herein, we studied a thermal method that provides the efficient and simple preparation of biphenyls from phenylboronic acid and aryl halides derivatives using magnetically recyclable BPMN-Ni complex as heterogeneous catalyst. (scheme1)



scheme1. Suzuki-Miyaura cross-coupling using the $NiFe_2O_4$@ TABTA–Ni complex.

The surface of silica nanoparticles can be functionalized through 3-iodopropyltriethoxysilane. With vigorously stirring, 400 µL of 3-IPTES and 600 µL of ammonia were added to 10 mL of $NiFe_2O_4$@SiO_2 MNPs solution suspended in dry toluene. The solution was refluxed for 24 h, filtered and washed subsequently with toluene, dichloromethane, and dried under reduced pressure at 80ºC for 10 h. A mixture of 3-Iodopropyl functionalized MNPs was added to a suspension of K_2CO_3 (5 mmol) and Malononitrile (5 mmol) in acetonitrile (30 ml). The mixture was refluxed for 48 h.

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Paper code: 941

Chemo-photothermal therapy of cancer cells using gold nanocages covered by smart polymers for controlled release

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Light-based therapies including photothermal therapy have been validated clinically for curative and palliative treatment of solid tumors. However, these monotherapies can suffer from incomplete tumor killing and have not displaced existing ablative modalities. The combination of photothermal therapy and chemotherapy, when carefully planned, has been shown to be an effective cancer treatment option clinically and preclinically [1]. Photosensitive caged compounds have enhanced our ability to address the complexity of biological systems by generating effectors with remarkable spatial/temporal resolutions. The caging effect is typically removed by photolysis with ultraviolet light to liberate the bioactive species. The ultraviolet light may cause damage to biological samples and is suitable only for in vitro studies because of its quick attenuation in tissue. Here we address these issues by developing a platform based on the photothermal effect of gold nanocages were prepared by coating timuli-responsive thiol-end capped ABC triblock copolymer. Gold nanocages represent a class of nanostructures with hollow interiors and porous walls [2]. They can have strong absorption (for the photothermal effect) in the near-infrared while maintaining a compact size. Furthermore, the anti-cancer drug doxorubicin (DOX) was conjugated onto the gold nanorod-cored micelles (GNR@polymer) by electrostatic force. When the surface of a gold nanocage is covered with a smart polymer, the pre-loaded effector can be released in a controllable fashion using a near-infrared laser.

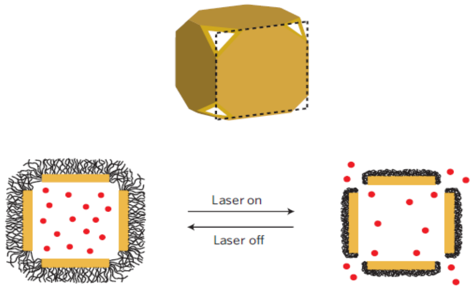

Fig.1. schematic of the controlled-release system

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Paper code: 947

Preparation, characterization and antimicrobial properties of some s-triazine/quinazolinone hybrids

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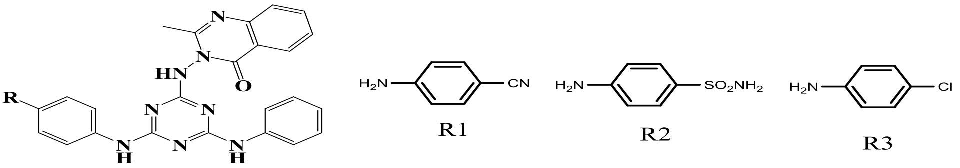
Heterocyclic structures are the basic elements of many pharmaceuticals products. The tri-substituted 1,3,5-triazine analogues is a very important pharmacophore due to its presence in an enormous amount of bioactive compounds [1-4]. In this study, a series of novel 2-methyl-3-((4-(4-arylamino)-6-(phenylamino)-1,3,5-triazin-2-yl)amino)quinazolin-4(3H)-one derivative as potential antimicrobial agents was designed and synthesized. The first chlorine group of the cyanuric chloride (CC) was replaced by aniline in acetic acid at 5 °C. The second chlorine group of the CC was replaced by 4-chlorobenzenamine, 4-aminobenzonitrile and sulfanilamide in the presence of sodium acetate. The last chlorine group of the CC was replaced by hydrazine molecule. Finally, 2-methyl-4H-1,3-benzoxazin-4-one was added to the above compounds and refluxed in ethanol for 10h (Scheme 1). The chemical structure and purity of these hybrid compounds were evaluated by elemental analyses, thin layer chromatography, Fourier transform infrared and, proton along with carbon nuclear magnetic resonance techniques. Antimicrobial activity of the hybrid compounds were study by three Gram-negative bacteria and three Gram-positive bacteria using the serial broth dilution method. Among them, compound with benzenesulfonamide group showed higher antimicrobial activity with a minimum inhibitory concentration (MIC) value of 16 and 32µg/mL. Furthermore, these compounds showed good activity against several tested strains.



Scheme 1: novel hybrid derivatives bearing s-triazine and quinazolinone moieties.

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Paper code: 951

Guanidine Acetic Acid Functionalized Magnetic Nanoparticles: Recoverable Green Catalyst for Transamidation

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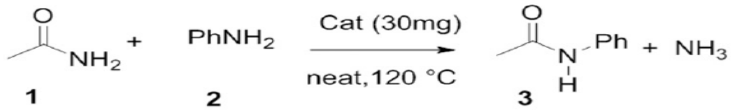
In the presence of a catalytic amount of Fe3O4-Guanidine acetic acid (GAA) nanoparticles, efficient transamidation of several amides with various amines is described under solvent-free conditions. Fe3O4-Guanidine acetic acid nanoparticles provide the first example of a magnetically recoverable organocatalyst for transamidation in the highest catalytic activity. The catalyst could be simply recycled with the assistance of an external magnet and reused for six runs without significant loss of its catalytic activity.

Amides are very important compounds with considerableapplications in both the industrial and academic communities.[1]The amide bond is an important functional group in top selling drugs such as valsartan, captopril, diltiazem, lidocaine, bupivacaineand acetazolamide.



Finally, we have supported guanidine acetic acid on the magnetic nanoparticles without using any supplemental linkers .The catalyst has been demonstrated to be an efficient catalyst for the transamidation of the transamidation products. But benzamide gives moderate to good yield.We also attempted transimidation completedby reaction between a primary amine with the phthalimide as shown atTable 4. Interestingly,the corresponding transimidation productswere obtained in good to excellent yields under solvent free conditions.Also, in the model transamidation reaction, the level ofreusability of this heterogeneous organocatalyst was evaluated.

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Paper code: 952

A one‑ pot synthetic strategy for the construction of chromenoimidazopyridines and chromenopyridopyrimidines containing intramolecular hydrogen bonds

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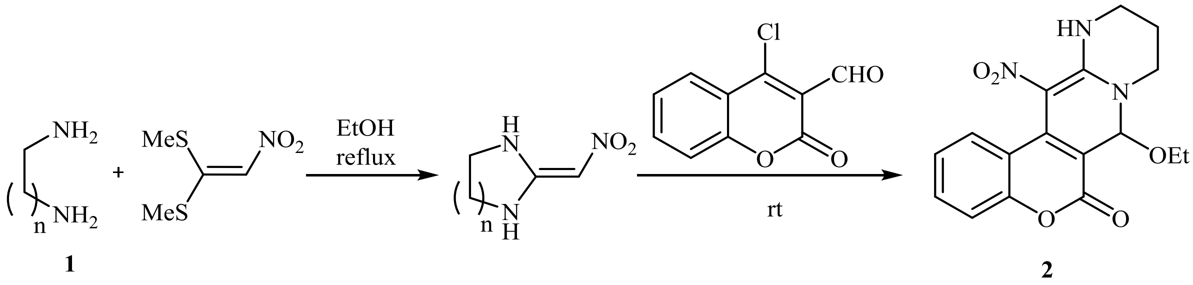
Chromen-2-ones are embedded in a number of natural products and pharmaceuticals. Chromen-2-ones with a fused *N*-ring are frequently found in natural products as lamellarin and ningalin B. As one category of chromen-2-ones with a fused *N*-ring, chromenopyridines have gained increasing interest due to their broad spectrum of bioactivities. For example, they are known as antibacterial and nonsteroidal progesterone receptor modulators.

Considering the importance of chromenopyridines, and based on our continued interest in the one-pot synthesis of heterocycles, herein we wish to report the efficient synthesis of chromenopyridines from the reaction of 1,1-bis(methylsulfanyl)-2-nitroethene, diamines **1**, and 4-chloro-2-oxo-2*H*-chromene-3-carbaldehyde. We used a one-pot sequential three-component procedure for the synthesis of chromenopyridopyrimidines **2** in EtOH at room temperature which resulted in the products with excellent yields (67%) in short reaction times.



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Paper code: 955

Synthesis of a new spiro derivative Catalyzed by p-Toluenesulfonic acid and using three component reaction

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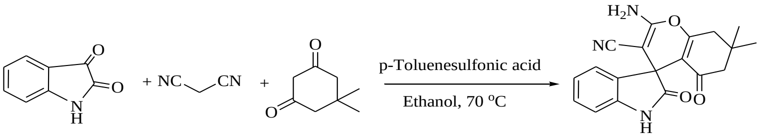
Multi component reactions are a suitable method for the preparation of multi chain molecules and complex heterocyclic compounds which are very significant due to their high efficiency, simplicity of procedure and saving of time, energy, raw materials and solvents. In this paper, a simple and efficient method is developed by using a three-component reaction between the Isatin derivatives, Malononitrile and active methylene compounds, such as 1,3-Diketones, in the vicinity of the catalytic p-Toluenesulfonic acid, which leads to the synthesis of the derivatives of spiropyranoxide. Spiropyranoxindole derivatives can be used as drug precursors in drug synthesis.

In this study, from reaction of the three-component Isatin, Malononitrile, with Dimedone in the vicinity of the acid catalyst of p-Toluenesulfonic acid .the 2-amino-7,7-dimethyl-2,5-dioxo-8,7,6,5-tetrahydrospiro(chromin-3,4-indolin)-3-carbonitrile is synthesized in ethanol solvent and 70°C temperature. (Reaction 1)The optimum reaction conditions were determined for temperature and catalytic value of the product, which contains 30 milligrams of catalysts per 1 mmol of the other ingredients of the reaction material at 70 ° C temperature. The IR and 1H_NMR and 13C_ NMR spectrums confirm the product.



Reaction 1- Preparation of 2-Amino-7,7-dimethyl-2,5-dioxo-8,7,6,5-tetrahydrosperiro (chroman-3,4-indolin) -3-carbonitrile

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Paper code: 959

Nano magnetite supported iron–phthalocyanine as a promising catalyst for the synthesis of β-amido ketones

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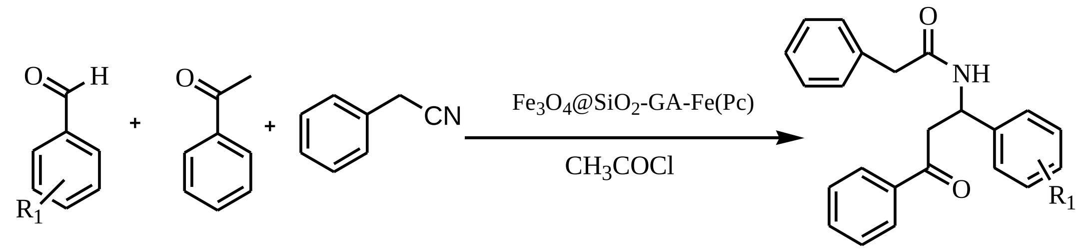
β-Amido ketones are precursors for synthesis of heterocycles, β-amino ketones and β-amino alcohols which are important units in biological compounds such as antibiotic and neopolyoxines [1]. Recently, nanoparticles have attracted attention due to their exclusive features. Owning high surface area, high density of active sites and excellent accessibility, nanomaterials have found use as efficient semi-heterogeneous catalyst in various reactions [2]. Metallophthalocyanines are metal-organic compounds exhibit special physical and chemical properties such as thermal stability, resistance to atmospheric oxidation electrical conductivity, light fastness and inertness to acids and alkalis [3].

In this research, we hope to report the preparation of some new β-amido ketones from acetophenone, benzyl cyanide, acetyl chloride and various aromatic aldehydes in the presence of $Fe_3O_4@SiO_2$-GA-FePc as a heterogamous catalyst at 70° C (Scheme 1). The products have been obtained in high yields and short reaction times. The structure of products has been assigned by nuclear magnetic resonance (NMR) and infrared (IR) together with physical and other spectroscopic data.



R_1= NO_2, Cl, Br, F, OMe

Scheme1. Synthesis of β-amido ketones

References

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Paper code: 966

Palladium nanoparticles supported on natural polymer (silk fibroin): the efficient and recyclable catalyst for Heck reaction

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The Heck reaction, one of the most utilized cross-coupling reactions, is the palladium-catalyzed arylation of an olefin with an aryl halide under basic conditions. It has drawn much attention due to high efficiency and simplicity. Heck methodology is attractive from a synthetic point of view because of its high chemoselectivity and mild reaction conditions along with low toxicity and cost of the reagent if, specifically, the catalyst is recycled.

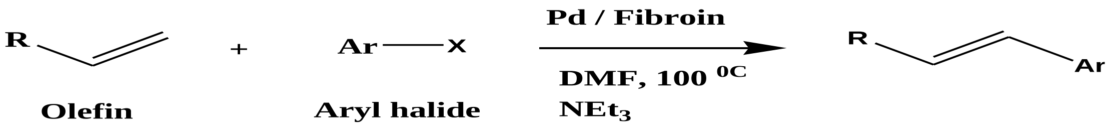

Fig (1): Heck reaction of an olefin with an aryl halide under basic conditions

The Heck reaction is described as a vinylation or arylation of olefins where a large variety of olefins can be used, like derivatives of acrylates, styrenes or intramolecular double bonds [2]. The aryl halide variants developed in addition to typical aryl bromides and iodides are aromatic triflates, aroyl chlorides, aryl sulfonyl chlorides, aromatic diazonium salts, aroyl anhydrides, aryl chlorides and arylsilanols [3]. The Fibroin/ Pd nanoparticles showed high catalytic activity in the heck coupling reaction. Attractive features of this protocol are high yields, simple procedure with an easy work-up, and recyclability and reusability of the catalyst.

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Paper code: 971

Biosynthesis of Ag/MgO nanocomposite using *Acalypha hispida* extract and its ability to the reduction of nitroarenes and organic dyes

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Up to now many different physical and chemical methods were reported to prepare the metal nanoparticles which suffer from many disadvantages. Thus, reporting the green methods as cost-effective and eco-friendly processes are inevitable [1,2]. The biological methods have advantages such as very mild and clean reaction conditions, high yields, avoidance of the dangerous materials, non-toxic solvents, high pressure and temperature. Through this work, a cost effective and environment friendly method for synthesis of Ag/MgO nanocomposite was presented using *Acalypha hispida* extract as reducing and stabilizer agent. In this study the water was used as a green and nontoxic solvent to obtaine the plant extract. Afterward, the catalytic activity of the Ag/MgO nanocomposite was examined for reduction of methylene blue, methyl orange, 4-nitrophenol, 2,4-dinitrophenilhydrazine using $NaBH_4$ in aqueous medium. The catalyst was characterized by TEM, FESEM, EDS and XRD.

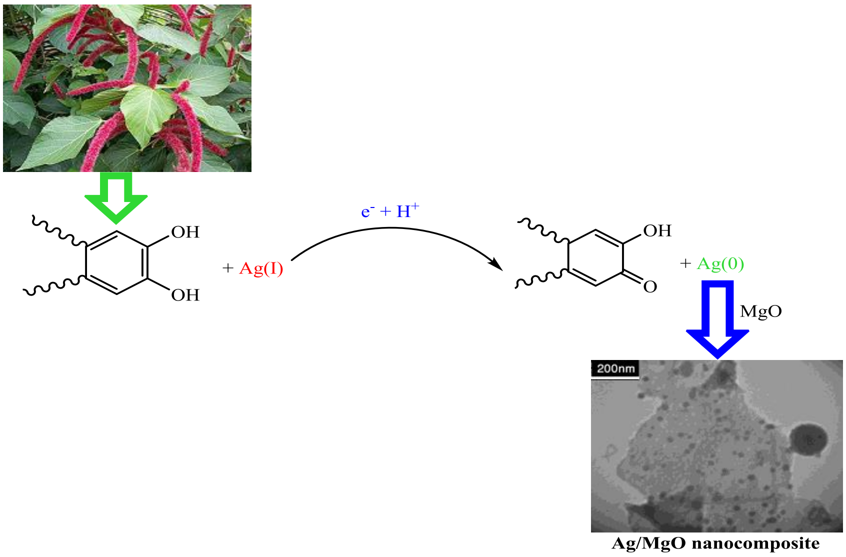

Fig. 1. Green synthesis of Ag/MgO nanocomposite.

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Paper code: 976

C−S Bond Formation *Via* C-H Bond Activation Catalyzed by Co(II)-Immobilized Silica- Based Magnetic Retrievable Nanocatalyst

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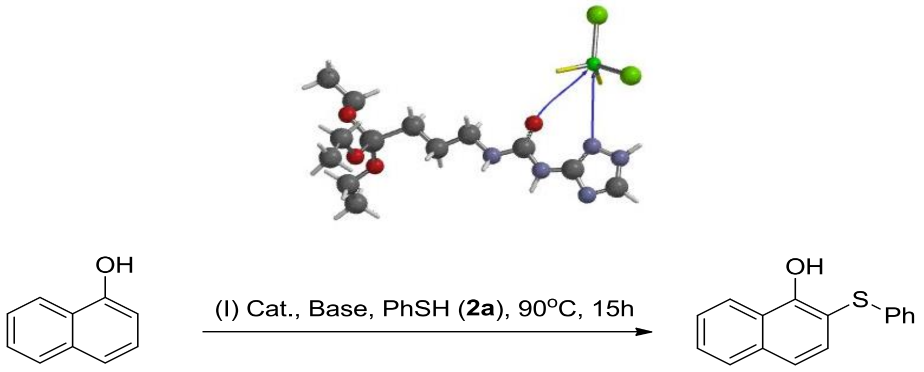
The formation of C−S bonds by method C-H bond activation leading to the synthesis of aryl sulfides is one of very significant strategies in organic chemistry, [1] as several bioactive compounds with broad spectrum therapeutic activities for the treatment of some disease such as Alzheimer, Parkinson, diabetes, anti HIV, anti-inflammatory and immune diseases contain aryl sulfides moieties [2]. Rostami et al. reported green and mild procedures for the C-S bond formation *via* C-N and C-O bond cleavage [3]. Recently, Zolfigol and co-workers have developed Synthesis of 2-(aryl/alkyl-thio) phenols *via* sp^2 C-H bond activation using the reaction of phenols with thiols in the presence of $CoCl_2$ as catalyst [4]. In continuation of our reseach on the development of task-specific catalyst, we wish to report a novel Co(II) supported-nanomagnetic core-shell catalyst for the preparation of aryl sulfide derivatives under mild and green reaction conditions. The presented protocol shows different advantages such as heterogeneous nature of the catalyst which allow an easy separation of the catalyst from the reaction mixture through applying a simple external magnet. Scheme 1 portrayed applied ligand which connected to the surface of magnetic nanoparticle and the style of reaction.



Scheme 1: Applied Co (II) complex, and the style of reaction

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Paper code: 978

An efficient green method for synthesis of 1,8 dioxooctahydroxanthenes in magnetized water as a new solvent

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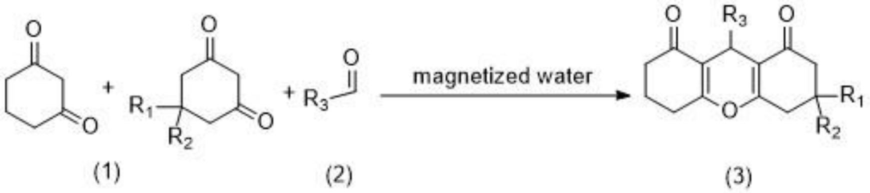
Xanthene's are one of the most broadly distributed groups of natural compounds. Most xanthene derivatives have several biological activities such as the anti-microbial, anti-viral, and anti-tumor [1-3] ones.Among the commonly used solvents in organic synthesis, water is quite non-toxic, and it is the most economical, most abundant, safest, and most environmentally friendly medium. Sometimes water shows a higher reactivity and selectivity in comparison with the other conventional organic solvents because of its strong hydrogen-bonding ability.

The water magnetization technique is an easy one without extra energy consumption when a permanent external magnet is utilized. A permanent external magnet can be installed on a previously established water tube system, resulting in no additional energy requirement for water magnetization.

Here, we wish to report the catalyst-free synthesis of 1,8-dioxooctahydroxanthenes**(3)***via* one-pot three-component reactions of 1,3-cyclohexandione/dimedone **(1)** with various aldehydes **(2)** in magnetized water (Scheme 1).



Scheme 1

To a 10-mL round-bottomed flask equipped with a magnetic stirrer bar and containing magnetized water (5 mL), were added an aldehyde (1.0 mmol) and 1,3-cyclohexandione or dimedone (2.0 mmol). The reaction mixture was stirred at room temperature, and the reaction progress was monitored by TLC using chloroform as the eluent. After completion of the reaction, the precipitate formed was filtered and purified by recrystallization from ethanol to afford the desired product.

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Paper code: 981

Synthesis of new derivatives of 2-alkynylamino-6-substituted-pyrimidine-5-carbaldehyde catalyzed by Pd-Cu

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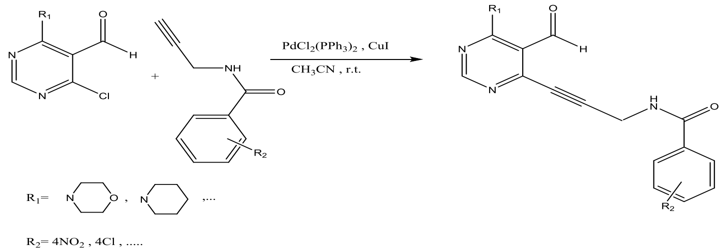
Pyrimidine derivatives are one of the most broadly distributed groups of natural compounds. Most pyrimidine-trione derivatives have several biological properties such as the anti-tumor, anti-cancer, HIV-1 and HIV-2 protease inhibitors, anti-convulsant, and anti-osteoporosis activities [1]. In the last few decades, the concept of catalyzed cascade reactions has been commenced through the advent of transition metal catalysis. Although many transition metal complexes have been found to efficiently catalyze cascade and sequential reactions, palladium complexes are clearly privileged and of paramount importance [3]. The Sonogashira coupling reaction catalyzed by palladium and copper is a powerful and straightforward method for the construction of arylated internal alkynes [4]. In this study, the reaction of 4-chloro-6-substituted-pyrimidine-5-carbaldehyde with various propargylamines catalyzed by Pd–Cu in the presence of triethyl amine as the base in CH_3CN leads to the one-pot formation of novel series of 2-alkynylamino-6-substituted-pyrimidine-5-carbaldehyde in moderate-to-high yields.



Scheme 1.reaction of 4-chloro-6-substituted-pyrimidine-5-carbaldehyde with propargylamines

A mixture of 4-chloro-6-substituted-pyrimidine-5-carbaldehyde (1 mmol), $PdCl_2(PPh_3)_2$ (3.5 mol%), CuI (7 mol%), and Et_3N (2 mmol) was stirred in CH_3CN (5 mL) at room temperature for 20 min under an argon atmosphere. Propargylamines (1.2 mmol) was then added and the mixture was stirred at room temperature for 5 h. After completion of the reaction, the resulting solution was concentrated in vacuo, and the crude product was subjected to silica gel column chromatography using n-hexane:ethyl acetate (9:1) as the eluent to afford the pure product.

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Paper code: 982

Efficient synthesis of novel 1,2,3-triazole-linked pyrimidine via copper-catalyzed click reactions

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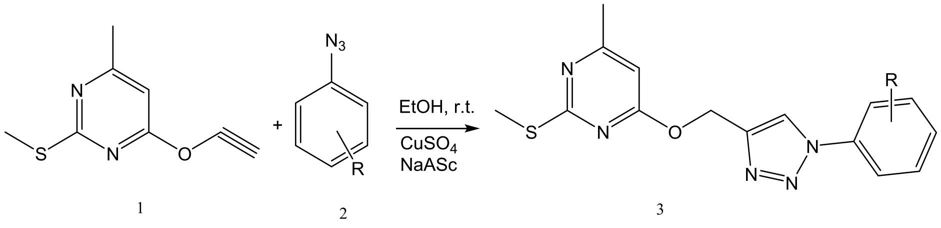
Click chemistry offers a highly efficient technique for connecting two potential building blocks to other functional groups under mild conditions with high tolerance. Click reaction has been widely applied to the synthesis of macromolecules4 and functionalization of biomolecules [1]. 1,2,3-Triazole compounds have an important role not only in organic chemistry but also in medicinal chemistry, drug discovery, agrochemicals, and also as dyes due to their easy synthesis by click chemistry and interesting features as well as multiple biological activities [2]. The pyrimidine skeleton is an important class of nitrogen-containing heterocyclic compounds with a significant pharmacological efficiency including the anti-bacterial [3]. Considering the above subjects, and on the basis of our progressive endeavors in developing Cu-catalyzed reactions of acetylenes leading to heterocyclic compounds of biological significance and environmental benign synthetic methodologies, herein we wish to report the synthesis of new derivatives of the 1,2,3-triazole-linked pyrimidine ring system via the copper-catalyzed click reactions (Scheme 1).



R=4-Me, 4-NO$_2$, 3Cl ,...

Scheme 1.The click reaction of pyrimidine-propargyle with arylazides in the presence of 10 mol% of CuSO$_4$ and 20 mol% of sodium ascorbate at room temperature in EtOH, The desired products, pyrimidine were obtained in good-to-high yields. .

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Paper code: 990

Synthesis of novel derivatives of 1,2,3-triazole-linked pyrazole catalyzed by copper(I)

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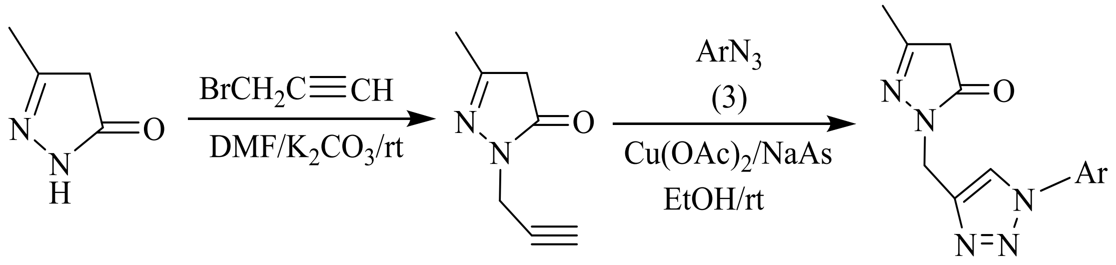
The synthesis of pyrazoles has attracted significant attention due to their pharmacological properties [1]. These derivatives possess a number of important biological roles. For instance, they exhibit anti-bacterial, anti-viral, anti-fungal, anti-histaminic, anti-cancer, anti-depressant, anti-inflammatory, anti-pyretic, and anti-convulsant activities[2,3]. Binding 1,2,3-triazole moieties to other pharmacophores via copper-catalyzed click reactions is important for the synthesis of biologically-active compounds. Copper-catalyzed azide-alkyne cycloaddition (CuAAC) reactions have several priorities over the thermal version including selectivity, increased reactivity of deactivated alkynes, and high yields. In this study, we decided to synthesize new derivatives of the 1,2,3-triazole-linked pyrazole ring system via the copper-catalyzed click reactions.

A mixture of pyrazole (1), K_2CO_3, and propargyl bromide in DMF was stirred for 20 h at room temperature until the disappearance of the starting materials. The resulting solid substance was filtered to afford 3-methyl-1-propargyl-1H-pyrazol-5(4H)-one (2) in good yield. The click reaction of compound (2) with arylazides (3) in the presence of 10 mol% of CuSO4 and 20 mol% of sodium ascorbate at room temperature in EtOH, The desired products, 3-methyl-1-[(1-aryl-1H-1,2,3-triazol-4-yl)methyl]-1H-pyrazol-5(4H)-one (4) were obtained in good-to-high yields.



(1) (2) (4)

Ar: 4-NO2C6H4,4-MeC6H4,4-ClC6H4,....

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Paper code: 991

Functionalized nickel ferrite nanoparticles with phthalocianine-nickel complex as a nano catalyst for microwave assisted synthesis of 1,2,4,5-tetra aryl imidazoles

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A novel, heterogeneous and magnetically recoverable phthalocyanine catalyst has been prepared by the coordinative anchoring the [PC-Ni(II)] complex on silica-coated magnetic nanoparticles ($NiFe_2O_4@SiO_2$) through an amine functionality [1]. The heterogeneous catalyst was characterized by X-ray diffraction spectrum (XRD), scanning electron microscopy (FE-SEM), and Fourier transform spectrometry (FT-IR). Multi-substituted imidazoles, an important class of pharmaceutical compounds, exhibit a wide spectrum of biological activity such as anti-inflammatory, antiallergic, antibacterial, antitumor [2]. The prepared catalysts have been successfully used in the synthesis of 1,2,4,5-tetra aryl imidazoles from reaction of benzyl, aldehyde, amine derivatives and ammonium acetate as catalyst in the ethanol solvent under microwave conditions . The pure products were identified and characterized by physical and spectroscopic data such as; melting point, IR, and ^1H NMR. The recycled $NiFe_2O_4@SiO_2PrA/PC\text{-}Ni(II)$ could be reused for five times without considerable loss of its catalytic activity and gave the corresponding product in high yields. The advantages of reported method are shorter reaction times, higher yields, a low amount of the catalyst, reusability of the catalyst and mild reaction conditions.

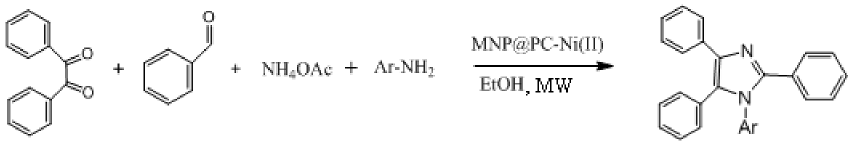

Fig. 1 Preparation of imidazole derivatives in the presence of a catalyst in microsphere and ethanol solvent

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Paper code: 992

Synthesis and Characterization of Fe_3O_4@C-SO_3H as a highly efficient Nano-Catalyst for the preparation of $2^{/}$-aminobenzothiazolomethylnaphthols and 1-amidoalkyl-2-naphthols

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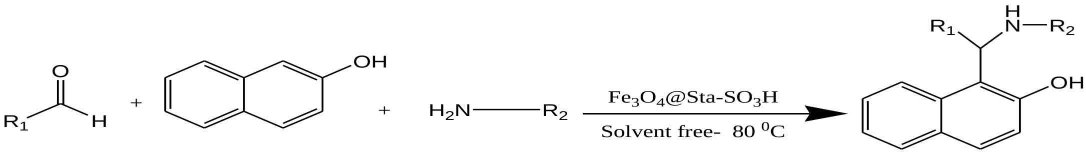
The enhanced activity of heterogeneous (Fe_3O_4@C-SO_3H) ascribed to the high stability of its acid sites, high density, carbon sheets hydrophobic property, and existence of –SO3H and –COOH groups in its molecular structure [1-5]. A stable core-shell structured magnetic solid acid catalyst Fe_3O_4@C-SO_3H, was prepared from Starch, concentrated sulfuric acid and modified magnetic particles of Fe_3O_4, which was used as the core. The effects of the carbonization and sulfonation processes on the activity of the catalysts were investigated. The result showed that preparation conditions had great influence on the quantity of the acidic groups (sulfonic, carboxyl, and hydroxyi groups) and the stability of magnetic catalysts.

Then we used the magnetically Fe_3O_4@Sta–SO_3H catalyst as a heterogeneous catalyst for the preparation of 2/-aminobenzothiazolomethylnaphthols and 1-amidoalkyl-2-naphthols via the one-pot three-component reaction of aldehyde, β naphthol and 2-aminobenzothiazole, acetamide or benzamide (Scheme).



Scheme

To our delight, the reaction was efficiently catalyzed by 0.03 g of Fe_3O_4@Sta–SO_3H at 80 ^{0}C under Solvent-free conditions, to give full conversion and high yield. It is clear from the result that the aromatic aldehydes bearing electron-withdrawing and electron-donating groups performed equally well in this reaction and give excellent yield of the products within 2–8 h.

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Paper code: 993

Catalyst-free method for the synthesis of pyranopyrazoles in magnetized water

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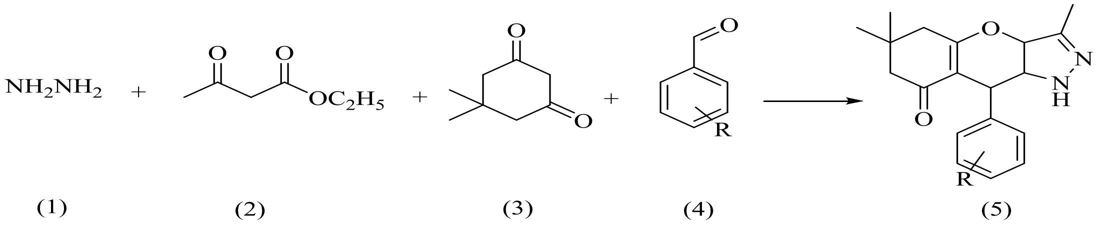
Pyranopyrazoles are fused heterocyclic compounds that possess many biological properties such as fungicidal, bactericidal, and act as anticancer agents[1].Multi-component reactions (MCRs), are those reactions in which three or more reactants react together to give the production a single step under suitable reaction conditions [2]. From the 1950s, we have known that water can be magnetized when exposed to an applied magnetic field, although the magnetization effect is very small [3]. Herein, we are reporting a simple and efficient synthesis of pyranopyrazoles (**5**) by a four component reaction of hydrazine (**1**), ethylacetoacetate (**2**), dimedone (**3**) and aromatic aldehydes (**4**) in magnetized water at 50 °C.

Preparation of magnetized water in order to prepare a magnetized water, 5 mL distilled water was first put in a test tube, which was then put between two neodymium magnets NdFeB (10cm×5cm×4cm) with a magnetic field of 0.8*T*. After20 min, the test tube was subsequently removed from the instrument and used for the reaction.

General procedure for synthesis of pyranopyrazoles To 10-mL round-bottomed flask equipped with a magnetic stirrer bar and containing magnetized water (5 mL), were added ethyl acetoacetate (1.0 mmol), hydrazine (1.0 mmol), an aldehyde (1.0 mmol), and dimedone (1.0 mmol). The reaction mixture was stirred at 50 °C, and monitored by thin layer chromatography (TLC) technique. After completion of the reaction, the precipitate thus formed was filtered and purified by recrystallization from ethanol to afford the desired product.



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Paper code: 994

Glycerin mediated-synthesis of 2-amino-4-aryl-3-cyano-4H-pyran derivatives

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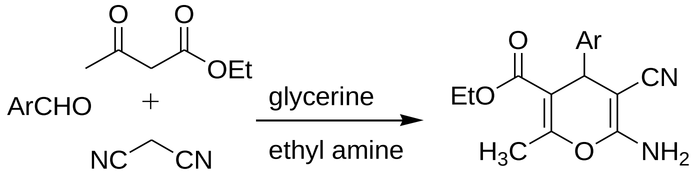
Polyfunctionalized 4H-pyrans are an important class of organic compounds due to their useful biological and pharmacological activities [1] such as antiallergic, antitumor, antibacterial activity, as potentially biodegradable agrochemicals, a structural unit of many natural products, and potential calcium channel antagonists [2].
In a one neck flask, ethyl acetoacetate (1 mmol), aryl aldehydes (1 mmol) and malononitrile (1 mmol) were mixed in glycerin and ethyl amine (1 ml) at 100 ºC. After completion of the reaction monitored by TLC, water was added and the product was obtained as a solid compound. The desired product was resulted after filtration, dried and recrystallized by ethanol and identified by Perkin Elmer FT-IR spectrometer and ^{1}HNMR spectra on Bruker DRX- 300 MHZ NMR instrument.
Aromatic aldehydes, malononitrile and ethyl acetoacetate were used in the synthesis of 2-amino-4-aryl-3-cyano-4H-pyran derivatives in glycerin and ethyl amine at100 ºC under reflux condition (Scheme 1). The experimental procedure is very simple and represents an attractive alternative to existing methods. This reaction protocol has the potential for developing combinatorial libraries.



Scheme1. Synthesis of 2-amino-4-aryl-3-cyano-4H-pyran derivatives

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Paper code: 997

Synthesis of new azo compounds based on thiazolidinone derivatives.

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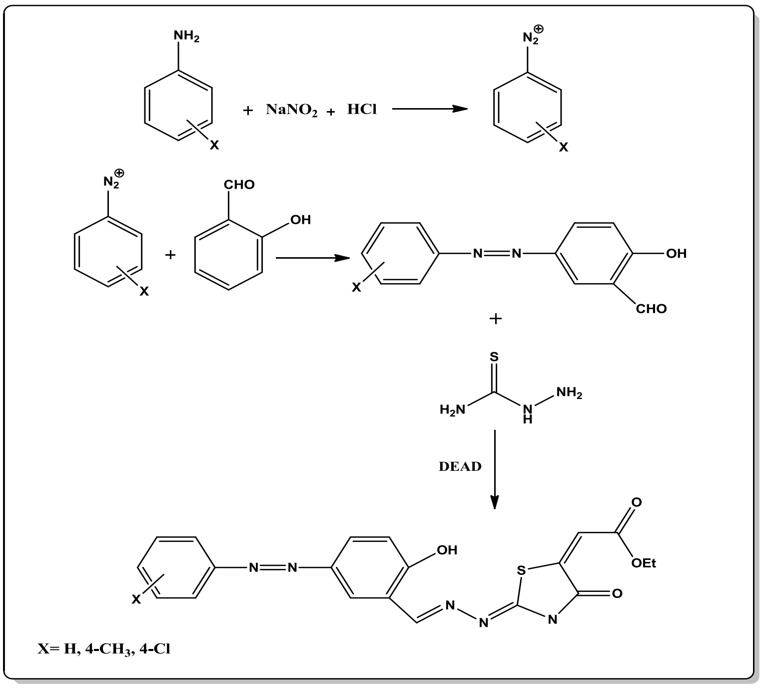
Azo compounds have been most widely used in many fields and technologies like textiles, paper, plastic, leather, ink jet printers, laser liquid crystalline displays [1-2]. Some novel azo compounds based on thiazolidinone were designed and synthesized. Diazonium ions synthesis of coupling reaction between aniline derivatives and with 2-hydroxy benzaldehyde. Then from the reaction of diazonium salts whit thiosemicarbazide and diethyl acetylene dicarboxylate products containing thiazole rings were synthesized. (Scheme 1)



shceme 1: Synthesis of new azo compounds based on thiazolidinone derivatives.

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Paper code: 999

Antibacterial activity of AgO- chitosan composite against aquaculture pathogenic bacteria (case study: *Edwardsiella tarda*)

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Chitosan is one of the bio-degradable natural products which can be used in heavy metal composites forms in antimicrobial agents and treatment measures [1, 2]. In this study, antibacterial activity of AgO-chitosan composite was tested against aquaculture bacterial disease agent, *Edwardsiella tarda*. Ag ions were adsorbed into the chitosan structure and surface chelation to form Ag-loaded composite. The physicochemical properties of the composites were determined by FTIR analysis, FESEM images and EDX. Disk diffusion method indicated that prepared composite has antibacterial activity. Minimum inhibitory concentration (MIC) and minimum bacterial concentration (MBC) of composites were determined at different times and antibacterial amounts. Antimicrobial activity assays indicated that prepared composite exhibited marked inhibitory activity against *Edwardsiella tarda*. The minimum inhibitory concentration (MIC) values were slightly lower than the MBC values for two composites at different time and concentrations. Results demonstrated that AgO-chitosan composites could inhibit the growth of tested bacteria. The antibacterial activity of AgO-chitosan composites provides the possibility of further clinical investigations leading to its application in aquaculture industry.

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Paper code: 1004

Synthesis of 2-hydroxy-1,4-naphthoquinone derivatives using Cu (II) immobilized on hyperbranched polyglycerol functionalized graphene oxide catalyst

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Molecules with the napthoquinone structure are of interest because of their occurrence in nature and their widespread biological properties. Also, quinone derivatives have been introduced as fluorescence materials [1]. Recently, two dimensional carbon based nanostructures such as graphene and graphene oxide have used as substrate for polymer matrices. Because of large surface area and presence of oxygen containing groups on basal surfaces and sheet edges of the GO materials, polymers can be adsorbed onto the graphene surface [2]. Hyperbranched polymers grafted covalently or non-covalently to a substrate which have been used for the generation of hybrid structures be it in the field for surface and particle functionalization. A class of hyperbranched polymers is polyglycerol with tree-like structure and a large number of hydroxyl functional groups in its backbone and environs [3]. The chemical grafting of HPG onto the surface of graphene oxide also supply a suitable surface for their functionalized with organic compound to obtain novel nanostructures. Herein, we would like to report the synthesis and application of Cu (II) immobilized on hyperbranched polyglycerol functionalized graphene oxide as an environmentally-benign, highly efficient and reusable catalyst for the preparation of aminonaphthoquinone derivatives via one-pot three-component condensation reaction under solvent-free conditions.

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Paper code: 1011

Electrospun Soluble Eggshell Membrane Protein/Galatin/Polycaprolactone for Tissue Engineering Applications

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In recent years natural polymers have been widely used in biomedical applications. Application of natural and biocompatible polymers in wound dressing, medical sutures and tissue engineering are extensively growing. Eggshell membrane (ESM) has potential as a natural scaffold because of its highly porous structure and good biocompatibility. The objective of this study is to prepare and evaluate a new type of soluble eggshell membrane protein (SEP)/ Galatin/PCL nanofibers using electrospinning method for tissue Engineering application. SEP/ Galatin/PCL nanofibers were successfully prepared with various blending ratios. The morphology, chemical composition, surface wettability, and mechanical properties of the nanofibers were characterized using scanning electron microscopy (SEM), contact angle measurement, Fourier transform-infrared spectroscopy (FTIR), and a universal testing machine. Results showed that the SEP/Galatin/PCL electrospun membrane was composed of uniform, bead-free nanofibers, which formed an interconnected porous network structure. The biological study results showed that SEP/ Galatin/PCL nanofibers could enhance cell attachment, spreading, and proliferation. The study indicated the potential of SEP/ Galatin/PCL nanofibers for Tissue Engineering application and provided a basis for future optimization.

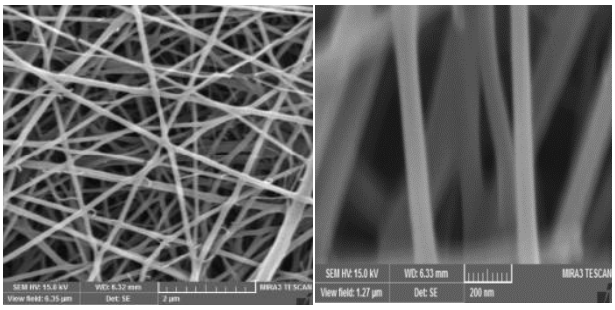

Fig. 1 SEM photographs of electrospun SEP/ Galatin/ PCL fibers.

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Paper code: 1018

A Sequential One-pot Three-component Synthesis of 2-Oxindole Scafold Containing Dihydropyrazine by Using Triethylammonium thiolates

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Pyrazines and its derivatives have shown different biological activities such as cytotoxic and antitumor, antimycobacterial, antituberculosis, antifungal, antibacterial and etc. The most common synthesis method of pyrazines is dehydrogenation of 2,3-dihydropyrazines which are prepared from reaction between 1,2-diamines and 1,2-dicarbonyl compounds. Furthermore, dihydropyazines also showed DNA strand-breaking activity and growth inhibition of *Escherichia coli*. Therefore, dihydropyrazines and pyrazines are amongst the most scaffolds used in natural products and chemotherapeutic agents.[1]

Oxindoles, especially substituted oxindoles at 3-Position have been exhibited antibacterial, antiinflammatory, antifungal, antimalarial, antitumor, antimicrobial, and antiviral activities. Moreover, the oxindole framework has been found in many biological and pharmaceutical active compounds and natural products.[2]

Because of the importance and applications of compounds contain of dihydropyrazine ring, and 2-oxindole skeleton, and in order to develop our studies on the synthesis of oxindole derivatives,[3] we report the one-pot three component reaction between triethylammonium (*Z*)-2-oxo-1-(2-oxoindolin-3-ylidene)-2-phenylethane-1-thiolate **1**, methyl iodide **2** and 1,2-diamines **3** in DMF at room temperature for the preparation of (*Z*)-3-(3-aryl-5,6-dihydro-2(1*H*)-pyrazinyliden)-1*H*-indol-2-ones **4** (Fig. 1).

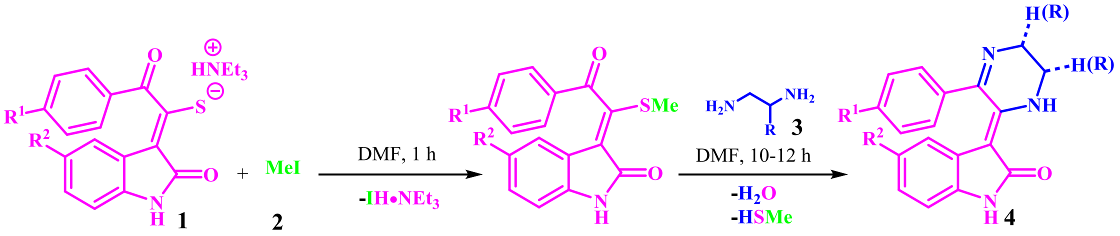

Fig. 1 the preparation of (*Z*)-3-(3-aryl-5,6-dihydro-2(1*H*)-pyrazinyliden)-1*H*-indol-2-ones **4**

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Paper code: 1022

A New Method for the Preparation of thiosulfonates from H_2O_2–Me_3ClSi

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Hydrogen peroxide, in the presence of Me_3ClSi , is a very efficient reagent for the direct oxidative conversion of thiol derivatives into the corresponding thiosulfonates. This method has been applied to a variety of substrates including nucleophilic and sterically hindered thiols, In most cases these reactions are highly selective, good to excellent yields, short reaction times, high efficiencies, cost-effectiveness, and, facile isolation of the desired products make the present methodology a practical alternative.

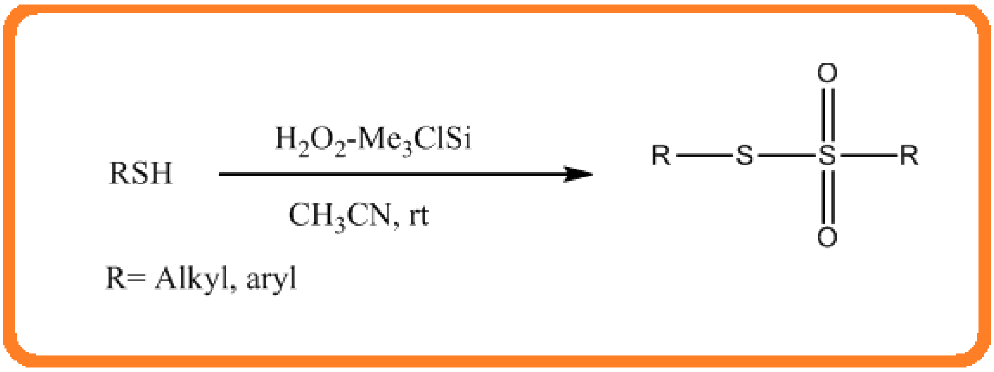

Fig. 1 Synthesis of thiosulfonates from thiols.

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Paper code: 1039

4H-benzochromene derivatives catalyzed by KCC-1@SO_3H nano heterogeneous solid acid

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During the last decade, 4H-benzochromene derivatives have received great attention in organic chemistry due to their biological and pharmaceutical properties such as antimicrobial, antiviral, sex pheromone, antitumor, anti-inflammatory, anti-tubercular, and cancer therapy [1]. These compounds were synthesized via multicomponent reaction of aromatic aldehyde with malononitrile and β-naphthol in the presence of various Bronsted and Lewis acids such as methane sulphonic acid, $TiCl_4$, $H_{14}[NaP_5W_{30}O_{110}]$, p-TSA, as well as basic catalysts such as g-alumina, Na_2CO_3, K_2CO_3, piperidine, nano sized MgO and NaOH. To overcome some drawbacks like the recovery of catalysts and promote the catalytic efficiency, Bronsted acids are supported on solid material producing heterogeneous solid acid. A KCC-1 silica nanosphere with high surface area, which comes from its fibrous morphology, is an excellent nominee to utilize as a support to design efficient heterogeneous nanocatalysts that would satisfy these conditions [3]. In this study, 4H-benzochromene derivatives were synthesized by multicomponent reaction of aromatic aldehyde with malononitrile and β-naphthol in the presence KCC-1@SO_3H in water media at reflux conditions. The results showed that the corresponding products were obtained in excellent yields (90-95%)(fig. 1). The catalyst was reused for several times without lack of activity.

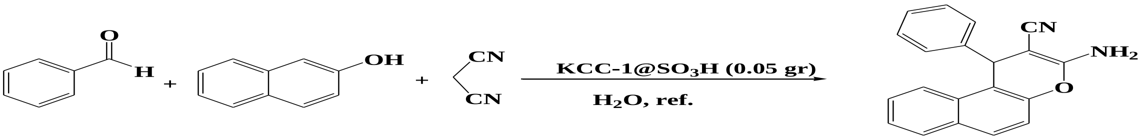

Fig. 1 Three-component synthesis of 2-amino-4H-chromenes

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Paper code: *1041*

N^1,*N*^{1},*N*^{2},*N*^{2}-Tetramethyl-*N*^{1},*N*^{2}-bis(sulfo)ethane-1,2-diaminium chloride as a highly effective catalyst for the synthesis of 3,4-dihydropyrimidin-2-(1*H*)-ones (-thiones)

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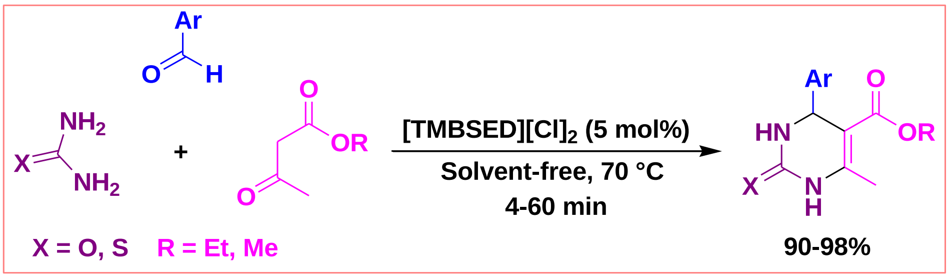
The important class of *N*-heterocycles is 3,4-dihydropyrimidin-2-(1*H*)-ones (-thiones). These compounds have attracted considerable attention in organic and medicinal chemistry, because of their pharmacological and therapeutic properties; e.g. antiviral, antitumor, antibacterial, antihypertensive and anti-inflammatory activities. Moreover, 3,4-dihydropyrimidin-2-(1*H*)-ones (-thiones) are used as calcium channel blockers, adrenergic antagonists and neuropeptide Y (NPY) antagonists [1,2].

Ionic liquids (ILs) have been extensively as useful solvents and catalysts in organic synthesis, because of possessing various unique properties, including high thermal and chemical stability, non-flammability, non-volatility and enhanced reactivity. Brønsted acidic ILs are an important class of these compounds, which have been designed especially to apply as efficient catalysts for organic transformations [3].

In this work, Brønsted acidic ionic liquid *N*^{1},*N*^{1},*N*^{2},*N*^{2}-tetramethyl-*N*^{1},*N*^{2}-bis(sulfo)ethane-1,2-diaminium chloride {[TMBSED][Cl]$_2$} has been used as a highly effective catalyst for the reaction of arylaldehydes with β-ketoesters and urea (or thiourea) under solvent-free conditions to synthesize 3,4-dihydropyrimidin-2-(1*H*)-ones (-thiones) (Scheme 1). Excellent yields, short reaction times, easy work-up and purification of the products, easy production of the catalyst and relatively mild conditions are some advantages of this procedure.



Scheme 1. The production of 3,4-dihydropyrimidin-2-(1*H*)-ones catalyzed by [TMBSED][Cl]$_2$.

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Paper code: 1043

A new application of KCC-1@SO_3H as a heterogeneous catalyst in crossed-aldol condensation reaction under solvent-free conditions

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Aldol condensation is an important reaction in the biosynthesis of carbohydrates, and it is used for the synthesis of α, β–unsaturated ketones, which have great potential and valuable intermediates in organic synthesis [1]. Numerous methods including homogeneous acids or bases as well as heterogeneous catalyst are known to generate the aldol products over the last three decades [2]. A KCC-1 silica nanospheres with high surface area, which comes from its fibrous morphology is an excellent nominee to utilize as a support to design efficient heterogeneous nanocatalysts that would satisfy these conditions [3]. In this study, KCC-1@SO_3H which is synthesized by supporting of chloro sulfonic acid onto the KCC-1 as a strong heterogeneous solid acid was used in Aldol-condensation reaction. The reactions were proceeded using Acyclic/cyclic ketone (1 mmol) with aromatic aldehyde derivatives in the catalytic amount of KCC-1@SO_3H under solvent –free conditions at 100 ^{0}C to produce α,ά- bis(substituted-benzylidene) alkanone. The results showed that the corresponding products were synthesized in good to excellent yields (90-95 %) (Fig. 1). The recovered nanocatalyst was successfully reused for several runs without significant loss in its catalytic activity.

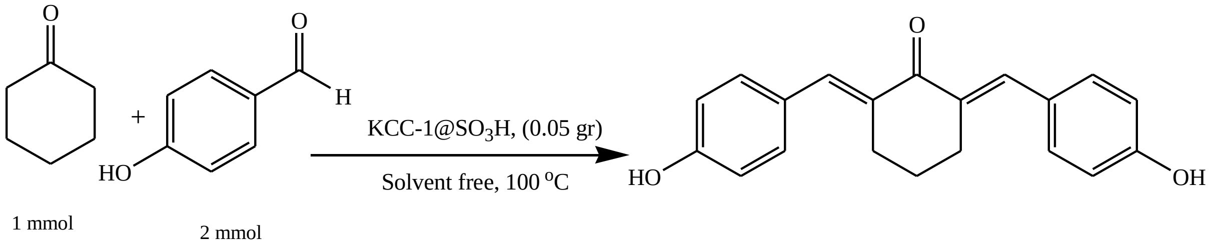

Fig. 1 Schematic illustration for synthesis of α,ά- bis(substituted-benzylidene) alkanoen

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Paper code: 1044

Sulfonic acid-functionalized phthalimide (SFP) as a highly Efficient catalyst for the synthesis of 4*H*-pyrano[2,3-*c*]pyrazole

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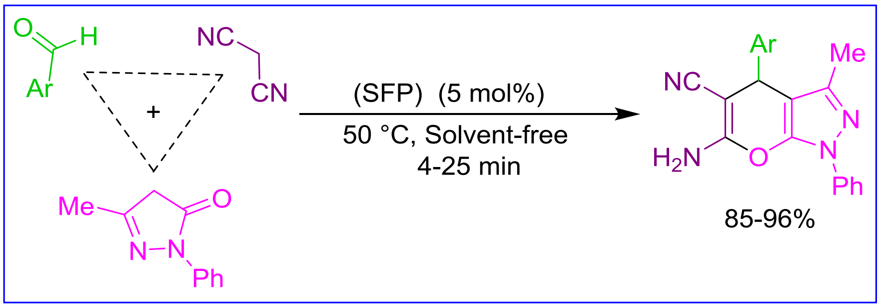
4*H*-Pyrano[2,3-*c*]pyrazole derivatives are of importance in medicinal chemistry, since they are used as precursors to potential drugs, and indicate different pharmaceutical activities, such as anti-inflammatory, antibacterial, anticonvulsant, analgesic, antimicrobial, antifungal, and anticancer properties [1,2].

In recent years, sulfonic acid-containing catalysts have attracted much attention in synthetic organic chemistry. The use of this class of catalysts to promote organic transformations, is associated with various benefits including: (i) enhanced reactivity as well as selectivity, (ii) uncomplicated work-up, (iii) easy accessibility of the starting materials for the catalyst synthesis, (iv) efficiency, (v) environmentally friendly reaction conditions, and (vi) ability to promote a wide range of reactions [3].

In this work, sulfonic acid-functionalized phthalimide (SFP) has been used as a highly efficient catalyst for the reaction of arylaldehydes, malononitrile and 3-methyl-1-phenyl-2-pyrazolin-5-one under solvent-free conditions to synthesize 4*H*-pyrano[2,3-*c*]pyrazoles (Scheme 1). Excellent yields, short reaction times, easy work-up and purification of the products, easy production of the catalyst and relatively mild conditions are some advantages of this procedure.



Scheme 1. The syntheis of 4*H*-pyrano[2,3-*c*]pyrazoles catalyzed by SFP.

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Paper code: 1047

A novel access to new pyrrolo[1,2-a]quinoxalines through palladium-catalyzed multi-component reactions

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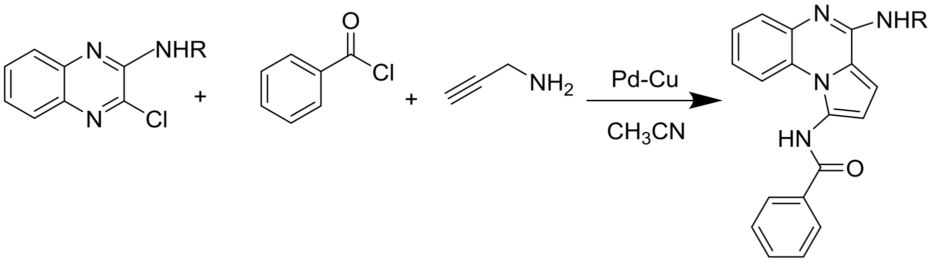
Quinoxaline and its derivatives are an important class of nitrogen-containing heterocyclic compounds, show a broad spectrum of biological activities including antitumor,[1] antiviral, and anti-inflammatory,[2] properties.

We herein present an efficient and successful approach for the synthesis of new pyrrolo[1,2-a]quinoxalines with good-to-high yields. The multi-component reaction of 3-amine substituted 2-chloroquinoxalines, benzoyl chlorides and prop-2-yn-1-amine in the presence of palladium-copper catalyst afforded functionalized pyrrolo[1,2-a]quinoxalines by amide and amine substituents at 1 and 4 positions respectively. This strategy provides the biologically active molecules in a one-pot process. All the new synthesis compounds were characterized by the analytical spectral data.



Scheme 1. One-pot multi-component synthesis of pyrrolo[1,2-*a*]quinoxalines through palladium-catalyzed reactions.

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Paper code: 1048

Novel multi-component synthesis of 4-ethynyl substituted pyrrolo[1,2-*a*]quinoxalines through palladium-catalyzed coupling-coupling reactions

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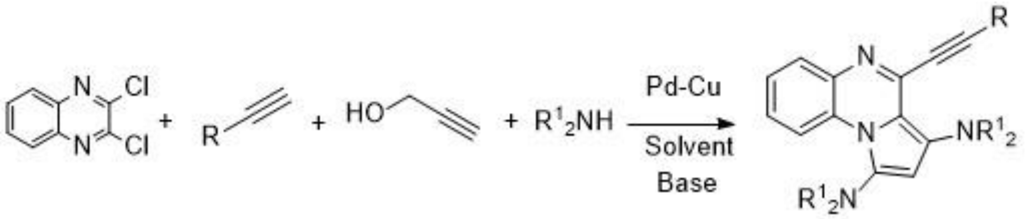
Quinoxaline and its derivatives are an important class of benzoheterocycles displaying a broad spectrum of biological activities which have made them privileged structures in pharmacologically active compounds [1]. Pyrrolo[1,2-a]quinoxalines and their analogues have outstanding roles in natural products [2], displaying broad pharmacological activities such as anti-tumor, adenosine A3 receptor modulator, anti-parasitic, and anti-HIV. Moreover, they are significant intermediates for the construction of 5-HT3 receptor agonists. Consequently, the progression of novel and highly efficient methods for the synthesis of pyrrolo[1,2-a]quinoxaline derivatives is highly favorable for drug discovery [3].

In this work, 4-ethynyl-1,3-disubstituted pyrrolo[1,2-*a*]quinoxalines were synthesized by a multi-component reaction of 1,2-dichloroquinoxaline, terminal alkynes, propargyl alcohol and secondary amines in the presence of a palladium-copper catalytic system. This one-pot process provides a novel synthetic approach for the preparation of 1,3,4-trisubstituted pyrrolo[1,2-*a*]quinoxalines by the formation of two C-C bonds through palladium-catalyzed two coupling reactions in a single reaction procedure. All the new synthesized compounds were characterized by the analytical spectral data.



Scheme 1. One-pot four-component synthesis of pyrrolo[1,2-*a*]quinoxalines.

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Paper code: 1050

A one-pot synthetic approach for construction of thiazolo[3,2-a]benzimidazole-linked quinoxaline scaffold via palladium-catalyzed reactions

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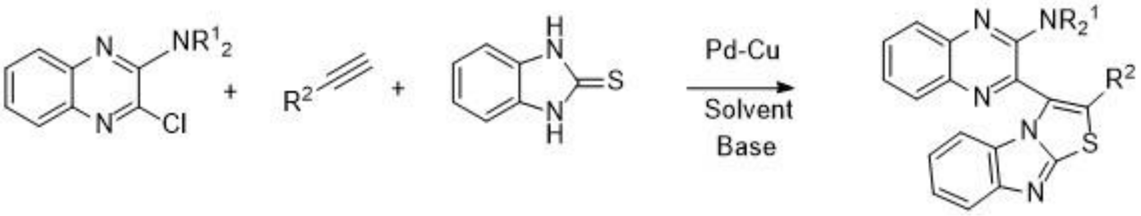
Nitrogen heterocyclic compounds are the most abundant and integral scaffolds that occur ubiquitously in a variety of synthetic drugs, bio-active natural products, pharmaceuticals, and agrochemicals. Due to their broad applications, these compounds have long been a subject of great interest, and fundamental efforts have been made for the development of synthetic strategies that could lead to the discovery of new bioactive compounds in medicinal chemistry. [1]

In this research work, a novel thiazolo[3,2-a]benzimidazole-linked quinoxaline system were synthesized by a multi-component reaction of 3-amine substituted 2-chloroquinoxalines, terminal alkynes and 1*H*-benzo[d]imidazole-2(3*H*)-thione in the presence of the palladium-copper catalyst. This one-pot process provided an efficient and successful approach for the construction of new thiazolo[3,2-a]benzimidazole-based quinoxaline scaffold with good-to-high yields. All the new synthesized compounds were characterized by the analytical spectral data.



Scheme 1. One-pot three-component synthesis of thiazolo[3,2-a]benzimidazole-linked quinoxaline scaffold.

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Paper code: 1051

One-pot Synthesis of quinoxaline Derivatives via Palladium-catalyzed reactions

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The pyrrolo[1,2-a]quinoxaline skeleton is present in various heterocyclic compounds possessing interesting biological activities. Quinoxaline derivatives display a broad spectrum of biological activities including anti-microbial,[1] anti-inflammatory [2] and anticancer [3] properties. A literature survey shows that the synthesis of quinoxalines, starting from the quinoxaline moiety, has been under explored. Consequently, the development of new synthetic strategies for the synthesis of quinoxaline derivatives from the quinoxaline scaffold are important.

In this research work, new quinoxalines were synthesized through the multi-component reaction of 3-substituted 2-chloroquinoxalines, benzoic acids and propargyl bromide in the presence of a palladium-copper catalytic system. This one-pot process provided an efficient and successful approach for the construction of 1,4-disubstituted quinoxalines with good-to-high yields. All the new synthesized compounds were characterized by the analytical spectral data.

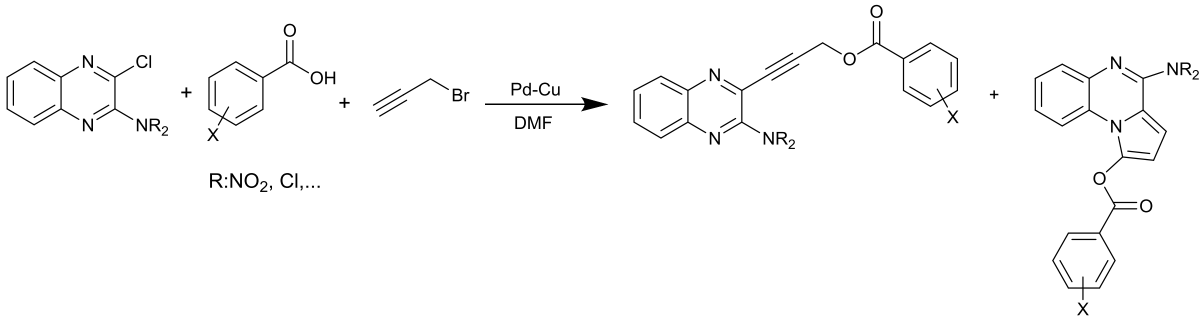

Fig. 1 One-pot synthesis of 1,4-disubstituted quinoxalines through palladium-catalyzed reactions.

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Paper code: 1058

Agar: a natural and environmentally friendly substrate composed with copper oxide nanoparticles for efficient synthesis of 1,2,3 triazoles

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Nanocatalysts are important substances in chemical processes, energy production, saving energy and prevention of environmental contaminants. By considering natural polymers to be the substrate of nanoparticles in nanocatalysts, they play an important role in organic synthesis. Agar, as a natural polymer, is extracted from an agarophyte which attracted a lot of attention due to its unique applications such as food industry, microbiology, pharmacy, cosmetics and dentistry [1]. Due to a large number of hydroxyl groups in their structure, they can be used as an efficient acidic catalyst in organic synthesis or considered a good hostage for metals which can catalyzed a verity of reactions. 1,2,3-triazole are heterocyclic rings formed by the bipolar azide ring and alkin in the presence of a copper catalyst [2]. The new $Cu_2O/Agar@Fe_3O_4$ nanoparticles was tested in the synthesis of 1,2,3-triazole via a one-pot three-component reaction in this study (Fig. 1) [3].

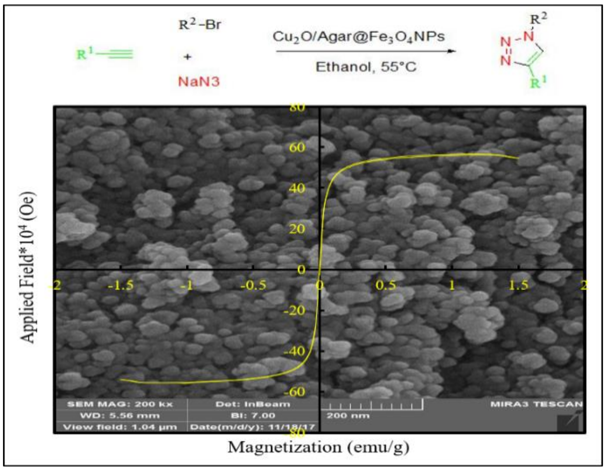

Fig. 1 Synthesis of 1,2,3-triazoles catalysed by Cu_2O/ $Agar@Fe_3O_4$ nanoparticles

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Paper code: 1059

Mica as an efficient catalyst for the synthesis of benzoimidazole derivatives

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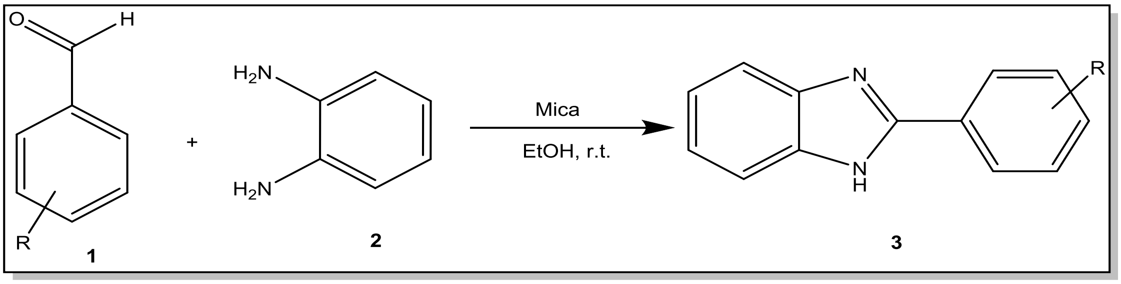
Nowadays, **clay mineral** with unique features such as eco-friendly, cheap and nanoscale size has attracted much attention and applied in different industry and sciences [1]. Mica has a layered structure, each layer consists of some combinations of two sheet types with silicon tetrahedral and aluminum octahedral as basic units. Mica due to chemical stable in acid and alkali solution can be used as a heterogeneous catalyst in the various organic reactions [2].

Imidazoles due to their interesting biological activities are an important class of heterocyclic compounds in pharmaceutical industry. In continuation of our research, herein, an efficient and selective synthesis of imidazole derivatives **3** were carried out by using benzaldehyde **1** and *o*-phenylenediamine **2** in mild condition and high yield by use of mica as an efficient, eco-friendly and heterogeneous catalyst (Scheme 1).



Scheme 1. Mica catalyzed synthesis of imidazole compounds.

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Paper code: 1073

A Green and Efficient Synthesis of 2-Thioxoquinazolinone Derivatives in Water Using Potassium Thiocyanate

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Green chemistry is one of the most important routes for the synthesis of heterocyclic compounds. In this regard, the synthesis of 2-thioxoquinazolinone derivatives was achieved by condensation of versatile materials including isatoic anhydride, amine, and potassium thiocyanate in green medium of water. This convenient and efficient method affords the desired products with good to excellent yields.

In this regard, new procedures were designed by chemists to reduce the environmental pollutions and to save energy [1]. Optimizing the reaction conditions in the presence of environmental friendly solvents (e.g. water and ethanol) instead of toxic solvents is noticeable for green synthesis of organic compounds especially heterocycles [2]. Although there are several methods for the synthesis of entitled heterocycles, but due to the importance of introducing green methods for the preparation of heterocycles in organic synthesis, the present methodology can be regarded as a versatile strategy for the synthesis of 2-thioxoquinazolinone derivatives. Considering the fact that most 2-thioxoquinazolinone derivatives show interesting biological activities, the new compounds synthesized in this paper are valuable for further pharmaceutical research.

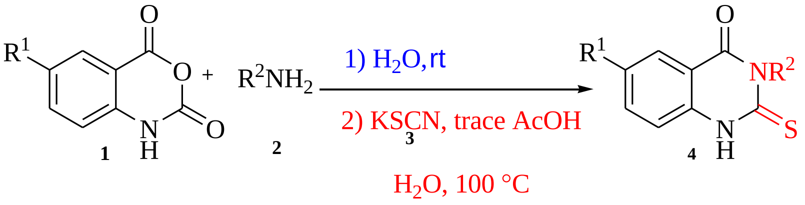

Fig. 1 Synthesis of 2-thioxoquinazolinone.

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Paper code: 1089

Mild and eco-friendly chemoselective acylation of amines in aqueous medium using superparamagnetic nanoparticles as a highly efficient and recyclable catalyst

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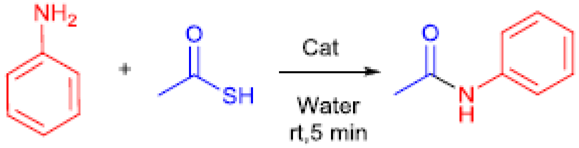
Acylation of amines is a basic and important reaction in organic chemistry. Many pharmacological molecules possess at least one amide bond [1]. Several methods for acylation have been developed, among them N-acylation reaction is commonly carried out with acetic anhydride or acetyl chloride in the presence of either acidic or basic catalysts under various conditions [2]. Guanidine acetic acid (GAA) is the essential precursor of creatine, and belongs to the class of guanidino compounds that are characterized by the presence of a basic guanidine group. GAA has a carboxylic acid group that facilitates the linkage of the compound to a magnetite support and the guanidino group renders it suitable to serve as a complexing agent for most transition metal ions. Herein, we report the rapid and highly selective N- acylation of amines using thioacids in water at room temperature mediated by copper- grafted GAA-modified magnetite nanoparticles (Fe_3O_4@GAA- Cu(II)).



Robust and effective Fe_3O_4@GAA-Cu(II) as a green, superparamagnetic and recoverable nanocatalyst for N-acylation of a variety of amines was synthesized and studied. When thioacetic acid is used as the acylation agent in water, N-acylation can be carried out to afford corresponding products in excellent yields and short time. This method is found to be highly selective for amines and not sensitive to other functional groups such as thiol, phenol and amino acids. Mild reaction conditions, high selectivity, efficiency, simple workup and excellent yields are some of the major advantages of the procedure.

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Paper code: 1092

A Facile Synthesis of quinoxalines and dicyano pyrazines using $Ca(IO_3)_2$ as efficient and recycling catalyst

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Quinoxaline derivatives are an important class of nitrogen containing heterocycles and have been widely used in dyes pharmaceuticals and electrical/photochemical materials. Also, quinoxaline ring moiety is a part of various antibiotics such as Echinomycin, Levomycin, and Actinoleutin that are known to inhibit growth of gram positive bacteria, and are active against various transplantable tumors [1]. Also, dicyanopyrazine derivatives have been synthesized and are valuable in a broad range of chemistry fields due to their applications as functional dyes, nonlinear optical materials, *etc.* [2]. Because of their importance, up to now, several methods have been reported for the synthesis of these compounds including the condensational reaction of an aryl 1,2-diamine with a 1,2-dicarbonyl compound in refluxing or in the presence of an acid catalyst under various reaction conditions [3].

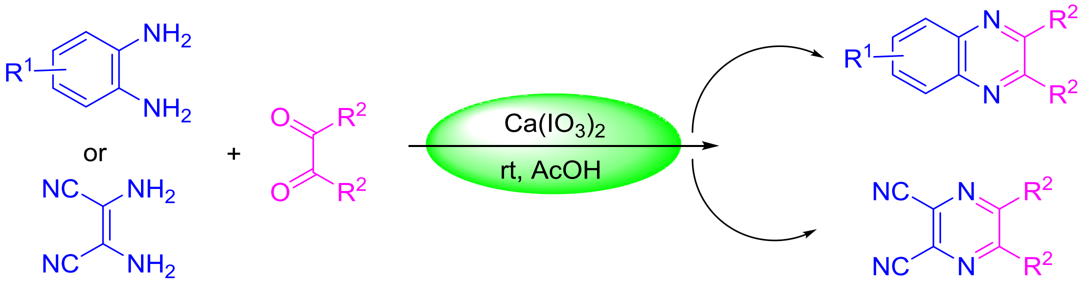

Fig. 1 The synthetic pathway for preparation of quinoxaline and dicyanopyrazine derivatives

Looking at the above facts, in this study, we report use of $Ca(IO_3)_2$ as an efficient heterogeneous catalyst for the preparation of 2,3-diaryl quinoxaline and dicyano pyrazine derivatives by reaction of *o*-arylenediamine or diaminomaleonitrile and 1,2-dicarbonyl compounds. The attractive features of this procedure are its good conversions, easy workup, and short reaction times, safely and recyclable catalyst, making it a useful practical method for the synthesis of the title compounds.

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Paper code: 1097

Stereoselective synthesis of spirooxindoles through multi component reaction catalyzed by guanidine under mild condition

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Oxindole with a six-membered spirocyclic moiety is an intriguing subset with potential bioactivity and is featured in a number of natural products, as exemplified by gelsemine as well as pharmaceutically relevant compounds with remarkable structural complexity and interesting biological activities. The art of accomplishment efficient chemical transformations to generate molecular complexity and miscellany with predefined functionality in natural and biologically relevant systems is a challenging benchmark which urges chemists to increase tools of their arsenal [1]. In this study, multi component reactions by virtue of their synthetic efficiency the decline of chemical steps and energy consumption in organic processes [2], formation of several bonds in one sequence without changing the reaction conditions, isolating the intermediates or adding reagents [3].

Here in, it was found a new type of cascade simple pseudo four-component reaction of isatins, cyclic ketones and two moles malononitrile catalyzed by guanidine at room temperature. The tetracyclic spirooxindoles were stereoselectively obtained as products in 70-90% yields and short reaction times. The special stereoselectivity was accomplished on two or three centers in this pseudo four-component reaction.

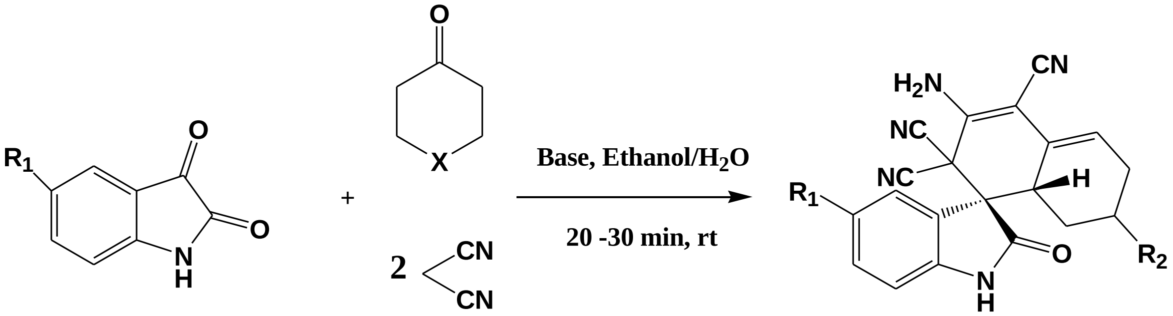

Fig. 1. One-pot multicomponent synthesis spirooxindoles

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Paper code: 1098

Sulfonic Acid-Anchored Isocyanurate-Based Periodic Mesoporous Organosilica (PMO-SO_3H): A Highly Efficient and Recoverable Nanoporous Catalyst in Biginelli reaction

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Multi-component reactions have attracted much attention as new research field for the synthesis of diverse and complex molecules especially heterocyclic compounds in pharmaceutical and organic chemistry [1]. Nitrogen containing heterocyclic compounds are one of the most important compounds in the pharmaceutical field and are used as agents for the synthesis of new drugs [2]. Biginelli reaction is one of the most important and effective methods for the production of 3,4-dihydropyridin-2(1*H*)-ones (DHPMs). DHPMs and their derivatives have attracted a lot of attention because having many biological and medicinal properties such as antiviral, antihypertension, anti-tumor, antibacterial and as calcium channel modulators [3]. The use of heterogeneous catalysts has been developed in recent years because its desirable properties and incorporating many principles of green chemistry. Mesoporous organosilica hybrids (PMOs) are an interesting and efficient category of these catalysts which prepared from bridged organosilane precursors ($(R'O)_3Si\text{-}R\text{-}Si(OR')_3$; R: organic bridging group, R′: methyl or ethyl). PMOs have large and adjustable pores, well-defined pore morphology and high surface area, which these properties allow facile and rapid diffusion of reagents into channels and improves reaction speed [4]. In this context, the preparation and catalytic application of sulfonic acid-anchored periodic mesoporous organosilica (PMO-SO_3H) as a novel and efficient heterogeneous catalyst is described. Furthermore, the catalyst was also recovered and reused. The catalytic application of the PMO-SO_3H nanoporous catalyst was then investigated in the Biginelli condensation of various aldehydes with β-ketoester⁄dimedon and urea/thiourea under solvent free condition [5].

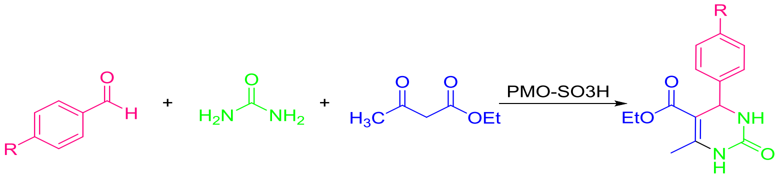

Fig. 1 Condensation of 3,4-dihydropyrimidinones with different aldehydes catalyzed by PMO-SO_3H

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Paper code: 1105

Protic acidic ionic liquids: green, efficient and reusable catalyst for synthesis of dihydropyridines

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In this methodology, at the beginning, environmentally friendly Protic acidic ionic liquids (HILs) have been synthesised by direct reaction of nitrogen heterocyclic compounds with various acids. Then, syntheis of dihydropyrimidines were investigated through one-pot, three-component reaction between substituted aromatic aldehydes, ethyl acetoacetate and urea (thiourea), using these green solvents at different temperature without any catalyst. The best results were afforded when [NImH]OAc was used at 100 oC for 5-10 min. It is worthwhile to mention that, the products were isolated and no further chromatographic purification was accomplished since no impurities were observed by NMR. Increasing the amount of catalyst, however, did not improve the yield significantly. Further investigation on the temperature effect indicated that high temperature did not reduce the reaction time.

Paper code: 1107

Synthesis a polymer-supported Fe_3O_4 nanoparticles and its application as a novel route for the synthesis of imidazole derivatives

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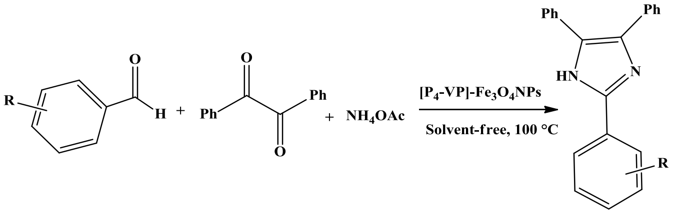
Magnetic iron oxide nanoparticles (MNPs) have attracted much attention than other nanoparticles arising from their unique physicochemical properties, great potential biomedical applications, large surface area, and fast response under applied external magnetic field and low Curie temperature [1-3]. Also polymeric reagents compared to monomeric reagents and catalysts benefit from important advantages including: insolubility in the reaction mixture and thus their rapid and simple workup, efficient reducing of the leaching of chemicals into reaction, solvent or environment in work-up procedures, safe handling, reusability of the reagents and reduction of environmental pollution in the presence of them because of their easy isolation by simple filtration. So by combining the positive properties of magnetic nanoparticles and polymeric reagents, we have a class of polymeric reagents and catalyst which shown excellent magnetic properties [4-6]. In this work cross-linked poly (4-vinylpyridine) supported Fe_3O_4 nanoparticles abbreviated as $[P_4\text{-VP}]\text{-}Fe_3O_4NPs$, was easily prepared as a new magnetic polymeric catalyst and efficiently used for the synthesis of imidazole. The Polymeric catalyst was characterized using various techniques including: field emission scanning electron microscope (FE-SEM), X-ray diffraction (XRD), vibrating sample magnetometer (VSM) and Fourier transform infrared spectroscopy (FT-IR) techniques. According to the obtained results of these techniques a good dispersion of Fe_3O_4 nanoparticles on the polymer support and also excellent magnetic property of the catalyst were approved. A novel method for the synthesis of imidazole derivatives also has been developed by one-pot condensation reaction of benzil, ammonium acetate and aldehydes in the presence of $[P_4\text{-VP}]\text{-}Fe_3O_4$ nanoparticles. The catalyst displayed good catalytic activity when applied in one-pot condensation reaction of benzil, ammonium acetate and aldehydes. Various imidazole derivatives are prepared in high to excellent yields (79-99%) with short reaction times and high purity. The imidazole products were characterized by FT-IR, ^1H and ^{13}C NMR spectroscopy and melting points. The physical properties were compared to the literature values of known compounds. The present method benefit from some advantages over conventional classical methods such as rapid and very simple work-up and also the catalyst is reusable many times without a significant loss in its activity.



Schem1. Synthesis of imidazole derivatives in the presence of $[P_4\text{-VP}]\text{-}Fe_3O_4NPs$

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Paper code: 1109

Simple and efficient strategy for the synthesis of pyridones derivatives

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Multicomponent reactions (MCRs) are useful methods in the sustainable and diversity-oriented synthesis of heterocyclic compounds, especially for the synthesis of heterocyclic drug-like compounds. MCRs have presented an excellent intent to approach variety as well as intricacy in molecular and chemical libraries in a short number of reaction steps by combining three or more starting materials in one-pot. Also, MCRs are in accommodation with the principles of green chemistry in terms of economy of steps and atom efficiency for organic synthesis.

Synthesis of heterocyclic compounds, especially an important class of biologically active nitrogen containing compounds, which present a wide range of therapeutic and pharmacological properties is finding out that currently available compounds could not responsive the needs of chemical drug-like compounds. Pyridone-based molecules have shown a broad range of biological properties such as antifungal, anti-HIV, antitumoral, anti-hepatitis B, anti-mycobacterium tuberculosis agents[1,2].

In continuation of our interest in the application of 1,1-bis(methylthio)-2-nitroethene in organic synthesis [3] herein we report an efficient and simple synthesis of pyridones derivatives, via a one-pot four-component reaction of nitro ketene aminals derived from the addition of various 1,n-diamines **1** to 1,1-bis(methylthio)-2-nitroethene **2** with aryl glyoxal **3** and methyl cyano acetate or ethyl cyano acetate **4** in EtOH as green solvent under reflux condition in good to excellent yields (Fig 1). This strategy has the advantages of easy workup, mild reaction conditions without using catalysts. All structures were determined by IR, MS, ^{1}H- and ^{13}C-NMR analysis.

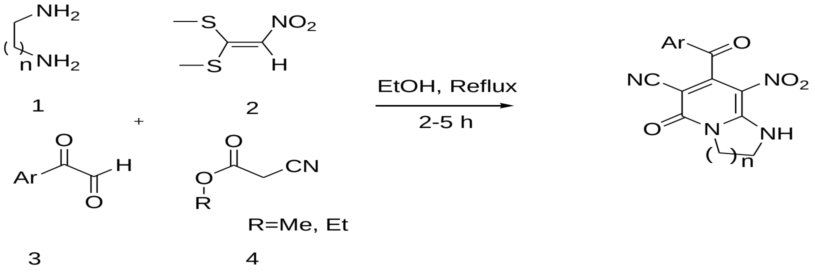

Fig. 1 Synthesis of pyridones derivatives.

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Paper code: 1114

Syntheses, characterizations, crystal structures and hirshfeld surface of two new oxidation agents of 1, 2- ethanediylbis (triphenylphosphonium) cation including perchlorate and chlorate anions

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Two new efficient oxidants 1, 2- ethane diylbis (triphenylphosphonium) diperchlorate (I), 1, 2 ethanediylbis (triphenylphosphonium) dichlorate (II) were prepared and used for oxidation of different benzylic alcohols to afford their corresponding carbonyl compounds. These new ionic liquids have been characterized by IR, NMR spectroscopies and single crystal X-ray analysis. These compounds have advantages over similar oxidizing agents [1], [2] such as short reaction time, high yields of the oxidized species, nontoxicity and stability of the reagent. The crystal structure and hirshfeld surface analysis of titled compounds revealed that the change of accompanying anionic moiety can affect the directional interactions of CH…O hydrogen bonds between anionic and cationic units which lead to various supramolecular aggregation on the crystal packing. In order to exploring the influence of crystal environment of anionic moieties on the geometry of main cationic unit, the relative contribution of various close contacts and 2D fingerprint plots of title compounds and fourteen analogous structures retrieved from Cambridge Structural Database (CSD) were investigated as well as the distortion of tetrahedral coordination geometry of P center of main cationic unit based on τ_4 parameter.

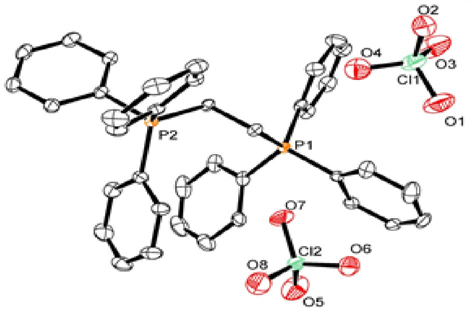

Fig. 1 Molecular structure of 1, 2 – ethanediylbis (triphenylphosphonium) diperchlorate.

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Paper code: 1115

Synthesis of highly functionalized 6-amino-4-(aryl)-5-nitro-2-oxo-1,2-dihydropyridine-3-carbonitrile derivatives

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Pyridones are an important class of heterocyclic compounds and are structural units found in a wide range of natural products, synthetic materials, and bioactive molecules. Pyridone derivatives are also a versatile synthon for the preparation of a variety of other nitrogen-containing heterocycles, such as quinolizidine, pyridine, piperidine, and indolizidine alkaloids [1]. Also they have been applied as a key synthetic intermediate to synthesize some complex natural products. Consequently, a large number of methods have been developed for the synthesis of pyridones and their derivatives. Due to the importance of pyridone skeleton, to develop new and efficient methodologies for construction of pyridone is still highly desired. Various pyridones are known to possess different important medicinal properties such as antifungal, anti-HIV, antitumoral, anti-hepatitis B, anti-mycobacterium tuberculosis agents [2].

In continuation of our previous work, here we wish to report the results of our studies in the application of 1,1-bis(methylthio)-2-nitroethene in organic synthesis [3], herein we report an effective and simple synthesis of pyridone derivatives, via a one-pot four-component reaction of ammonia **1** to 1,1-bis(methylthio)-2-nitroethene **2** with different aldehyde **3** and methyl cyanoacetate or ethyl cyanoacetate **4** in EtOH as solvent under reflux condition (Fig 1). This strategy has the advantages of simple procedure, mild reaction conditions, easy workup and good to excellent yields without using catalysts. All structures were determined by IR, MS, ^{1}H- and ^{13}C-NMR analyses.

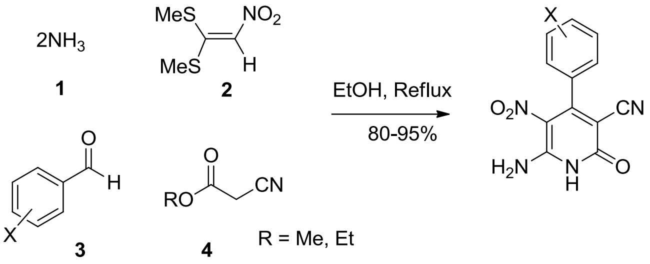

Fig. 1 Synthesis of pyridone derivatives.

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Paper code: 1125

κ-Carrageenan as an efficient, green, bifunctional and reusable catalyst for one-pot synthesis of Hantzsch 1,4-dihydropyridine

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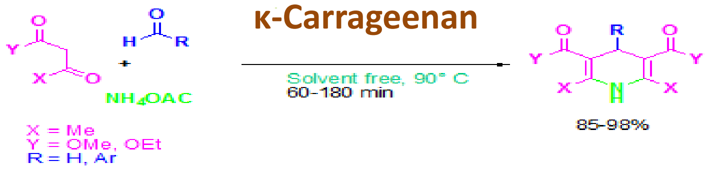
Developing chemical processes using more environmentally acceptable catalysts, chemicals and atom efficient procedures have been emerged as subjects of innovation in green chemistry. For instance, the terrible impact of non-biodegradable wastes is still an open challenge in either developed or developing countries. In this regard, great efforts have been performed to use different bio-based feedstocks such as chitosan, chitin, starch, cellulose, gelatin, wool and alginates as biopolymeric support in the transition metal-based heterogeneous catalytic systems. On the other hand, multicomponent reactions have been recognized as a vast improvement for synthetic chemists. Multicomponent reactions are the reactions with three or more substratets, which lead to the production of complex molecules, especially heterocyclic complex products.[1-3] Carrageenan is a natural carbohydrate (polysaccharide) obtained from edible red seaweeds. Carrageenans are used in a variety of commercial applications as gelling, thickening, and stabilising agents, especially in food products and sauces. Carrageenans are also used in pharmaceutical, drug delivery, cosmetics, experimental medicine and textile industries.[4]

Kappa-Carrageenan was found to be an efficient, bifunctional, recyclable, economical, environment-friendly and green catalyst for the one-pot multicomponent synthesis of 1,4-dihydropyridines (1,4-DHPs) via the Hantzsch reaction. The mild reaction conditions, short reaction times, good yields and the nontoxic catalyst make this method especially attractive.[5, 6]



Scheme 1. Multicomponent reaction of aldehydes and ethyl acetoacetate (methyl acetoacetate) and ammonium acetate catalyzed by κ-carrageenan under solvent-free conditions at 90 ºC temperature.

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Paper code: 1127

Sulfonic Acid-Anchored Isocyanurate-Based Periodic Mesoporous Organosilica (PMO-SO_3H): A Highly Efficient and Recoverable Nanoporous Catalyst in Biginelli reaction

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Multi-component reactions have attracted much attention as new research field for the synthesis of diverse and complex molecules especially heterocyclic compounds in pharmaceutical and organic chemistry [1]. Nitrogen containing heterocyclic compounds are one of the most important compounds in the pharmaceutical field and are used as agents for the synthesis of new drugs [2]. Biginelli reaction is one of the most important and effective methods for the production of 3,4-dihydropyridin-2(1*H*)-ones (DHPMs). DHPMs and their derivatives have attracted a lot of attention because having many biological and medicinal properties such as antiviral, antihypertension, anti-tumor, antibacterial and as calcium channel modulators [3]. The use of heterogeneous catalysts has been developed in recent years because its desirable properties and incorporating many principles of green chemistry. Mesoporous organosilica hybrids (PMOs) are an interesting and efficient category of these catalysts which prepared from bridged organosilane precursors ($(R'O)_3Si\text{-}R\text{-}Si(OR')_3$; R: organic bridging group, R′: methyl or ethyl). PMOs have large and adjustable pores, well-defined pore morphology and high surface area, which these properties allow facile and rapid diffusion of reagents into channels and improves reaction speed [4]. In this context, the preparation and catalytic application of sulfonic acid-anchored periodic mesoporous organosilica (PMO-SO_3H) as a novel and efficient heterogeneous catalyst is described. Furthermore, the catalyst was also recovered and reused. The catalytic application of the PMO-SO_3H nanoporous catalyst was then investigated in the Biginelli condensation of various aldehydes with β-ketoester⁄dimedon and urea/thiourea under solvent free condition [5].

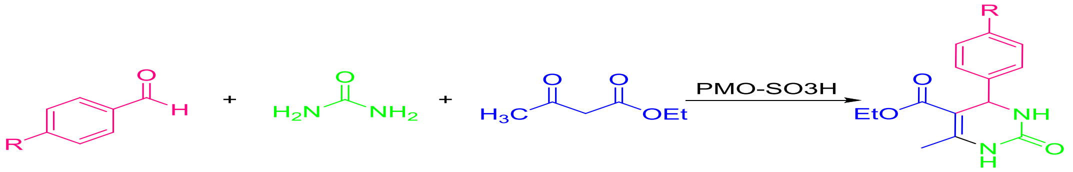

Fig. 1 Condensation of 3,4-dihydropyrimidinones with different aldehydes catalyzed by PMO-SO_3H

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Paper code: 1145

A Combination of natural deep eutectic solvents and microflow technology: a sustainable innovation for the tandem synthesis of 3-aminohexahydrocoumarins

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Nowadays, in different research areas the interest in deep eutectic solvents (DESs) is growing as green substitutes to conventional ionic liquids (ILs), such as electrochemistry, extraction, or biocatalysts. These compounds are basically formed from two or three safe, inexpensive and environmentally friendly components [1].

On the other hand, microreactors as a functional component of microfluidic devices, have many advantages compared to batch reactors, including a short reaction time, low cost, portability, reduced reagent consumption, and a high surface-to-volume ratio [2].

Dihydrocoumarin and aminocoumarin derivatives possess significant bioactivities such as cytotoxic, anti-inflammatory, inhibiting histone deacetylase, and antibiotic.

Upon the aforementioned explanation and in continuation of our recent investigation on green chemistry especially developing microflow synthesis, herein we would like to present the first efficient, and environmentally friendly consecutive microflow synthesis of the *N*-(2,5-dioxo-3,4,5,6,7,8-hexahydro-2Hchromen-3-yl)acetamide framework utilizing hippuric acid, aryl aldehyde, acetic anhydride and 1,3-dicarbonyl compounds in choline chloride (ChCl)/urea as a biorenewable solvent. This reaction is the first flow methodology described using NADES as eco-friendly, nontoxic, and green solvent and catalyst compared to the common volatile organic compounds (VOC).

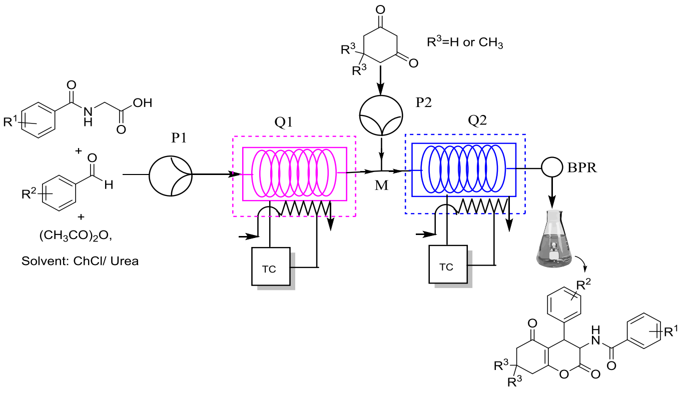

Fig. 1 Preparation of 3-aminohexahyrdocoumarins using microreactor.

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Paper code: 1147

Metal-Free Aerobic Oxidative Esterification of Aldehydes in the Presence of Potassium Fluoride

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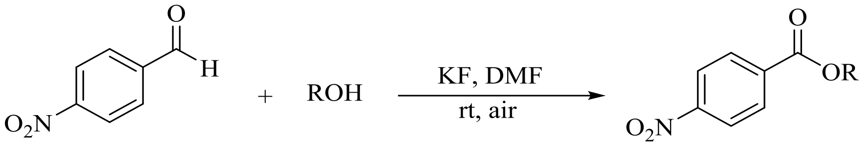
Ester functionality is among the most abundant functional groups in natural products, polymers, and pharmaceuticals [1]. In the recent years, direct catalytic transformation of aldehydes to esters has achieved considerable interest. This method have a drawback related to the catalyst cost which represent an impractical aspect for large-scale. For this reason, direct esterification of aldehydes under catalyst-free conditions is a challenging task in organic chemistry [2].

Herein, we describe the direct synthesis of esters from aldehydes in presence of potassium fluoride and alcohols *via* metal-free aerobic oxidative esterification reaction in DMF (Scheme 1).



Scheme 1. Esterification of aldehydes under metal-free conditions

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Paper code: 1149

Application of Magnetic Fe_3O_4 Nanoparticles in the Synthesis of β-Lactams Containing Amino Group

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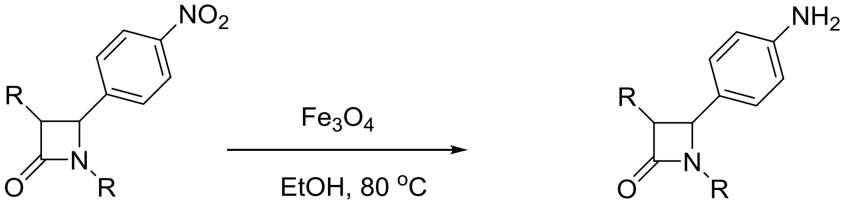
β-Lactam antibiotics are the most important antibacterial agents for human health and it began with the discovery of penicillin by Alexander Fleming in 1928. In addition, β-lactams are an important class of heterocyclic compounds due to their wide range applications in other biological activities [1]. With the alarming trends in bacterial resistance to many β-lactam antibiotics it has become necessary to synthesize some novel β-lactams for bioassay of antibacterial activity and the need for drugs with more specific antibacterial activity. Therefore, the synthesis of the new β-lactams is the subject of extensive study. The reduction of nitroarenes to aromatic amines is an important step in the production of agrochemicals, pharmaceuticals and dyes. Therefore, various methods have been developed to reduce the nitro group [2]. On the other hand, the existing methods for the preparation of β-lactams containing the amine group are very difficult and take place in several steps. In this project, green method using ethanol solvent and Fe_3O_4 catalyst has been reported to reduction of nitro group on β-lactams (Scheme 1). In this reaction iron oxide is responsible for the electron transfer and ethanol acting as proton source. The catalyst can be used several times without decrease in catalytic activity. The chemical structure of products was identified using spectral data.



Scheme 1. Synthesis of β-lactams containing amino group

References

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Paper code: 1152

Synthesis of Xanthene and Dihydroquinazolin-4(1H)-ones by fructose catalyst

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Xanthene, Benzoxanthene and 2-Amino-chromene and its derivatives represent an important class and very useful compounds in various fields of chemistry. These molecules are biologically active and find application in pharmacological, medicinal [1]. Also, Dihydroquinazolin-4 (1H) -ones constitute an important class of heterocyclic compounds that have been widely exhibited spectrum of biological, physiological activities and pharmacological properties [2], such as anticancer, antidiuretic, anticonvulsant, antibacterial, antifungal activity [3] and mono-amine oxidase inhibition and are also used as 5-hydroxytryptamine (5-HT) receptor ligands. Recently, Lindsley and coworkers observed the metabotropic glutamate receptor (mGluR) properties of this class of compounds. In this project, sulfonated fructose used as a new, non-toxic and effective catalyst for benzaldehyde, 2-naphthol and dimedone for the synthesis of tetrahydrobenzo [a] xanthene-11-one and the reaction of aldehyde and 2-naphthol to synthesize 14H-DI benzo [a, j] Xanthene. Advantages of this method are: the use of inexpensive, affordable and non-toxic catalyst, high efficiency, relatively short response times, simple product purifications, good to excellent yields.

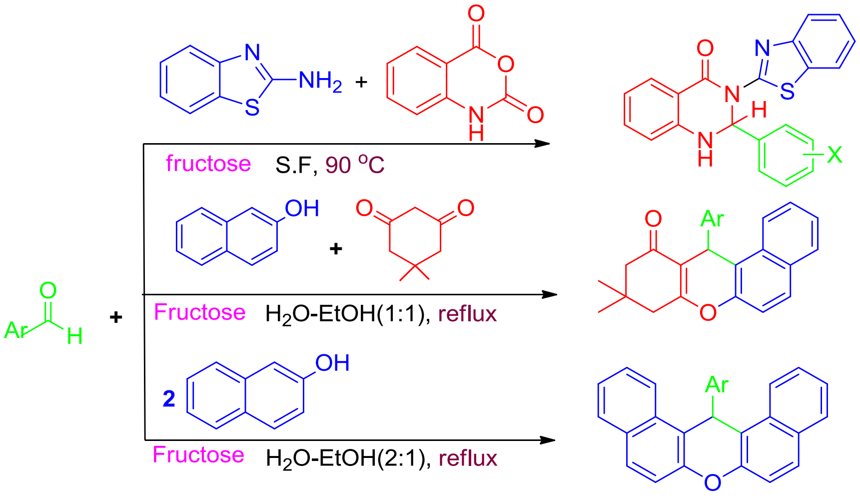

Fig. 1 Synthesis of Xanthene and Quinazoline derivatives in the presence of sulfonated fructose

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Paper code: 1153

An Efficient Green Synthesis of Pyrimidine and Pyridopyrimidine Derivatives In The Presence of Eutectic Solvents

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Pyrimidine and pyridopyrimidine derivatives belong to two significant heterocyclic building blocks which have been found abundantly in the structure of natural products [1]. Besides, many biological characteristics have been reported for these derivatives, amongst them, antibacterial [2], antifungal, antituberculosis, antioxidant and anticonvulsant [3] features can be briefly referred herein. Introducing novel synthetic protocols based on green chemistry fundamentals is one of the very active areas of research in recent years. Substituted solvents such as ionic liquids and deep eutectic solvents have been widely used as replacement media in place of hazardous organic solvents to provide an efficient route for the synthesis of organic chemicals. In this research project, more facile and efficient methodologies were introduced for the preparation of some new pyrimidine and pyridopyrimidine derivatives according to applying deep eutectic solvents (Cholin Chloride-Urea(1:2)) as media and promoters (Fig. 1). The antibacterial and antifungal features of some these derivatives were also studied.

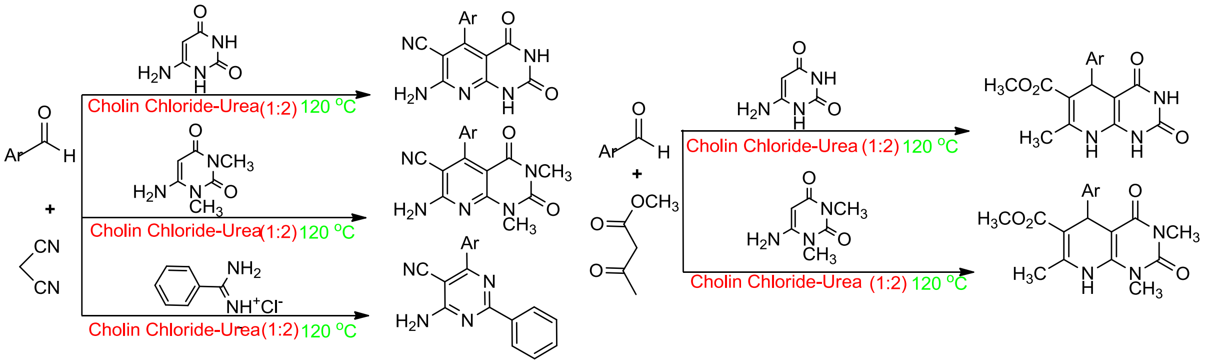

Fig. 1 The synthesis of pyrimidine and pyridopyrimidine derivatives in the presence of Cholin Chloride-Urea(1:2)

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Paper code: 1157

Synthesis of Aryl Sulfides via Transition-Metal Free Cross-Coupling of Thiols with Hydrazines.

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Transition-metal-catalyzed carbon−heteroatom cross-coupling reactions have made a great contribution to the recent growth of organic synthesis. Although the aryl sulfides have broad application in the pharmaceutical industry and material science and as intermediates in organic synthesis, the formation of carbon−sulfur bonds has received less attention. Difficulties in C−S bond formation can be attributed to the sulfur species rapidly and irreversibly deactivating the catalyst. So the efficient formation of the C−S bond is a most important aspect of organic chemistry. Many research groups have made great effort to overcome this problem in recent years, and several excellent catalytic systems that used Pd, Cu, Ni, Fe, and other metals as catalysts have been found for C−S bond formation by couplings of aryl halides with thiols or disulfides [1]. Aryl Sulfides are also becoming more prevalent structural motifs in pharmaceuticals. Examples include axitinib (a tyrosine kinase inhibitor), albendazole (a treatment for parasitic worm infestations), vortioxetine (an antidepressant), and fenticonazole (an antifungal) [2]. In this project, the optimum conditions for reaction such as solvent type, temperature type are studied, in order to finally obtain a product with purity and acceptable yield. Various benefits, such as relatively short response times, simple purifications, good to excellent yields are among the important features of the proposed method.

Fig. 1 Synthesis of Aryl Sulfides via Transition-Metal and Ligand-Free with oxidant and base in green solvent.

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Paper code: 1178

Synthesis of Pyrimidin derivatives using Fe_3O_4@Ag-*β*-CD nanoparticles as a green and magnetically recyclable nanocatalyst

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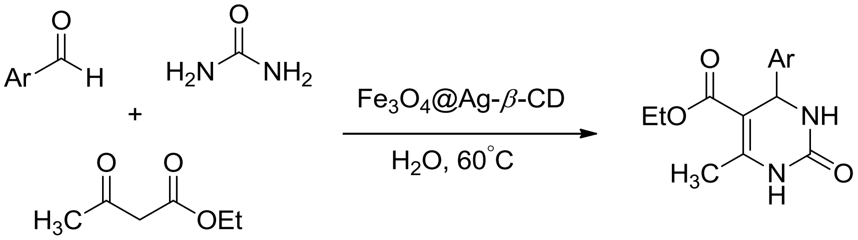
Insolubility of most organic substances in water as well as the distribution or deactivation of many active substrates, reagents, and catalysts by water molecules are the two significant limitations of organic reactions in aqueous media [1]. To overcome these constraints, there are some strategies that facilitate the use of water as a solvent for a wide variety of organic reactions. *β*-CD forms inclusion complexes with smaller molecules and they can be exist in aqueous solution. The hydrophobic cavity of the *β*-CD allows this molecule to encapsulate a variety of non-polar molecules of suitable size [2]. Ag nanoparticles have been recently shown to be efficient catalyst for some important reactions [3]. In the present paper, Ag-*β*-CD nanoparticles have been successfully linked on the surface of magnetic Fe_3O_4 nanoparticles. The morphology, composition and crystallinity of the Fe_3O_4@Ag-*β*-CD nanocomposites were characterized by FT-IR, XRD, TEM and EDS techniques. This new catalyst was employed for one-pot synthesis of pyrimidin derivatives in aqueous solution under mild conditions (Scheme). Compared with the classical Biginelli reactions this procedure showed several advantages including mild reaction conditions with environmental benign, excellent yields, short reaction times, and also this catalyst can be recovered easily and reused many times without significant loss of its catalytic activity.



Scheme: Fe_3O_4@Ag-β-CD-catalyzed synthesis of pyrimidin derivatives.

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Paper code: 1189

Iodine catalyzed mild 4CR protocol for synthesis of Tetrahydroimidazo[1,2-a]pyridines

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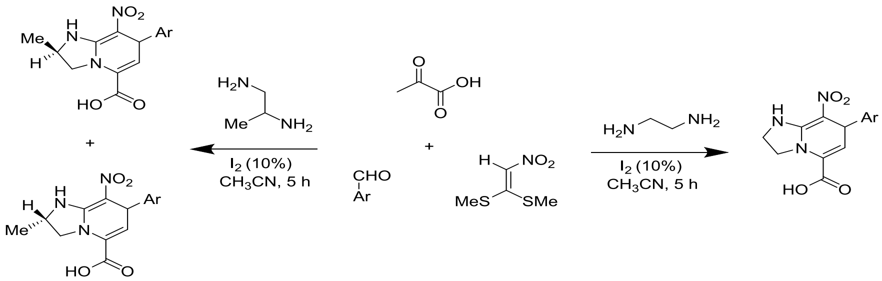
A highly convergent and straight forward synthesis of *N*-fused heterocycles, including 1,2,3,7-tetrahydroimidazo[1,2-a]pyridine-5-carboxylic acids is successfully achieved via a one-pot four-component cascade reaction utilizing pyruvic acid, aldehydes, diamines and 1,1-bis(methylthio)-2-nitroethylene (BMTNE) in the presence of a catalytic amount of molecular iodine in acetonitrile. The new efficient domino protocol generates two rings by the concomitant formation of C-N (three) and C-C (two) multiple bonds presumably involving a sequence of N,N-acetal formation, Knoevenagel reaction, aza-ene reaction, imine-enamine/keto-enol tautomerization, and N-cyclization as key steps. The merit of this protocol is highlighted by its easily available and economical starting materials, operational simplicity, efficient utilization of all the reactants, clean reaction profile, simple workup procedure, and tolerance of a wide variety of functional groups.

The importance of our synthetic method is to use nitro ketene aminal (NKA) intermediates as an important versatile synthetic intermediate, to produce the useful and pharmacologically azaheterocycle molecules [1]. In this research we used the molecular Iodine as a nontoxic and powerful catalyst to obtain products in excellent yields as an eco-friendly method [2].



Scheme 1. One-Pot Synthesis of Tetrahydroimidazo[1,2-a]pyridine-5-carboxylic acids via Domino SN/Knoevenagel condensation/Michael Addition/Cyclization Reaction.

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Paper code: 1190

A mild and efficient method for Synthesis of novel fused thiopyrano[2,3-*b*] indole derivatives

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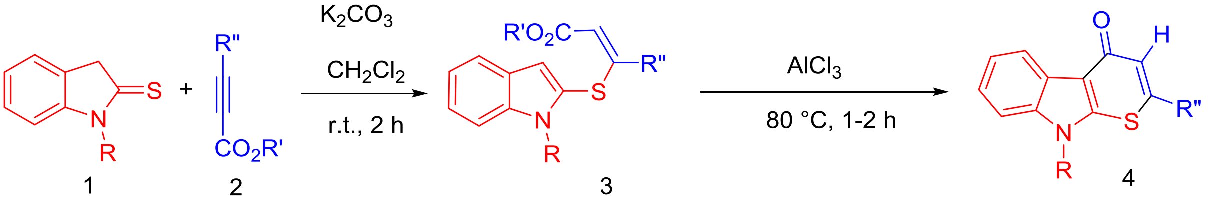
Thiopyran and fused-thiopyran derivatives are main classes of sulfur-containing heterocycles due to the frequency of occurrence in the molecular structure of natural products [1]. and have been found to exhibit of bioactivities, such as anti-bacterial and anti-cancer activities On the other hand, the indole scaffold is a structural motif common to a large and varied group of natural products with a remarkable array of biological activities [2]. Over recent decades, synthesis of anti-cancer thioflavone derivatives as a thiopyran analogues have also been developed [3].

In this research, a facile and efficient protocol for the regioselective synthesis of thiopyrano[2,3-b]indole-2-carboxylates using $AlCl_3$ is developed. The reaction of various acetylenecarboxylates and indoline-2(3H)-thiones using of Eaton's reagent affords indole-fused heterocyclic compounds in good to excellent yields. This procedure has advantages of mild reaction conditions, short reaction times, and ease of product isolation.



R= Me, Et, Ph
R"= CO_2Me, CO_2Et, H
R'= Me, Et

Scheme 1. Two steps synthesis of fused thiopyrano[2,3-b]indole derivatives.

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Paper code: 1198

Selective Deuteration of pyridinecarboxylic acid derivatives by decarboxylation and D_2O

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Nowadays isotopic labeling -as presented in Deuterium-labelled compounds- is known as a unique technique to track the passage of an isotope through a reaction, metabolic pathway, or cell. The reactants are labeled by replacing specific atoms with their isotopes and then allowed them to undergo the certain reaction and therefore, this method is employed for mechanistic investigations of catalytic cycles and reaction pathways [1, 2].

The most common protocol involves halogen/D exchange; this is usually mediated by strong bases, with the consequent limitation in functional group scope. In addition employing transition metal catalyst is believed as an alternative for this purpose [3]. In this work, a practical, mild and highly selective protocol for the monodeuteration of pyridinecarboxylic acid derivatives is presented. Decarboxylation process was promoted under Ag catalyst in DMSO/D_2O media, facilitating the deutero-decarboxylation of heteroaromatic α-carboxylic acids in high yields with excellent levels of deuterium incorporation.

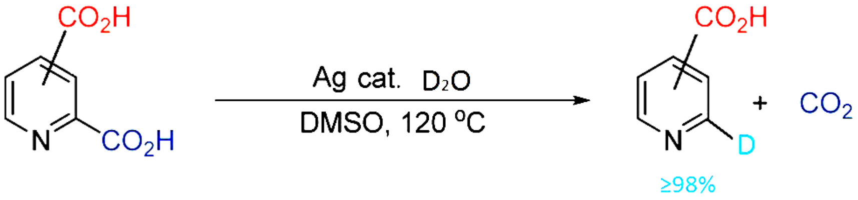

Fig. 1 deutero-decarboxylations of pyridinedicarboxylic acids.

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Paper code: 1199

Deuteration of aniline aromatic ring in the presence of Heterogeneous Platinum Catalyst

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Deuterated arylamines demonstrate great potential for use in optoelectronic Devices. In this study, a quite simple and post-synthetic method has been reported for D labeling of aniline using a combination of platinum metal on carbon as catalyst and deuterium oxide (D_2O) as a D source in the presence of hydrogen gas. Typically, the reactions were carried out in a sealed tube, a mixture of a substrate, heterogeneous Pt/C (20 wt% of the substrate) in D_2O was stirred at 80 °C under ordinary hydrogen gas atmosphere for 24h, chemical purity and deuterium isotopic enrichment of the aromatic ring determined by NMR spectroscopy and using internal standard addition method.

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Paper code: 1200

Preparation of deuterated methyl iodide through trimethylsulfoxonium iodide intermediate

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Since deuterium (D) is different from its most abundant isotope hydrogen (H), the additional neutron makes a notable difference in the properties of deuterated compounds. While drug molecules easily transform to metabolites by metabolic enzymes that the body can excrete, deuterium introducing to drugs appears to strengthen the resistance of drugs toward metabolism. The higher the stability, the longer the drug can work, which may result in lower dosage, therefore less side effects [1].

As a potential source of deuteromethyl group, methyl iodide-*d*₃ is very valuable compound in deuterium chemistry, which is used as an intermediate in the manufacture of some pharmaceuticals, in methylation processes and in the field of microscopy [2].

To synthesis of methyl iodide-*d*₃ we prepared trimethylsulfoxonium iodide from dimethylsulfoxide and methyl iodide [3]. The isotope exchange of this salt was accomplished with the deuterium oxide and a catalytic amount of base. The obtained deuterated salt, upon pyrolysis, is converted back to the deuterated starting materials [Fig. 1].

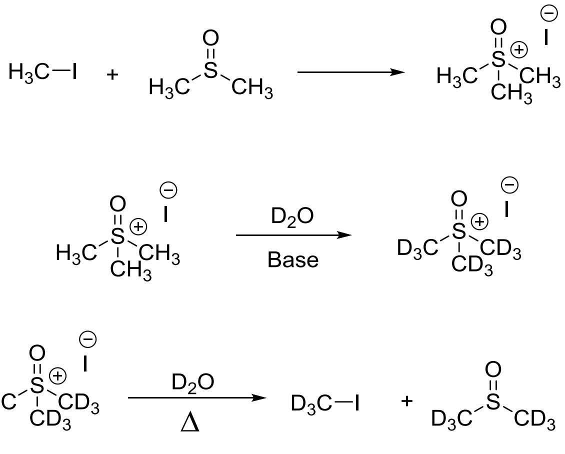

Fig. 1 General pathway for the synthesis of deuterated methyl iodide.

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Paper code: 1201

Synthesis and Characterization of Deuterated Glycine d-5: comparison of deuterated and non-deuterated glycine spectra

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Recent developments particularly in the field of nuclear magnetic resonance spectrometry suggest that there is a growing demand for compounds labelled with stable isotopes [1]. Deuterium is one of two stable isotopes of hydrogen, can be used as a labeling agent to distinguish a molecule from its protonated analogues and, the kinetic isotope effect, which deuterium exhibits by virtue of its increased bonding strength, permits a more detailed study of specific mechanisms of amino acid reactions.

In this study, the synthesis of deuterium-labelled [$^2H_5$]-glycine is described. The isotopically labelled compounds are applied as internal standards in liquid chromatography–mass spectrometry (LC–MS) assays and enzyme activity determination. Comparison of its spectrum with that of ordinary glycine exhibited the significant differences in the FT-IR and NMR spectra. A convenient method for the synthesis of glycine has been elaborated [Fig. 1]. Deuteration with high isotopic purity (%D ≥ 98) followed by reaction of the 2-ethylacetamidomalonate with D_2O/DCl 20% gave deuteroglycine-d6(I) salt. Conversion of this salt to the neutral glycine-d5(II) was performed using addition of trimethylamine [2].

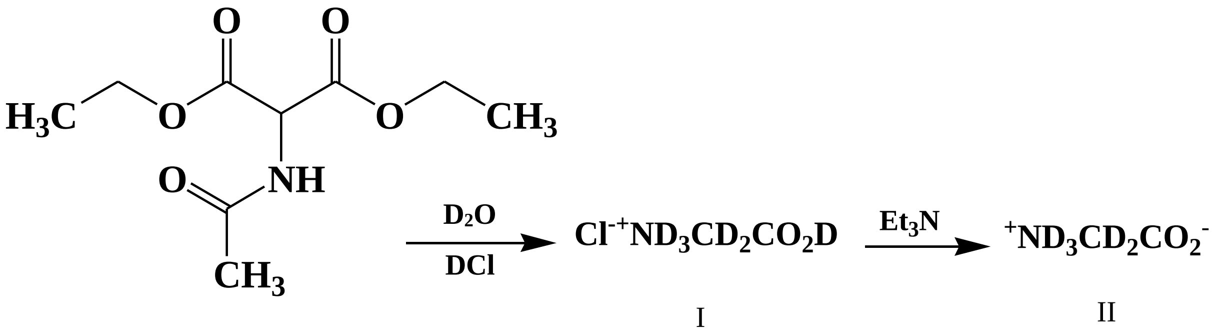

Fig. 1 conversion of 2-ethylacetamidomalonate to the deutero-glycine in acidic media

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Paper code: 1202

Metal catalyst Synthesis of methyl-d_3-amine hydrochloride by nitro group reduction

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This report relates to the synthetic method and production procedure for (methyl-d_3) amine salts, the important intermediates for chemical synthesis, can be used to make chemical, biological and pharmaceutical compounds [1]. Here, we report an efficient, mild and general methodology for conversion of deuterated nitromethane to the methyl-d3 amine using iron metal catalyst in the presence of deuterium chloride as acid and deuterium oxide as solvent. The reaction was completed in two steps: (i) deuterium exchange reaction between deuterium oxide and nitromethane in the presence of a base catalyst [2], and (ii) reduction of deuterated nitromethane to the methyl-d_3-amine using iron powder catalyst deuterium oxide solvent in the presence of deuterium chloride [3]. Isotopic enrichment was measured by NMR spectroscopy technique and GC-FID was applied for determining chemical purity of deuterated product.

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Paper code: 1204

Synthesis of Tetrahydrobenzo[b]pyran Derivatives using SO_3H–functionalized Nano-MGO-D-NH_2 in Aqueous Media

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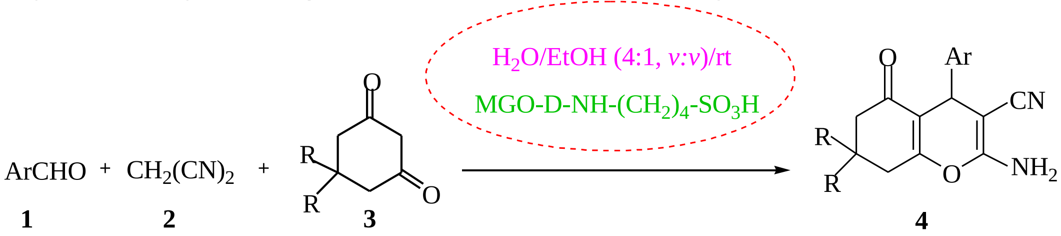
In organic transformations, catalysts play a significant role, and most of these reactions are acid catalyzed. The most generally acidic catalysts are sulfuric, hydrochloric, nitric and phosphoric acids. However, corrosive properties, inability to be reused and tough separation are their drawbacks. Immobilization of organic molecules with active catalytic sites on the surface of insoluble solids such as inorganic materials, synthetic organic polymers or hybrid materials is a common way for the preparation of heterogeneous catalysts. One of the most useful heterocycles for the mild and defined incorporation of sulfonate groups into organic molecules are sultones (as cyclic sulfonate esters). Sultones behave as a sulfoalkylating agents by reacting with a wide variety of nucleophiles via carbon–oxygen bond cleavage. As green chemistry becoming a vital topic in both industrial and academic investigation in the last decades [1] the growth of environmentally benign and unpolluted synthetic procedures have become the aim of present-day organic synthesis in multi-component reaction. Due to the diverse biological properties associated with tetrahydrobenzo[*b*]pyrans, there is extensive interest in the synthesis of such compounds. Tetrahydrobenzo[b]pyrans and their derivatives are an important class of heterocyclic compounds and have prominent properties such as antitumor, antibacterial, antihypertensive, hepatoprotective, cardiotonic, vasodilator and bronchodilators [2]. An efficient one-pot three-component procedure has been progressed for the preparation of tetrahydrobenzo[*b*]pyrans using SO_3H–functionalized Nano-MGO-D-NH_2 as a novel catalyst in aqueous media at room temperature, in this study. Some benefits of this methodology have been listed below: use of the reusable catalyst, easy access, short reaction times, high yields, easy work-up and use the non-toxic and green solvent.



Scheme 1 MGO-D-NH-$(CH_2)_4$-SO_3H–catalyzed synthesis of tetrahydrobenzo[b]pyrans

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Paper code: 1208

Innovative applications Of ionic liquids in Chemistry and chemical engineering

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During past few years, ionic liquids (ILs) have kept attracting much attention as “green and designer” media for chemical reactions. Room-temperature ILs have emerged as a potential replacement for organic solvents in catalytic processes on both laboratory and industrial scales [1, 2]. Effectively, ILs, among a unique set of chemical and physical properties, have no measurable vapor pressure, which lends them as ideal replacements for volatile, conventional organic solvents. The wide and readily accessible range of room-temperature ILs with corresponding variations in physical properties, prepared by simple structural modifications to the cations or changes in anions, offers the opportunity to design an ionic liquid-solvent system optimized for particular processes. Highlights recent advances of ILs are as versatile “green” engineering liquids in a variety of industrial applications including heat transfer fluids, azeotrope-breaking liquids, lubricants, electrolytes, liquid crystals, supported IL membranes, plasticizers, and more. This paper highlights specific examples of ionic liquid Innovative applications in chemistry and chemical engineering.

Fig. ionic liquids

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Paper code: 1245

Synthesis, characterization and molecular docking study of new 4-acetamidoalkyl pyrazoles as B-raf /COX-2 inhibitors

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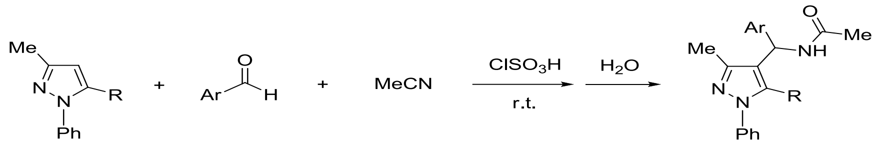
The success of COX-2 inhibitors containing a pyrazole moiety has highlighted the importance of these heterocyclics in medicinal chemistry [1]. Meanwhile, recent researches have shown the potency and selectivity of pyrazoline derivatives against B-RafV600E after being identified through high-throughput screening [2]. Both pyrazole and pyrazoline are reported to be backbone moieties of anti-cancer molecules [3]. These compounds are also reported to possess significant antipyretic, antidepressant, antiviral, antifungal, antitumor, and anti-inflammatory activities [4-6]. Some new 4-acetamidoalkyl pyrazoles were synthesized by efficient, one-pot three-component reaction of 3,5-dimethyl-1-phenyl-1*H*-pyrazole or 3-methyl-1-phenyl-1*H*-pyrazol-5-ol, aromatic aldehydes and acetonitrile in the presence of chlorosulfonic acid at room temperature. The products were characterized on the basis of IR, ^{1}H NMR, and ^{13}C NMR data and evaluated as potential COX-2 and B-Raf inhibitors by molecular docking studies.



1a and **1b** **2a-2d** **3** **4a-4f**

90-95%

1a: R = Me
1b: R = OH
2a: Ar = C_6H_5
2b: Ar = 4-BrC_6H_4
2c: Ar = 4-ClC_6H_4
2d: Ar = 4-FC_6H_4

4a: R = Me, Ar = 4-BrC_6H_4
4b: R = Me, Ar = 4-ClC_6H_4
4c: R = Me, Ar = 4-FC_6H_4
4d: R = OH, Ar = C_6H_5
4e: R = OH, Ar = 4-BrC_6H_4
4f: R = OH, Ar = 4-ClC_6H_4

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Paper code: 1273

Rational design, synthesis and application of task-specific materials in organic synthesis

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In recent years, the subject of green and sustainable chemistry has been accompanied by introducing task-specific materials such as ionic liquids and nanostructured catalyst. Accordingly, in the scope of catalysis science and technology, Brønsted acidic ionic liquids and nanostructured catalyst have been designed to replace solid acids and traditional mineral liquid acids like sulfuric acid and hydrochloric acid in chemical procedures. Ionic Liquids (ILs) have been used as solvent, catalyst and reagent. Anion exchange is a subjective way for designing and synthesis of ionic liquids with other anions that cannot be directly prepared. Over the years, much attention has been paid to study the changing the properties of ionic liquids by the exchange of counter ions, which change physical properties such as viscosity, melting point, vapor pressure of fluids and fluorescence properties [1]. Nanoarchitectonics is expected to achieve an effective guidance in fabricating functional nano materials. Nano-orientation of materials is a widely demanding tool in nanoarchitecturing to reach out new task-specific materials with higher surface area. Applications of nano catalysts are some advantages in organic functional groups transformations including (i) high yields, (ii) short reaction times, (iii) low catalyst loading (iv) inexpensive catalysts (v) regioselectivity and (vi) safety of reaction conditions. Thus, there is a great demand for designing and synthesis of easy and safe chemicals and chemical processes [2]. With this aim, our research group has developed the knowledge-based designing, synthesis and application of task-specific novel ionic liquids and nanostructured catalysts for the synthesis of various organic compounds (Fig.1).

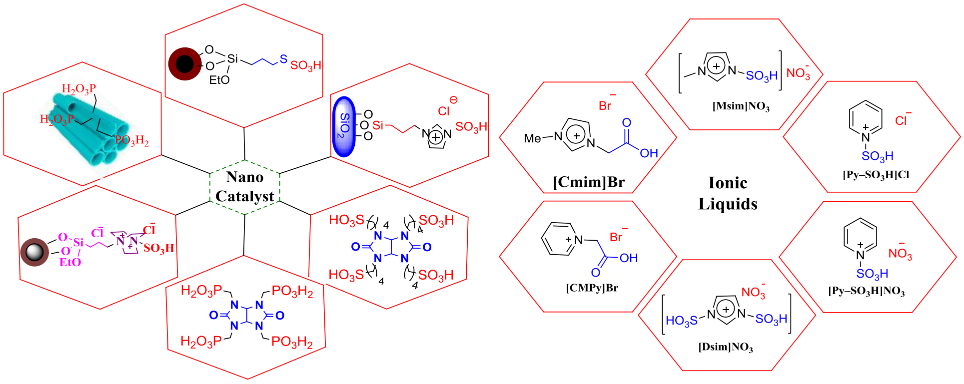

Fig.1: Structure of some task-specific materials.

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Paper code: 1247

Tosylation of Cellulose Nanowhisker in Aqueous Solution

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Natural polymers such as cellulose can be employed to hydrolyze the amorphous region of the polymer. The uses of polysaccharide nanoparticles are receiving a significant amount of attention because of their nontoxicity. This propertie make them excellent candidates for implant materials and drug carriers. The work presented here involves the chemical modification of cellulose nanowhisker with poly (ethylene imine). the cellulose used in this study was cotton linters with degree of polymerization of 850. Briefly Cellulose nano crystals were prepared through dissolution of cellulose in NaOH/Urea then in sulfuric acid aqueous solutions [1], [2], [3] and then were tosylated by p-toluenesulfonyl chloride. 0.5 gr tosylated cellulose Nanowhisker was used as macro initiator and placed in reaction tube then 2-ethyl-2-oxazoline added under nitrogen atmosphere and kept at 90 ºC for 50h, resulted (CNW-g-PEOX) was washed with methanol. Finally CNW-g-PEOX was hydrolyzed in %10 solution of NaOH at 98 ºC for 3h. The nano crystalline cellulose are found embedded in the depth of lignocellulosic matrix enclosed by less ordered amorphous regions which can be removed after different chemical and physical treatments. AFM photograph of CNW`s are shown in Figure 1. After the acid-treatment process, cellulose has been destructed to be nanowhiskers with a size range of 30–80 nm.

Resulted CNW`s were grafted by PEOX and then PEOX moiety in graft copolymer was hydrolyzed to PEI. The structure of products was confirmed by FTIR and ^1H NMR spectroscopes. the ^1H NMR spectra of CNW-g-PEI shows characteristic absorption for cellulose (3-5 ppm) and PEI peaks (3.4 ppm). Also the crystalline structure and thermal properties of modified cellulose nanowhiskers were studied using DSC and XRD. The collected data showed that crystalline structure of cellulose nanowhiskers have not changed during chemical modification reaction.

Successful surface modification was confirmed using FTIR and NMR spectroscopy and also DSC and XRD techniques. The described surface modification clearly changes the character of the nanocrystal surfaces as a cationic graft polymer. These modified nanocrystals will be tested as nonviral vectors for gen delivery systems.

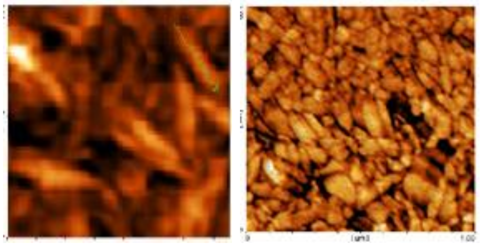

Fig. 1 AMF Images of cellulose Nano whisker

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Physical Chemistry

Paper code: 13

Theoretical Study on the Kinetics and Dynamics of the Reaction of HNO ($^3A''$) with HO_2 ($^2A''$)

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In this study, the kinetics, dynamics and mechanism of the reaction of nitroxyl (paramagnetic HNO ($^3A''$)) with the ground state hydroproxy radical (HO_2 ($^2A''$)) is theoretically investigated at the CBS-QB3 level of theory. Quantum mechanically proposed potential energy surface of HNO ($^3A''$) + HO_2 ($^2A''$) reaction includes one energized intermediate. The *ab initio* results are used to investigate the rate constants by means of RRKM calculations along with stochastic one-dimensional chemical master equation (CME) [1] modeling and steady state assumption (RRKM-SSA) [2]. The temperature and pressure dependence of the reaction over a wide range of temperature (300-3000 K) and pressure (0.1-2000 Torr) are studied. The major products of the title reaction in the stated temperature range studied are trans-HNOH, O_2 ($X^3\Sigma_g^-$), HNOO (T) and OH (D). The master equation calculations determine negligible OH+HNOO formation due to the corresponding high energy barrier. No sign of pressure dependence was observed for the title reaction over the stated range of pressure. The calculated rate constants from the CME simulation (weak collision model) are compared with those obtained from RRKM-SSA that is based on strong collision assumption. Our results indicate that the strong collision assumption increases the calculated rate constant for the formation of the main product (HNOH+O_2($X^3\Sigma_g^-$)) at lower temperature and 1 atm, compared to the results of CME simulation, although the results are in good agreement at higher temperatures.

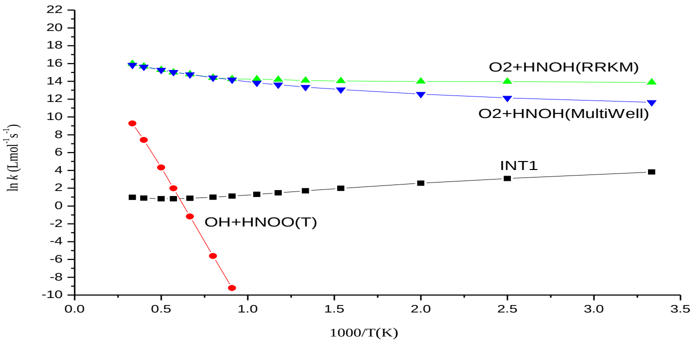

Fig. 1 Arrhenius plot for various channels in HNO (T) + HOO (D) reaction

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Paper code: 14

Dynamics Study on an Interpolated Potential Energy Surface of the Imidogen with Hydroxyl Radical Reaction

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A goal of chemical dynamics is to obtain a microscopic picture of how energy flows as atoms move during the course of a chemical reaction [1]. For this purpose, in this work, semi-classical dynamics simulation of the HN(T)+OH(D) reaction on an interpolated *ab initio* potential energy surface (PES) has been carried out. A global *ab initio* interpolated PES for the title reaction is constructed using the GROW package [2]. An important aspect of the Grow methodology is monitoring the derived dynamical quantities as points are added to the *ab initio* data set defining the interpolation. Dynamics of the reaction is investigated on the ground state of the potential energy surface (PES) based on B3LYP calculations. H_2O, HNO products and two stable wells trans-HNOH and H_2NO were classically observed over the range of relative translational energy (10.5 to 157.5 kJmol^{-1}). The reaction probabilities and reactive cross sections for different channels are reported. The total reaction cross section of the title reaction has been calculated and fitted to an exponential model. Quasiclassical trajectory (QCT) studies on lowest doublet surface shows that the total reaction rate constant is close to the experimental rate constant obtained at lower temperatures (~24.5 Lmol^{-1}s^{-1} at 300 K).

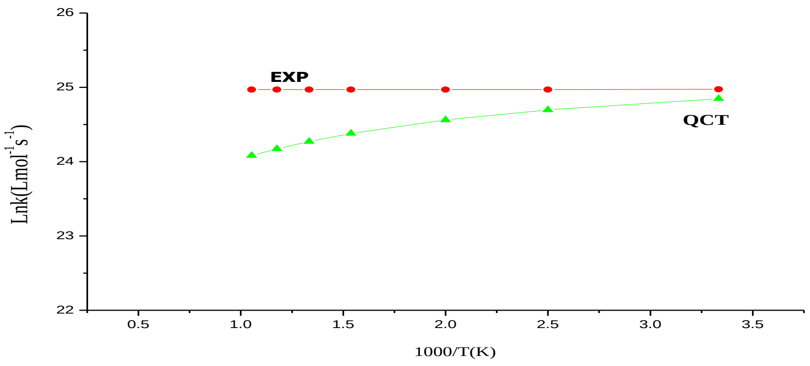

Fig. 1. Arrhenius plot for the formation of HNOH. (QCT) present study.

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Paper code: 25

Kinetic Monte Carlo Simulation of hydrogen production from formic acid decomposition on Ni(100) catalyst

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Hydrogen is a non-polluting fuel. In oxidation, water is the main product. Hydrogen is most abundant element in the universe and it has many uses. hydrogen has the high energy per unit weight. In this research, we investigated the properties of formic acid decomposition on Ni (100) catalyst, by using kinetic Monte Carlo simulation. A mechanism for hydrogen production was suggested. To get a better understanding of the mechanism of formic acid decomposition on Ni(100) surface, several mechanisms have been chosen. Each elementary reaction is represented by using its initial and final states, gas species participating in the reaction, different surface sites, activation energy and the pre-exponential factors. In our simulation, the catalyst surface was modelled as a collection of active sites. On a lattice, each site can be possibly occupied by an adsorbate. The surface of Ni(100) single crystal was considered as a square lattice of 2800×2800 adsorption sites with periodic boundary conditions The kinetics parameters (activation energies and exponential factors) of reactions have been obtained by simulation. It is considered that the square lattice contains four adsorption sites per unit cell, one top, one hollow and two independent bridge sites. In this research it was shown that the simulated kinetics data are in good agreement with experimental data. Both experiment (solid line) and simulated (dashed line) TPD spectra of H_2 desorption from Ni (100) are shown in Fig. 1.

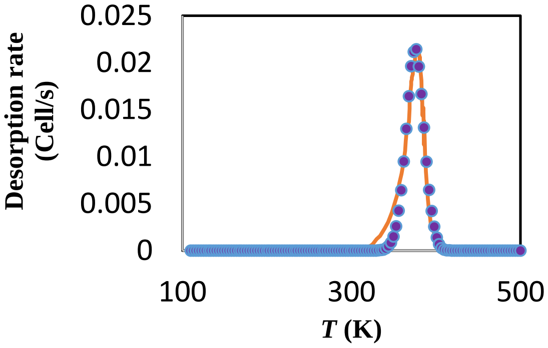

Fig. 1 The experimental (solid line) and simulated (circles) data of hydrogen desorption on Ni (100).

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Paper code: 26

Forest like $BiFeO_3$ thin film obtained from Sol-EPD: photocatalytic and photoelectrochemical activities

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Recently, photocatalytic thin film was attracted for specific application such as photodegradation of pollutant, production storable energy from water splitting and solar cell [1-3]. As shown in Fig.1, forest like bismuth ferrite ($BiFeO_3$) film was synthesized from sol solution by novel sol-electrophoretic deposition (Sol-EPD) method. The crystal structure and the shape of the film and its elemental composition are examined by X-ray diffraction (XRD) and scanning electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDS), respectively. Also atomic force microscopy (AFM) and magnetic force microscopy (MFM) were applied for morphology and magnetism studies. Photoelectrochemical (PEC) studies was performed in 0.5 M Na_2SO_4 as electrolyte under visible light illumination. Photocurrent was moved to positive values (60 µA) and created photovoltage under illumination which indicated sensivity of film under visible light irradiation. Finally, the prepared thin film was used for photodegradation of phenol in a photocatalytic reactor.

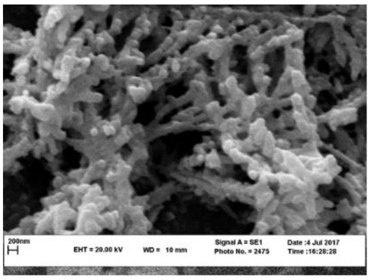

Fig. 1: SEM image of forest like $BiFeO_3$ thin film.

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Paper code: 30

Electron-hole transfer in the dye-based solar cells: A computational study on indoloquinoxaline and triphenylamine derivatives

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Herein, we report some key results related to the photovoltaic properties of a novel dye structure with a double triphenylamine donor and an indoloquinoxaline as the subordinate acceptor (QX22; Fig. 1). To find out whether this dye is applicable to the dye-sensitized solar cell (DSSC) and whether charge transfers are possible in the DSSC, natural bond orbital (NBO) analysis and ground/excited state studies were applied [1]. To obtain photovoltaic parameters, density functional theory (DFT) [2] and time-dependence DFT (TD-DFT) computations were used [3]. Since the LUMO energy level of QX22 is upper than the conductor band (CB) of TiO2 and its HOMO state is lower than the oxidation potential of (I^-/I_3^-) electrolyte, it can be applied as a sensitizer in the DSSC. Negative values of Gibbs energy of the electron/hole injections ($\Delta G_{inj.}$ /$\Delta G_{reg.}$) Show an efficient charge transfer in the DSSC. Negative value of ΔG_{inj} means that electron easily transfers from the dye to TiO_2, which can prevent the charge recombination. Also, $\Delta G_{reg.}$ Values show a proper regeneration process in the DSSC, which can prevent this photovoltaic system from quenching process.

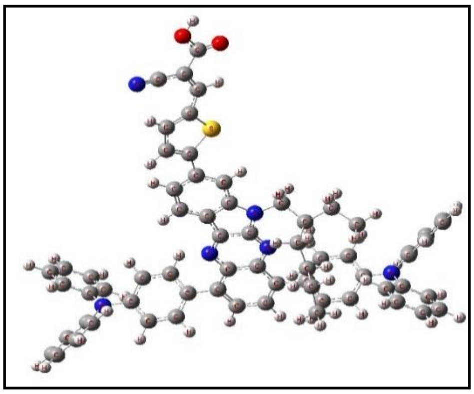

Fig. 1 The optimized molecular structure of the QX22 dye.

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Paper code: 33

Energy conversion efficiency in the solar cells based on the methylammonium lead halide perovskites: Molecular Approach

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In this research, a theoretical investigation of the perovskite-based solar cells (PSCs) was performed to rationalize the the incident photon to current conversion efficiency (IPCE). To achieve this goal, we described photovoltaic processes quantitatively/qualitatively. The ground to excited state transition electric dipole moments ($r_{k,k'}$) and the quantum chemistry reactivity indices such as electrophilicity (ω) of the methylammonium make halide perovskites ($MAPbCl_3$/$MAPbBr_3$: (Fig. 1)) attractive for energy conversion.

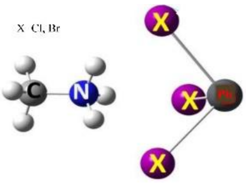

Fig. 1. Schematic presentation of the studied perovskites.

These properties were investigated through density functional theory (DFT), natural bond orbital (NBO) and time-dependent DFT (TD-DFT) at B3LYP/(6-311G++(d,p):for C, H, N) and B3LYP/(6-311G++(d,p): for Pb, Cl, Br) levels of theory [1, 2]. According to the ground state of the studied perovskites, $MAPbCl_3$ has a less tendency of electron donating, which in turn enhances the electron transfer path to be loaded in external circuit. Also, it shows a greater oscillating strength (f) than $MAPbBr_3$, which means a greater probability of charge transfer between the molecular orbitals in the Cl-based perovskite. Also, obtained results show a higher value of $r_{k,k'}$ in $MAPbCl_3$ and IPCE in $MAPbCl_3$-based solar cell (Fig. 2). This behavior may be interpreted by an advance in the efficient electron-hole separation in $MAPbCl_3$. Finally, on the basis of different analyses, $MAPbCl_3$ is proposed as a good candidate to be applied in the PSC, in agreement with the previous studies [3, 4].

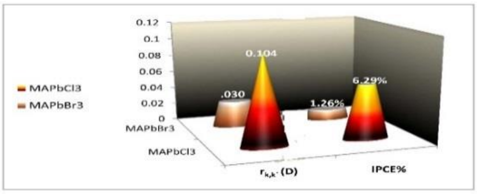

Fig. 2 Comparison of the IPCE and $r_{k,k'}$ in the perovskites.

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Paper code: 34

Carrier lifetime improvement in D-π-A systems; Molecular engineering of the dye-sensitized solar cell

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This work is a computational study on the molecular engineering of the dye-sensitized solar cells (DSSCs). The studied dyes have been designed in the donor-π spacer-acceptor (D-π-A) forms marked as 5'-(9-(4-Fluorophenyl)-9*H*-carbazol-3-yl)-[2,2'-bithiophene]-5-carbaldehyde (3p), (*E*)-5'-(4-(Pyrrolidin-1-yldiazenyl)phenyl)-[2,2'-bithiophene]-5-carbaldehyde (3v) (Fig. 1).The study of the ground state and molecular orbitals of the dyes have been done via density functional theory (DFT) and natural bond orbital (NBO) analysis [1]. Since excited state lifetime of the dyes is one of the most important challenges related to the performance of the dyes, it has been investigated through the time-dependence DFT (TD-DFT) method [2]. According to the energy alignment of the molecular orbitals, the selected molecules can be applied as the dyes in the DSSCs. Here, the effects of different donors on the performance of the DSSCs have been considered, specially. Results show a stronger D part can facilitate electron injection from the dye to the TiO_2, due to a greater intramolecular electron transfer. Moreover, a more efficient D-π-A model of the dye leads to an improved life time of the excited states. The calculated Gibbs energies of the electron injection from the dyes to the semiconductor in the DSSCs are enough low to transfer electrons in an efficient path.

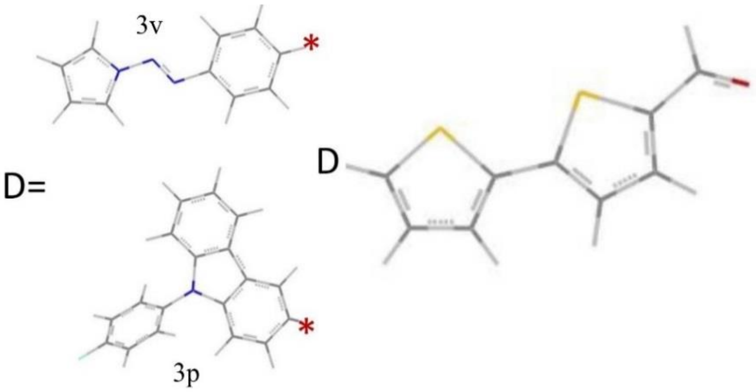

Fig. 1 Schematic representation of the D-π-A dyes.

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Paper code: 44

Thermodynamic modeling of NaCl+RbCl electrolytes in water-Ethanol solvent mixtures based on the electrochemical data and the Pitzer theory

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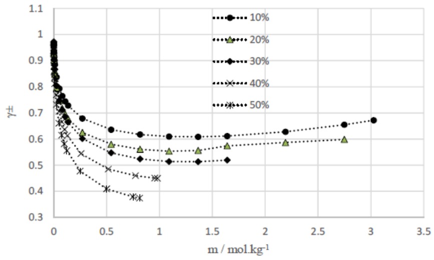
The knowledge of the thermodynamic properties of mixed solvent mixed electrolyte solution are needed for understanding the nature of various ionic interactions and controlling many industrial and environmental process. As we know, rubidium and its salts are rare in the world and cannot form mineral salts because they are extremely reactive. Also, due to its high price, the market for these compounds is very small; so, there is less thermodynamic data for this metal and its salts than other alkali metals and related compounds. Studies on this metal and its salts showed that they have applications like night-vision equipment, batteries, fiber optic telecommunication systems and an ingredient of metal-ion catalysts [1].

in this research, we showed the thermodynamic properties of $NaCl+RbCl+H_2O+C_2H_5OH$ at 298.15 K. A galvanic cell without a liquid junction containing a Na^+-glass membrane and Ag/AgCl electrodes were used along with a computerized data acquisition system for collecting the potentiometric experimental data over the ionic strength ranging from 5.10^{-4} and up to about 4 mol/kg at 298.15 K. Different theoretical electrolyte models were used for investigation of these electrolytic systems. The use of the Pitzer model permitted the determination of parameters ($C^{\phi}, \beta^{(1)}, \beta^{(0)}$) for single salts and mixing ion-interaction (ψ_{ijk}, θ_{ij}) parameters for these investigated systems[2]. The interaction parameters obtained for this system and the graph of the values of the experimental mean activity coefficients in different mass percentages of Ethanol in water are given below.



EeOH	$\beta^{(0)}$/ mol. kg^{-1}	$\beta^{(1)}$/ mol. kg^{-1}	$C^{(\phi)}$/ $mol^2.kg^{-2}$	I_{max}/ mol. kg^{-1}	σ(mV)
10%	0.1256	0.0936	-0.0063	3.5	0.31-0.86
20%	0.1440	0.1025	-0.0024	2.5	0.44-0.84
30%	0.1410	0.1385	-	≤ 2	0.36-0.54
40%	0.1369	0.1115	-	< 1	0.33-0.51
50%	0.2688	0.0150	-	0.75	0.15-0.43

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Paper code: 47

N-Heterocyclic germylenes in focus: Steric effects on nucleophilicity of novel tetrazole-5-germylenes at DFT

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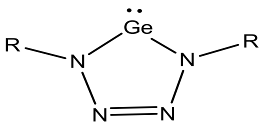
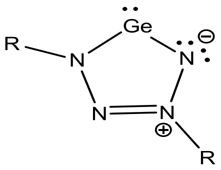
Discovery of N-heterocyclic germylenes (NHGes) began years before Arduengo's report on N-hetrocyclic carbenes (NHCs) in 1991[1]. In this work 20 novel NHGes are characterized at B3LYP/6-311++G**level of theory. Nucleophilicity (*N*) is anticipated to be a crucial factor for coordination of NHGes to transition metal complexes[2]. Hence, comparison is made between *N* of a series of 1,4-disubstituted tetrazol-5-germylidens (“normal”, **1R**), and their corresponding ten 1,3-disubstituted isomers (“mesoionic, or abnormal”, **2R**), where R = H, methyl, ethyl, *i*-propyl, and *t*-butyl. In contrast to their corresponding carbenes where a singlet is more nucleophilic than its corresponding triplet, all our ten triplet NHGes appear more nucleophilic than their related singlet isomers. Similarly, singlet NHGes appear rather aromatic (NICS ≥ -20.7) while their corresponding triplets are nonaromatic (NICS ≥ 0.23). In addition, *N* increases as the size of the substituent increases. The global electrophilicity (ω) trend takes on an exactly opposite direction. Stabilities of **1R** and **2R** are presumed to be related to their singlet–triplet energy gaps ($\Delta E_{S\text{-}T}$, kcal mol-1). Every normal **1R** appears more stable than its corresponding abnormal **2R** isomer. This is except for **1ethyl** which is less stable than **2ethyl**.

The most stable germylenes among the normal and abnormal series are **1H** and **2H**; while the least stable ones are **1ethyl** and **2methyl**, respectively.



1R



2R

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Paper code: 48

Multichannel RRKM-SSA and CVT Rate Constant Calculations for the Reaction of $H_2S(^1A_1)$ with $HO_2(^2A'')$

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An understanding of the oxidation of sulfur containing species such as H_2S, is important to describing both the oxidation of sulfur-containing fuels and the behavior of sulfur pollutants in the atmosphere.

The kinetics and mechanism of the reaction of hydrogen sulfide ($H_2S(^1A_1)$) with hydroperoxyl radical ($HO_2(^2A'')$) on the lowest doublet potential energy surface have been theoretically studied. The potential energy surface for each possible pathway has been investigated by employing CBS, DFT, and CCSD(T) methods. Three different pathways are suggested to be possible for the title reaction. The most probable channel consists of one hydrogen-bonded complex (vdw1) and two energized intermediates.

Multichannel RRKM-SSA method[1] and direct dynamics canonical variational transition-state theory (CVT)[2] calculations have been carried out to compute the temperature dependence of the individual rate constants for different channels and also the overall rate constant for the consumption of the reactants. We have shown that the major products of the title reaction are H_2O_2 and SH while at high temperatures, formation of other products such as H_2O, HOS, HSOH and OH also become important.

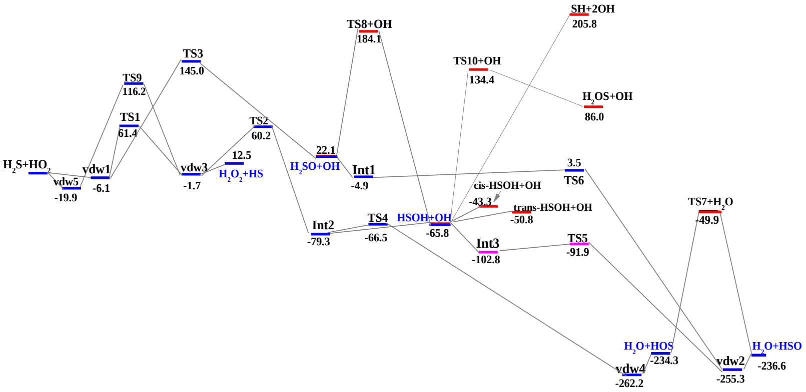

Fig. 1 The ZPE corrected potential energy surface for the reaction of $H_2S(^1A_1)$ with $HO_2(^2A'')$ at the CCSD(T)/Aug-cc-pVTZ//B3LYP/Aug-cc-pVTZ level of theory.

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Paper code: 49

Theoretical studies on the kinetics and mechanism of the unimolecular reactions of hydrogen thioperoxide

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Hydrogen thioperoxide (HSOH($^2A''$)) can be considered as the simple sulfur-substituted analog of the common hydrogen peroxide chemical, and as the simplest hydrogen chalcogenide containing more than one type of chalcogen.
The kinetics and mechanism of the unimolecular reactions of Hydrogen thioperoxide on the lowest doublet potential energy surface have been theoretically studied. The potential energy surface for each possible pathway has been investigated by employing CBS, DFT, and CCSD(T) methods. Hydrogen thioperoxide molecules have a gauche conformation. Internal rotation about the S-O bond of the chemically activated HSOH can form the *cis* and *trans* transition states by torsional barriers of 22.5 and 15.0 kJ mol^{-1}, respectively. HSOH may isomerize to H_2SO or H_2OS by surmounting or tunneling through saddle point.
The MEP calculations are carried out by the IRC theory at the B3LYP/Aug-cc-pVTZ level, and energetic information is further modified by the CCSD(T)/Aug-cc-pVTZ level. Dual-level dynamics calculations are carried out with the variational transition state theory with interpolated optimized corrections (VTST-IOC).[1] The calculated rate constants for isomerization reactions of HSOH to H_2OS and H_2SO to HSOH are displayed in Figure 1. These results indicated that the tunneling effect is very important for calculation of rate constant of channel H_2SO to HSOH.

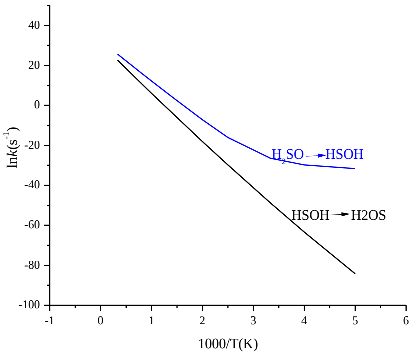

Fig. 1 Arrhenius plot at the CCSD(T)/Aug-cc-pVTZ level for the reaction channels.

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Paper code: 59

Molecular dynamics Simulation of Self- assembly Soybean Oil- based Nanoemulsion System

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Today, the use of nanoemulsions has been considered as penetration enhancers in pharmaceutical applications. In this paper, the structural properties of soybean oil -based nanoemulsion system with Tween80 as the non-ionic surfactants were investigated with molecular dynamics simulation using GROMACS. This system was simulated with the ratios obtained from experiment in 100 nanoseconds. The equilibrium of system was analyzed through the trajectory, the number of clusters, and the radius of gyration. The number of assemblies remained unchanged after 50 ns. Using the free energy landscapes, the most stable shape of assembly, 31, in system was observed asymmetric and non-spherical. The average solvent accessible surface area (SASA) value of the assembly 31 calculated to be 139.73 ± 14.00 nm2. The arrangement of the molecules in the assembly showed that the carboxyl groups (COOH) of oil and the hydroxyl groups (OH) of Tween80 were placed on the surface while the accessible water molecules and the rest of the molecule are located inside the assembly. Also, the plot of radial distribution function between H (water) and O (Tween 80) show the interactions between the O hydroxyl groups (Tween 80) and H (water) is greater than O ether group, and H (water). The results of molecular dynamic simulation studies of nanoemulsion systems can be used in interpretation of practical applications of them as chemical enhancer and drug carriers.

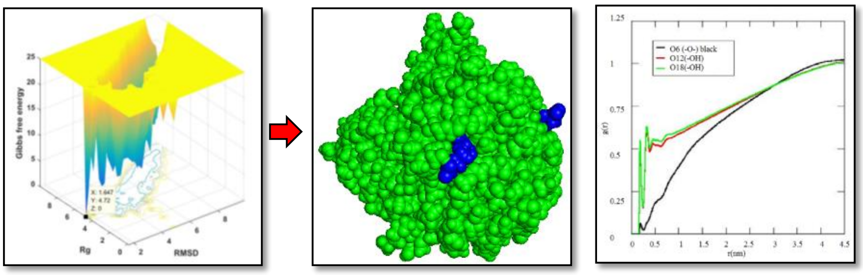

Fig. 1 presentations of the free-energy landscapes for the largest assembly (31) in time of 100 ns and plot of radial distribution function between H (water) and O (Tween 80)

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Paper code: 61

The theoretical study on the coumarin-based Mn(II) complex

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Coumarins (2H-benzo-pyran-2-ones) derivatives, constitute a unique class of fused ring heterocycles that have attracted significant attention owing to their wide distribution in nature [1]. Several natural compounds containing this heterocyclic framework exhibit interesting biological and pharmacological properties [2]. In the present work, the structure of $Mn(Couma\text{-}H^+)_2(MeOH)_2$ (Fig. 1) was investigation theoretically and the results of experimental [3] and theoretical were compared with each other. Full geometry optimization of the crystal structure of Mn(II) complex was carried out using Gaussian 09 suite of program package at B3LYP/6-31G level of theory in the gas phase. Density functional theory (DFT) simulation was used to further understand the electronic structure of Mn(II) complex. The results show that the molecule lies on a center of symmetry. The Mn ion is 6-coordinated bonded to two monodeprotonated, bidentate ligands, which form 6-membered chelate rings. The coordination sphere is completed by two methanol molecules hydrogen bonded to the oxygen of a neighboring molecule. The values of bond lengths and angles calculated with B3LYP method are in agreement with the experimental crystal structure. However, for this complex, the ribbon structure is reinforced by some π-interactions involving carbonyl groups of the coumarin and there are no significant inter-ribbon interactions.

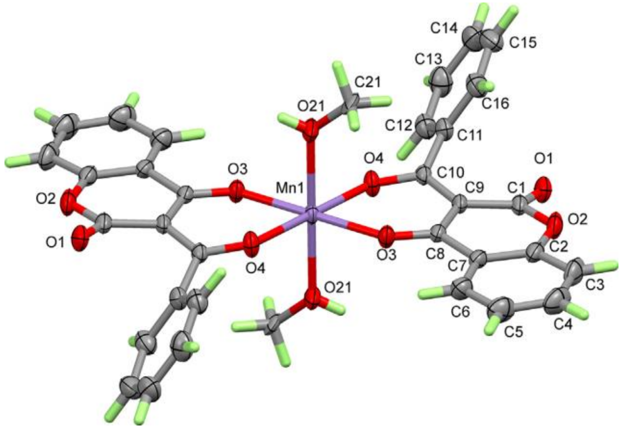

Fig. 1 Molecular structure of Mn(II) complex.

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Paper code: 75

Is single-reference calculation adequate to address kinetics of CH($X^2\Pi$) reaction with N_2($^1\Sigma_g$)?

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CH ($X^2\Pi$) radical (methylidyne) is an omnipresent radical that plays an important role in atmospheric, interstellar and combustive systems [1]. This radical can interact with N_2 and result into prompt NO formation and ozone layer depletion through production of HCN+N [2]. Though there are several experimental studies reported about this reaction, theoretical data are limited. Therefore, this study explores detailed mechanism of this reaction using single-reference calculations at CCSD(T)/aug-cc-pVTZ//M06/aug-cc-pVTZ level of theory (Fig. 1). According to the calculated reaction enthalpies, the results of CCSD(T)/aug-cc-pVTZ, G2M(RCC) [2] and multi-reference CASPT2/aug-cc-pVTZ [2] calculations are about 8.0 to 23.6, 0.5 to 9.2 and 38.1 kJ mol^{-1} different from the corresponding experimental values. Furthermore, there are three transition states that have been reported by G2M(RCC) and/or CASPT2 studies but cannot be found at the CCSD(T) level of theory. With respect to these observations, the related T1 diagnostic values were extracted, which suggested that, except TSn4, all transition states have strong multi-reference characters and should be treated with multi-reference calculations. The strong multi-reference character might be due to the presence of CH radical with the T1 diagnostic value of 0.108, at CCSD(T)/aug-cc-pVTZ//M06/aug-cc-pVTZ level of theory. Meantime, the apparent activation energy of the overall reaction, ^{2}H+^{3}NCN formation and ^{2}N+^{1}HCN production were calculated as 90.2 (81.6), 90.2 (73.3) and 56.9 kJ mol^{-1} at the CCSD(T) (CASPT2 [2]) level of theory, which can be compared with the experimental values of 92.7, 71.2 and 53.1 to 58.2 kJ mol^{-1}, respectively. Therefore, both single and multi-reference calculations of this reaction might involve some discrepancies with respect to the experimental results. Regardless of the level of theory, ^{2}N+^{1}HCN, ^{2}H+^{3}NCN, ^{2}N+^{1}HNC, ^{2}H+^{1}Tri.CNN, ^{2}H+^{3}CNN and ^{3}C+^{2}HNN are the most to the least stable products of this reaction, along with ^{2}HNCN, which is the most stable reaction intermediate. See Fig. 1 for more details.

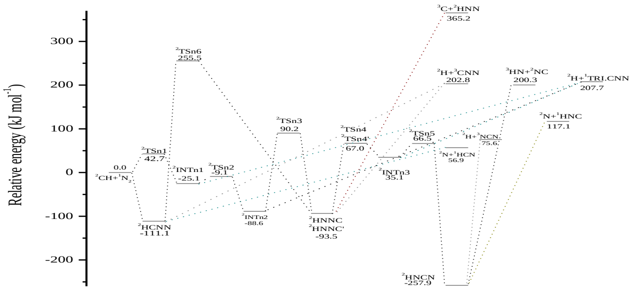

Fig. 1 Doublet potential energy surface of ^{2}CH+$^1N_2$ reaction, at CCSD(T)/aug-cc-pVTZ level of theory.

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Paper code: 77

Permeability-Solubility Compensation by Molecular Dynamics Simulation

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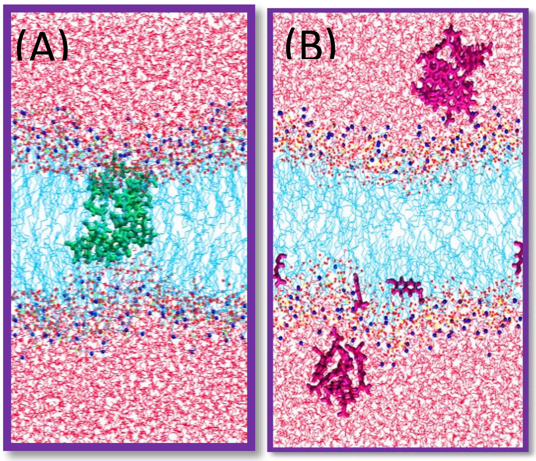
The primary motivation for this study is to gain better insight to the prediction of membrane permeability by using molecular dynamics simulation. The present study attempts to evaluate the impact of intermolecular hydrogen bonds between drug molecules on biological activity. We have chosen octanol-water partition coefficient (log P_{oct}) [1] as our starting point because it is measured routinely in pharmaceutical industry. We test whether octanol/water partition coefficients of these drugs correlate with ensemble average membrane permeability's. All simulations were performed using the GROMACS package. [2] For the initial lipid bilayer structure, a well-equilibrated system containing 128 DPPC lipids was used. Around 7000 water molecules were added to this system to provide the water/membrane ensemble. After about 50 ns of simulation, the aspirin molecules (Fig 1A and 2) are totally aggregated near the center of bilayer. Aspirin occurred in both leaflets because it can transverse the bilayer center spontaneously. Interestingly, the migration process becomes much slower in the case of naproxen (Fig 1B and 2) and equilibrate at the water/DPPC interface even after 110 ns of simulation. We found that changes in the membrane permeability, water solubility, and lipophilicity of drugs depend on strength of the hydrogen bond interaction and geometry of the molecular assemblies.



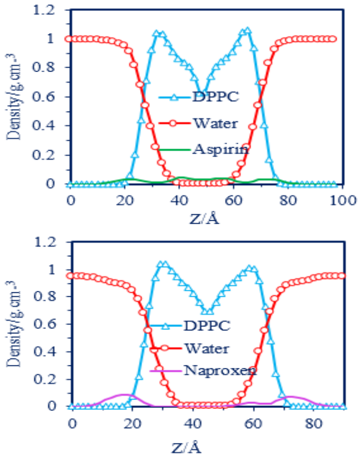


Fig. 1 Sample snapshots of (A) water/Aspirin/DPPC , Fig. 2 Density profiles. water/Naproxen/DPPC system.

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Paper code: 81

Application of Master Equation to Multi Well System of CH_3OH+HO_2

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Master equation method is employed to investigate kinetics and dynamics of CH_3OH+HO_2 system in the presence of N_2 as the bath gas. In solving the master equation, the Lennard-Jones potential is used to model collisions between the colliding gases. The reaction mechanism is quantum mechanically explored through lowest doublet potential energy surface (PES) at QCISD(T)/Aug-cc-pVTZ//CBS-QB3 level of theory. Our proposed mechanism over the lowest doublet PES at QCISD(T)/Aug-cc-pVTZ//CBS-QB3 level of theory involves a chemically activated intermediate and three van der Waals complexes. The fractional population of intermediate and products of the title reaction as a function of time is tested to determine the role of the energized intermediate and van der Waals complexes in the kinetics of this reaction. Theoretical bimolecular reaction rate constant is computed by chemical master equation (CME) while one dimensional tunneling through an asymmetric Eckart [1] barrier is applied to study dynamics and kinetics of title reaction. The formation rate constant of the products is in agreement with the reported experimental values in the literature. Master equation predicts the formation of $CH_2OH + H_2O_2$ and $CH_3O+H_2O_2$ in the CH_3OH+HO_2 system as the major products in accordance with the previous studies. Dominance of rate constant for the formation of $CH_2OH + H_2O_2$ over $CH_3O+H_2O_2$ is coupled with the fact that the CH_3O radical is considerably higher [2] in energy than CH_2OH. No sign of temperature and pressure dependence was observed for the title reaction over the range of 300 to 1300 K and 0.1 to 7 atm, respectively.

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Paper code: 82

Direct Dynamics Study on the Reaction of CH_3^+ with $O(^1P)$ Atom

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Gas phase ion–atom reactions are a class of important reactions that take place in combustion or atmospheric processes where cosmic light is involved. This study focuses on the dynamics and kinetics of the reaction of CH_3^+ with $O(^1P)$ atoms in presence of N_2 molecules as the bath gas. The mechanism of the title reaction is explored at the CCSD(T)/aug-cc-pVTZ level of theory over the lowest singlet surface. The barrier-less initiation step in this system is governed by the capture probability in the entrance channel to form an energized adduct once the centrifugal barrier is surmounted. The reaction takes place over a multiwell multichannel potential energy surface (PES) that is based on the computations at CCSD(T)/aug-cc-pVTZ level of theory. Low values of T1 diagnostic test indicates that the single determinant wave function is dominated [1]. The dynamics and kinetics of the title reaction is simulated by solving a one-dimensional chemical master equation (CME) [2]. The temperature and pressure dependence of the reaction over a wide range of temperature (300−3000 K) and pressure (0.1−5000 Torr) are examined. No sign of pressure dependence was being observed for the title reaction over the stated range of pressure. The results from solving the chemical Master equation indicates that CH_2O^+ and H are the major products in our study.Theoretical bimolecular reaction rate constants over the lowest PES are computed. The results from direct-dynamics canonical variational transition-state theory calculations depict the importance of tunneling in hydrogen transfer isomerization reactions of CH_2O^+ to trans-$HCOH^+$ and HOC^+ to HCO^+.

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Paper code: 102

Electrochemical oxidation of some dihydroxybenzene derivatives in the presence of some Meldrum's acid derivatives: Mechanistic and thermodynamic study

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Electrochemical oxidation dihydroxybenzene derivatives in the absence and in the presence of different nucleophiles were studied by many researchers. It was reported that the mechanisms of the reactions are dependent on the nucleophiles and changes with changing the nucleophile [1,2]. Also, it was reported that the reaction mechanism is dependent on a total change in Gibbs free energy (ΔG_{tot}) of the electrochemical oxidation and species with more positive oxidation potential have larger ΔG_{tot} values [3]. In this work firstly, electrochemical oxidations of some dihydroxybenzene derivatives were studied in aqueous solution at various pHs by the use of cyclic voltammetry. Potential-pH diagram of studied species constructed and oxidation potential of them in pH = 0.0 have been calculated. Also, ΔG_{tot} of the electrochemical oxidation of studied species were calculated using a general thermodynamic cycle (Born- Haber cycle). The theoretical results were calculated at DFT (B3LYP, BP86) levels of theory and different basis sets. The plots of calculated ΔG_{tot} versus E_{p0} constructed and it was found that the best correlation is related to the BP86 level of theory and 6–31G (p,d) basis set. Therefore, this level of theory was used to obtain further data. The electrochemical oxidation of catechol, hydroquinone, 3-methoxycatechol, 3-methylecatechol, 2,3-dihydroxybenzoic acid (both anionic and non-anionic forms), 4-methylecatechol and 4-tert-catechol has been studied in the presence of methyl-meldrum's acid, meldrum's acid and phenyl-meldrum's acid as nucleophiles. The calculated results indicate that oxidation potentials of studied species are directly dependent on their ΔG_{tot}. It was found that not only electrochemical oxidation of one electrophile in the presence of different nucleophile has different mechanisms, but also electrochemical oxidations of various electrophiles in the presence of one nucleophile have different mechanism too. The results showed that the electrochemically generated species which are produced during controlled-potential coulometry, based on their ΔG_{tot}, will participate in the subsequent electrochemical and chemical reactions, and reactions proceed in the thermodynamically favored directions.

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Paper code: 110

Density functional calculations on the adsorption of Ampyra drug on graphene nanosheet

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In this study, the interaction between graphene nanosheet (GNS) and Ampyra drug is investigated using density functional computations to exploit graphene potential application as a drug delivery system. All calculations on the GNS and different configurations are performed using density functional theory at M06-2X [1,2] functional along with the 6–31G(d,p) basis set in the gas phase as well as the water solution.

DFT calculations give valuable information on the structural properties, orientation, adsorption energy and charge transfer between Ampyra molecule and graphene nanosheet in the equilibrium GNS-Ampyra complexes in the gas phase and water solution.

The optimization of different GNS-Ampyra geometries shows that drug molecule tends to adsorb via its six-membered aromatic ring to the hexagonal ring of Graphene nanosheet by π–π stacking interaction at the most stable physisorption (Fig. 1).

Incorporation of aqueous medium imparts significant impact on the solvation energy and dipole moments of the GNS-Ampyra systems which indicate GNS applicability as a drug carrier in the living system.

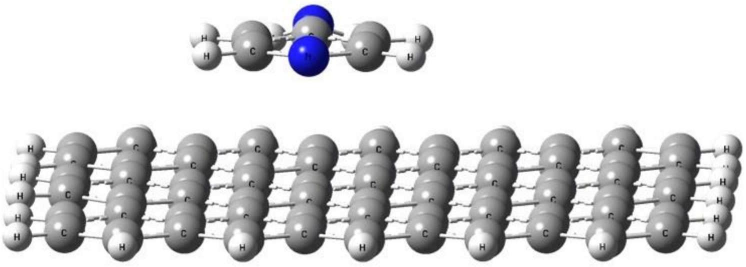

Fig. 1 Optimized structure of the most stable adsorption configuration of Ampyra drug on the graphene nanosheet in the water solution.

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Paper code: 114

Molecular structure and electronic properties of adsorbed Ampyra drug on the functionalized graphene nanosheet: A DFT study

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In this study, the adsorption of Ampyra (Am) molecule (C5H6N2) on the graphene nanosheets functionalized with hydroxyl (G-OH), epoxide (G-O), carbonyl (G-CO), and carboxyl (G-COOH) groups have been investigated by density functional theory. All calculations have been done using M06-2X [1] functional along with the 6-31G(d,p) basis set in the gas phase.

Table 1 shows that, by functionalization of graphene nanosheet with a carboxyl group, the maximum adsorption energy (E_{ads}) between Ampyra drug and the nanosheet is obtained. Diminish in energy gap (E_g) and global hardness (η) with the adsorption of Ampyra on the functionalized nanosheets shows that the reactivity of functionalized complexes increases upon loading of the drug molecule.

When Ampyra molecule approaches on the functionalized nanosheets, electrons are transferred from higher chemical potential to the lower electronic chemical potential, until the electronic chemical potentials become identical. Considering the amount of chemical potential values of Table confirm that electrons will flow from a definite occupied orbital in the TG drug to definite empty orbital in G-COOH, G-O, G-CO and G-OH nanosheets. These results are in accordance with the obtained electrophilicity index values of the studied segments at the considered functionalized complexes.

These results reveal that the chemical modification of graphene nanosheet using covalent functionalization scheme is an effectual approach for loading and delivery of Ampyra drug molecule within biological systems.

Table 1. Adsorption energy (E_{ads}), energy gap (E_g), chemical potential (μ), global hardness (η) and electrophilicity index (ω) for Ampyra drug, functionalized nanosheets and the considered complexes in gas phase.

	Eads(kj/mol)	Eg(eV)	μ(eV)	η(eV)	ω(eV)
G-CO/Am	-28.924	3.309	-3.897	1.655	4.589
G-COOH/Am	-55.169	0.86	-3.702	0.43	15.943
G-O/Am	-43.134	0.974	-3.909	0.487	15.698
G-OH/Am	-28.262	2.846	-3.903	1.423	5.353
Am	-	8.518	-3.274	4.259	1.258
G-CO	-	3.32	-3.798	1.66	4.345
G-COOH	-	0.86	-3.964	0.43	18.278
G-O	-	0.964	-3.849	0.482	15.373
G-OH	-	2.939	-3.866	1.47	5.084

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Paper code: 119

Theoretical investigation dielectric coefficient tautomerization process in gas and solution phase of 5-(x-amino)-1,3,4-oxadiazol -2(3H)-one(x=Br)

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Investigation of tautomerism and transition states in a derivative of 1,3,4-oxadiazole (A, B, C and D) In this combination of atomic bromine as halogen is used. in the gas and solution phase was performed by calculations at the DFT-B3LYP/6-311++G(d,p) level of theory. The geometries of four possible tautomers of 5-(x-amino)-1,3,4-oxadiazole-2(3H)-one were optimized in the gas and solution phase.

It was found that in the gas and solution phase, transition states **C** → **D** and **A** → **D** tautomers are the most stable and unstable forms, respectively. The results show that the tautomeric interconversion C → **D** has the lowest Gibbs free energy changes and so the highest equilibrium constant in the gas and water phase . The calculated results show that the highest rate k forward in the transition states **C** → **D** In the substituent gas phase and lowest rate k forward in the transition states **A** → **D** In the substituent Br in the water phase and highest rate k reverse in the transition states **A** → **D** In the substituent Br in the gas phase and lowest rate k reverse in the transition states **C** → **D** In the substituent Br in the solution phase .

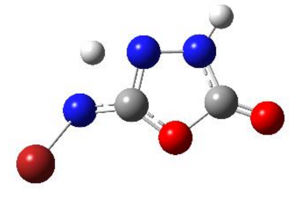
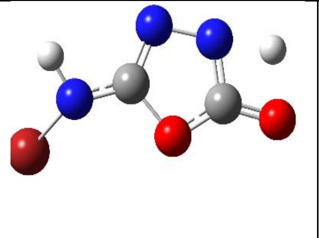
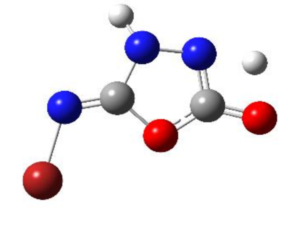
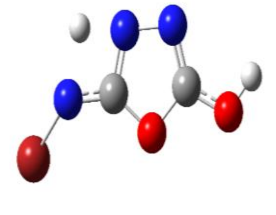
A	B	C	D
			

Fig. 1 The figure(a,b,c,d) four tautomerse in this research. That Nitrogen is blue and Hydrogen is white and Oxygen is red and Carbon is Gray and Bromine is dark red .

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Paper code: 120

Molecular dynamics as a tool to study effect of Na^+ cations on diffusion of SO_2 in Y zeolite

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Since most carbonaceous or hydrocarbon fuels and the ores of many metals contain sulfidic sulfur, as a result, vast volumes are produced in the processing and utilization of hydrocarbon fuels such as power plants, refineries and metallurgical units of metal extraction. High levels of sulfur dioxide production releasing it into the atmosphere is one of the chemical threats to the environment. On the other hand, sulfur dioxide has widespread uses in the wood pulp industry and the manufacture of paper, textile and food processing. However, the outstanding use (more than 98%) is the production of sulfuric acid [1]. The existence of these mutual characteristics has led to the development of adsorption and removal processes. The present study evaluates the diffusion of SO_2 gas in silica Y zeolite cages (Si/Al=∞) and Y zeolite with 48 or 64 Na^+ cations per unit cell (Si/Al=3,2) by MD simulation. All simulations have been done using DL_POLY_2.17 [2] program. The MD simulations were performed within the NVE ensemble at 300, 400, 500 and 600 K. The behavior of SO_2 was investigated for loading of 24 molecules per unit cell (mol/u.c.). Self-diffusion coefficients of guest molecules in Y zeolite are presented in Table 1.

Table 1. The computed self-diffusion coefficients, D in 10^{-9} $m^2.s^{-1}$ of SO_2 in Y zeolite, at different temperatures and loading 24 mol/u.c.

T(K)	Silica Y	Si/Al=3	Si/Al=2
300	6.92	0.69	0.75
400	9.38	1.62	2.93
500	13.57	5.78	6.15
600	13.61	7.83	8.23

As the temperature increases, the self-diffusion coefficient increases in all three types Y zeolite, because molecular movements at higher temperatures lead to more successful jump between sites. The presence of Na^+ cations in two zeolites Si/Al=2,3 will lead to a decrease in the diffusion of SO_2. The SO_2 molecules preferentially reside near the cations due to the stronger attraction [3].

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Paper code: 133

The pristine and C, Si or Ge substituted (5, 5) BeO nanotube: A Computational DFT study of NMR parameters

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To investigate the influence of C, Si or Ge doping on electrostatic structure properties including bond length, bond angles, tip diameters, dipole moments, band gaps and NMR parameters we considered an armchair model of (5,5) beryllium oxide nanotubes (BeONTs) of 1.67 nm length, consisting of 60 Be and 60 O atoms. To this aim Density Functional Theory calculations were performed at the B3LYP/6-31G* level of theory, the Gaussian 03 Program suites. The calculations revealed that Bond distances and tip diameters did not detect any changes in the doped models. The dipole moments of the doped structures show significant changes due to the dopant effect with respect to the pristine model.

In comparison with the pristine model, band gaps of doped models are reduced, and increased their electrical conductance. Our results revealed that Si-doped BeONTs are more reactive than C or Ge-doped BeONTs for Contributing in intermolecular interactions. The results of NMR revealed that the activity of these nanotubes to participate in intermolecular interactions increases with the arrival of impurities, in particular carbon and silicon. Quantum data such as electronica, softness, and chemical potential all confirm these results.

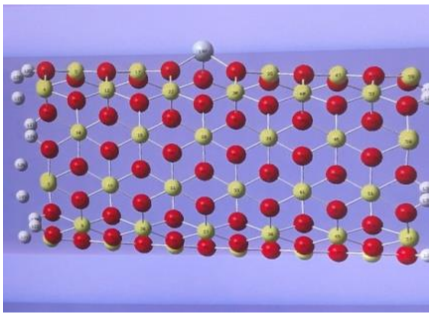

Fig. 1 the Beryllium oxide nanotube doped by silicon

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Paper code: 138

The study of synergism between N-lauryl sarcosine sodium and lithium dodecyl sulfate using conductometric technique

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Surfactants tend to associate as micelles; self-aggregation of surfactants in an aqueous medium is a subject of much interest in the field of surface chemistry. Synergism in the formation of mixed micelle survives as the cmc of mixed system is lower than that of each amphiphiles. In this work we have investigated the mixed of two anionic surfactants at different mole fraction.

Two anionic surfactants with commercial names N-lauryl sarcosine sodium(NDS) salt and lithium dodecyl sulfate (LDS) used in this work. Specific conductivities (k) of the solutions (either pure or different mole fractions) were measured using a Consort conductometer (model C860) at 30.0 °C.

In this study reports the interaction between two anionic surfactants (NDS and LDS) in the water at different mole fractions by conductometric method. The critical micelle concentration (CMC) calculated in pure and mixture state. Also, the micellar mole fractions of surfactants (X_1^{id} and X_1^m), interaction parameters (β^m), degree of counterion binding (α) and standard Gibbs free energies of micellization(ΔG_{mic}^0) values were evaluated and discussed[1-2]. Fig. 1 shows plots of specific conductivity, *k*, *vs* concentration of surfactant in pure of LDS and mixture; above a certain concentration, the slope changes; this concentration is taken as the cmc.

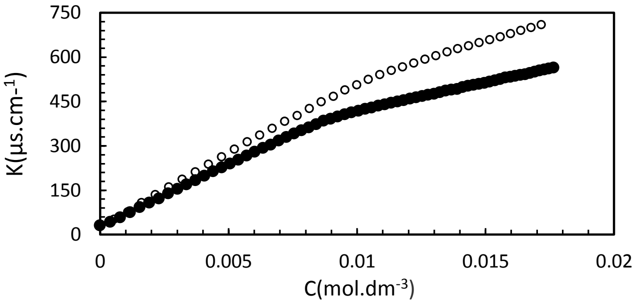

Fig 1. Plot of specific conductivity against concentration of pure LDS (O) and 0.2 mole fraction of LDS(●).

For all mixtures of NDS/LDS, the results indicate an attractive interaction (negative β^m -values), which confirming synergistic interactions between two surfactants. Also, activity coefficients (f_1^m and f_2^m) are always less than unity suggesting non-ideality in the mixtures.

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Paper code: 139

A comparison between three methods for determination of the critical micelle concenteration in ionic surfactants

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Micelles are small colloidal particles; the micelle formation depends strongly on molecular structure (hydrophobic and hydrophilic groups). The concentration above which micelles form is called the critical micelle concentration (CMC). The value of the CMC can be determined by the change in the physicochemical properties of the surfactant solution as the surfactant concentration increases. In this work, CMC values of number of cationic surfactants (DETAB, DOTAB, TTAB, CTAB and IL ([C_{12}mim]Br)) and anionic surfactants (LDS, NDS and SDS) determined by three methods(spectroscopic, conductometric and tensiometry). Fig. 1 shows the effect of increasing surfactant (NDS) concentration on the UV-absorption spectrum of aqueous BZA solutions of 0.07mM (as probe). Below the CMC no changes are observed in the presence of surfactant monomers; above the CMC the absorption band centered at λ = 312 nm (due to the enolic form) is augmented, typically [1].

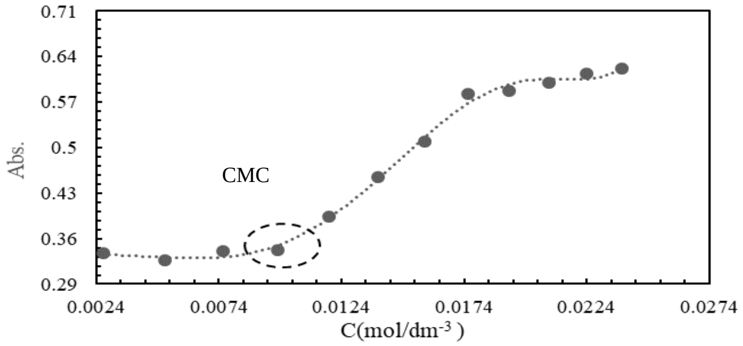

Fig. 1: Absorbance of BZA as a function of [NDS] at 312 nm

The advantages and disadvantages of each method are indicated and compared. Also, it is important to recognize that there may be systematic differences among methods for determining the CMC. The results obtained (CMC values) show a good consistency between two methods (conductometric and tensiometry). The electrical conductance method of ionic surfactant was carried out to determine the CMC, degree of dissociation of counter-ions (β) and standard Gibbs free energies of micellization (ΔG^0_{mic}) values according to the Carpena *et al*. method [2].

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Paper code: 147

Spectroscopic properties of a metal-free indoloquinoxaline-based dye

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In this research, the spectroscopic properties of a metal-free dye based on the indoloquinoxaline has been evaluated (QX25; Fig. 1). To describe the behavior of this molecule against the radiation of sunlight, time dependent-density functional theory (TD-DFT) by the Gaussian 09 program was applied [1]. To obtain more accurate results, all calculations were performed at the M062X/6-311++ (2d, 2p) level of theory. The probability of electron transfer and the ability of the studied compound were estimated at different frequencies of sunlight [2]. The corresponding compound can absorb the wavelengths from 340 to 440 nm. It shows two peaks at 360 and 410 nm. Both of the maximum absorption intensities are equal to the highest light harvesting efficiency (LHE) of the studied molecule. It means that the dye has a greater ability to harvest the sunlight in the wavelengths of 360 and 410 nm. Fig. 2 shows the behavior of the LHE as a function of different wavelengths of light.

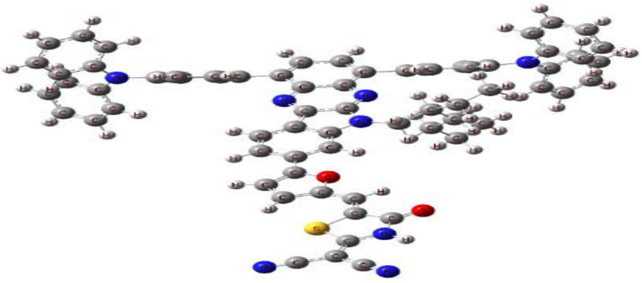

Fig. 1 The optimized molecular structure of the QX25 dye.

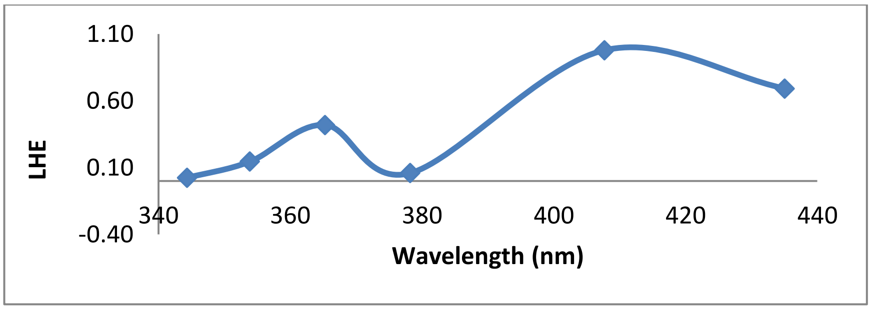

Fig. 2 LHE behavior against different wavelengths of light.

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Paper code: 157

Reactive molecular dynamics simulation for isotope exchange reactions in H/D systems: ReaxFF$_{HD}$ development

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We developed the ReaxFF$_{HD}$ force field for the H_2/D_2 isotope exchange reactions. To the best of our knowledge, the ReaxFF$_{CHO}$ force field has not used to the isotope exchange reactions. Quantum calculations for the isotope exchange reactions are very massive and there are a few *ab initio* information for these reactions. The ReaxFF$_{HD}$ force field was developed by using experimental and computational results on both the concentration and the structural characteristics of all products in the H_2/D_2 isotope exchange process. In this work, we developed the reactive molecular dynamics (RMD) simulations for the reaction $H_2 + D_2 \rightarrow 2HD$ in an electric field. The parameters are modified in such a way that the results are consistent with the previous results. The ReaxFF$_{HD}$ can predict the reaction of H_2 and D_2 at different temperatures and concentrations under an external electric field. We find out that in the reaction between H_2 and D_2 in a discharge chamber the production of three atomic molecules at lower temperatures is more favorable. The simulation results show that at low pressure, the production of H_2D and D_2H is very unlikely. By RMD simulations on a few H_2/D_2 systems, it was found that three atomic molecules are produced by consuming the diatomic molecules. The configuration of the produced three atomic molecules is triangular at all temperatures and concentrations.

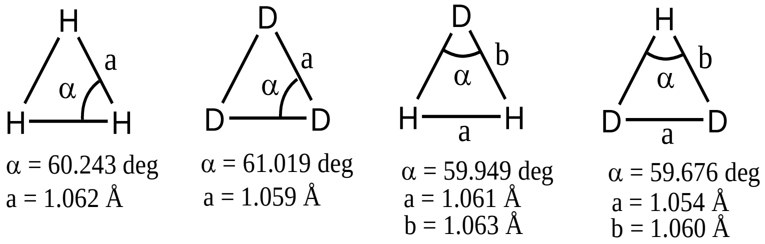

Fig. 1 Schematic representation of all three atomic molecules produced in the simulations of this research. In this picture, the a and b letters are representing the average bond length and α is representing the average bond angle.

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Paper code: 158

Antibacterial activity investigation of magnetic metal nanoparticles decorated ionic liquids

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Magnetic structures were prepared with co-precipitation method. Surface of Fe_3O_4 was modified with BMIM[NTf_2] ionic liquid. The samples became antibacterial by loading metal nanoparticles (Au, Ag, Cu) and denoted as X/IL/Fe_3O_4 (X=Ag, Au, Cu). X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX), thermal gravimetric analysis (TGA), Atomic absorption spectroscopy (AAS), Fourier transform infrared (FTIR) and vibration sample magnetometer (VSM) technics were applied for catalysts characterization. Modified nanocomposites were used for inactivation of Escherichia coli as the gram negative and Staphylococcus aureus as the gram positive of bacteria. Transmition electron micrscopy (TEM) images indicated that highest bacteria cell walls destruction is achieved when the surface of the magnetic nanoparticle is coated with Au particles. Ionic liquid with forming hydrogen bond with cell wall create a channel that metal ions transfer to outer layer of bacteria. Ionic liquid by hydrogen bonding interactions absorb the bacteria to the composite surface and facilitate the ion transfer and bacteria wall destroying. Minimum inhibitory concentration (MIC) study approved the positive effect of Ionic liquid for better antibacterial activity.

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2.

Paper code: 176

Optimization of synthesis parameters of iron oxide nanoparticles prepared by reverse microemulsion method

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Iron oxide-hydroxide nanoparticles have been prepared by a microemulsion route using n-heptane as oil phase, di-n-dodecyldimethylammonium bromide (DDAB) as double-tailed cationic surfactant, polyoxyethylene(23)lauryl ether (Brij 35) as non-ionic surfactant and ammonia (NH_3) solution as precipitant. Inside micelles, the chemical reaction of Fe precursor (ferric nitrate) and NH_3 resulted in formation of precipitate ($Fe(OH)_3$) which was centrifuged, washed with acetone and highly pure water, dried and calcined. Properties such as specific surface area (S_{BET}) and average pore size (a_p) were determined [1]. In this research, in order to evaluation of the influence of parameters, determination of the effective parameter and finally, optimization of synthesis conditions, response surface methodology (RSM) was applied. It was found that the surfactant concentration was the most influencing parameter on the surface area and pore size. The best conditions in terms of higher surface area and smaller pore size was obtained when the water to surfactant ratio of 21.49 and surfactant concentration of 0.19 M were employed. In these conditions, the smallest droplets and the highest number and concentration of droplet were obtained. This explanation was proved by small-angle neutron scattering (SANS) [2].

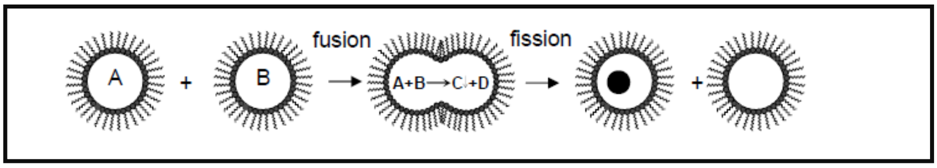

Fig. 1 Schematic of nanoparticle formation by micro-emulsion method

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Paper code: 187

Theoretical study of adsorption behaviour of Thioguanine anticancer drug on the surface of fullerene C_{60} nanocage

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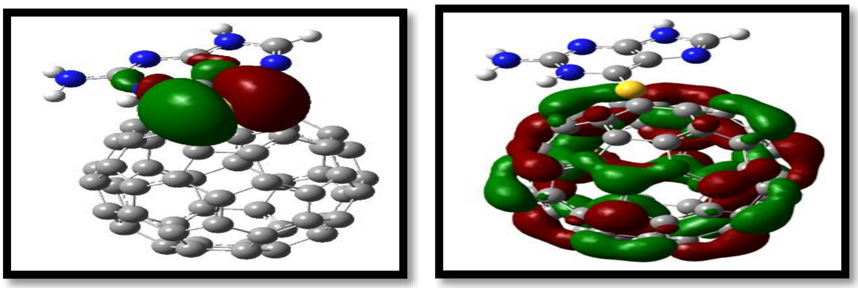
At present work, the adsorption properties of the Thioguanine (TG) interacting with (fullerene C_{60}) are investigated by density functional theory (DFT) calculations. Thioguanine is a chemotherapeutic drug which has significantly curative effect for acute lymphoblastic leukemia and other tumors [1]. Fullerenes are of great interest due to their unique properties, which makes them very attractive for a wide range of applications [2].

The interaction mechanism of TG with C_{60} was investigated by using DFT calculation of the special level of B3LYP/6-31G*. Several possible configurations were selected for TG approaching the side-wall of fullerene. The corresponding adsorption energy value in the most stable structure is -1.61 kJ/mol in the water phase, showing that process of drug adsorption is exothermic.This weak interaction indicates the existence of physisorption between TG and C_{60}. The results of NBO analysis on studied configurations indicated that The important charge transfer in the most stable configuration related to electron donating from lone pair of N atom of TG to the anti-bonding acceptors σ*(C-C) of C_{60}. In other words, drug molecule acts as donor NBO and C_{60} acts as acceptor NBO. After TG is adsorbed, in the most stable complex, the HOMO is positioned on the drug molecule, while the LUMO is located on the surface of fullerene, indicating that electron transfer from TG molecule to C_{60}. It is found that the Eg of C_{60} by interacting with TG altered very slightly, so that we can claim that it is an electronically harmless interaction and the nanocarrier would not significantly alter the drug properties.



HOMO LUMO

Fig. 1. Molecular orbitals of the HOMO and LUMO of the most stable complex.

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Paper code: 189

Theoretical study on adsorption of methane molecule on nanostructured functionalized graphene with hydroxyl and epoxide

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In the present work, density functional theory was employed to analyze the effect of functional groups on the adsorption behavior of CH_4 in nanostructured functionalized graphene (G). Methane which is abundant in earth is found to be an energy carrier [1] and high use of it would result in the reduction of greenhouse gas emission. It is well known that graphene and derivatized forms of graphene offer applications as gas sensors [2].

Two oxygen-containing functional groups such as hydroxyl(OH) and epoxy(O) are applied to modify the graphene surface to clarify the role of a functional group of graphene on the gas adsorption strength. Wood et al demonstrated binding of CO2 and CH4 to model zigzag graphene nanoribbons edge-functionalized with COOH, OH, NH2,H2PO3,NO2, and CH3, while we investigated adsorption of methane molecule on hydroxyl and epoxide on the basal plane of graphene. The interaction mechanism of CH_4 with G(OH) and G(O) was demonstrated by using DFT calculation at the special level of B3LYP/6-31G*. The optimized structures of CH_4 on G(OH) and G(O) were shown in Figure 1. The adsorption energies (E_{ads}) for CH_4 on G-OH and G-O are -3.85 and -3.55 kJ/mol, respectively. Based on the calculated adsorption energy, it can be concluded that the interaction between the gas molecule and the functionalized graphene is weak. Furthermore, values of E_{ads} does not considerably change upon functional groups, indicating the type of functional group has not a significant effect on interaction of the Methane and nanostructures.

Moreover, the values of HOMO–LUMO energy gap are G(OH) =0.064 ev Eg G(O) =0.114 ev, CH_4/ G(OH)= 0.064 ev and CH_4/ G(O)= 0.114 ev respectively, indicating that the adsorption of CH4 has no significant effect on the electronic properties of the functionalized graphene.

Fig 1. Optimized geometries of CH_4 with G(OH) and G(O)

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Paper code: 209

H_2S adsorption on hexagonal boron nitride: A DFT study

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Graphene-like nanostructures such as graphene oxide and hexagonal boron nitride (h-BN) sheet have attracted significant attention because of their potential use for electronic nanodevices and biosensors. Among these materials, h-BN sheet structure is a type of semiconductor material with a wide band gap, which possesses a two-dimensional hexagonal. The peeling of monolayer h-BN was recently realized in experiments, making the application and study on this material more attractive. One potential application is for gas capture and storage [1-2].

In this study we examine adsorption mechanism of H_2S gas molecule on h-BN sheet by using density functional theory (DFT) at B3LYP functional along with 6-31G** basis set as implemented in the Gaussian 03 program package. The interaction energy and geometry parameters of all studied configurations (see Fig. 1) have been systematically explored. It is found that the H_2S molecule presents weak physisorption on the nanosheet surface. The theoretical results indicate that adsorption energy for the studied complexes varies from -4.20 to -0.26 kJ/mol and the most stable configuration is configuration D.

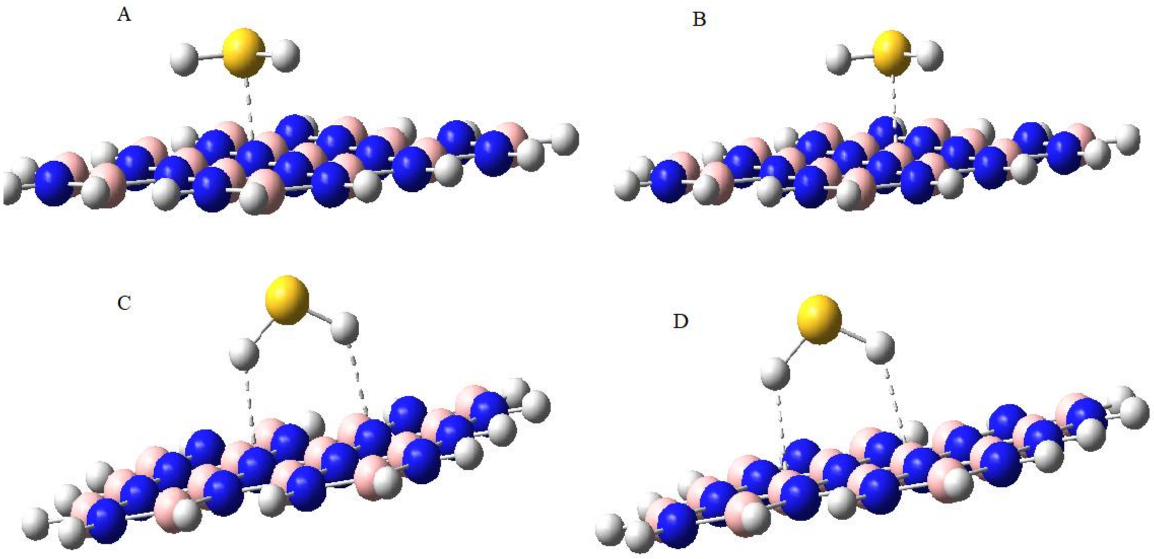

Fig. 1 All of the adsorption configurations of gas molecule on h-BN surface.

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Paper code: 210

Investigation of adsorption properties of CS_2 on hexagonal boron nitride

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Carbon disulfide (CS_2) is ubiquitous throughout the environment. It has been detected in air, water, sediment, and soil; however, it is present primarily in the air. CS_2 is not only extensively used in industry and laboratories as solvent or a reactive reagent but also frequently used for dry cleaning and as an insecticide for the conservation of grains. mobile liquid at room temperature. Due to detect CS_2 concentration in the air, gas sensors have been considered promising alternatives for environmental measurements due to their low cost, high sensitivity, fast response and direct electronic interface [1-2].

In this work, the CS_2 adsorption on the surfaces of hexagonal boron nitride (h-NT) studied using density functional theory (DFT) at B3LYP functional along with 6-31G** basis set as implemented in the Gaussian 03 program package, with the aim of understanding the adsorption behavior at various sites (see Fig. 1). DFT calculations confirmed the energetic stability of the optimized geometries and revealed that CS_2 molecule adsorbed on the h-BN through weak van der Waals (vdW) interaction, which means that the adsorption is physisorption process. Our results show that the adsorption energy for our complexes varies from -1.575 to -0.525 kJ/mol and the most stable configuration is configuration A, which atom sulfur gas molecule prefers attach to N atom of h-BN.

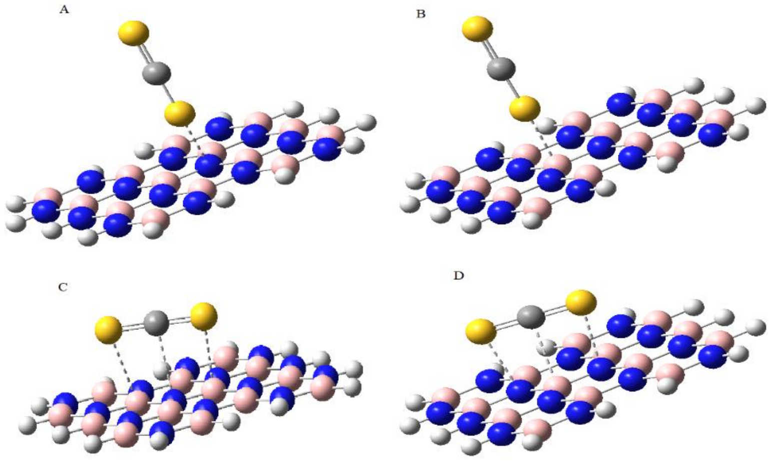

Fig. 1 All of the adsorption configurations of gas molecule on h-BN surface.

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Paper code: 229

Understanding the molecular mechanism of thermal decomposition of methyl benzoylformate using bonding evolution theory

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Understanding of bond breaking/forming, creation/annihilation of lone pairs, and electron rearrangement along an elementary reaction is possible by joint use of the Rene Thom's catastrophe theory (CT) and topological analysis of electron localization function (ELF) that is known as bonding evolution theory (BET) [1]. In the present work molecular mechanism of thermal decomposition of methyl benzoylformate (*see* Figure) [2] has been studied using the MPWB1K/6-31G* level of theory.

Decomposition of methyl benzoylformate involves eleven structural stability domains (SSDs) and can be characterized by the sequence of ten catastrophes (turning points). Breaking of C_8–O_3 and C_8–C_7 bonds occur at *s* ≈ –1.72 amu$^{1/2}$Bohr and at *s* ≈ –0.69 amu$^{1/2}$Bohr, respectively, before the transition state is achieved. When the transition state is reached and left behind new C_7–O_3 bond formation takes place at *s* ≈ 3.78 amu$^{1/2}$Bohr using the C_7– to O_3– coupling of *pseudoradical* centers localized on the atoms.

Along the reaction course of thermal decomposition of methyl benzoylformate, electron flow redistribution is asynchronous and bond breaking/forming do not takes place simultaneously demonstrating that the reaction is concerted yet highly asynchronous process.

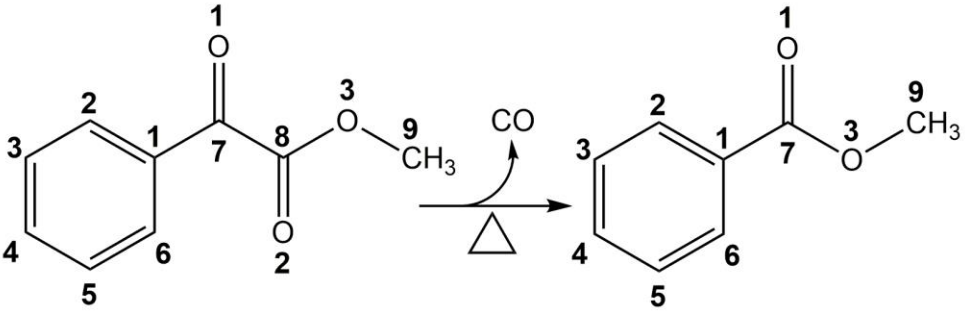

Fig. Thermal decomposition of methyl benzoylformate (left) and atom numbering system.

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Paper code: 236

Time-dependent properties and major electronic transitions in diphenylbacteriochlorin as a dye in DSSC: A quantum chemistry study

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A metal-free type organic molecule, LS-00, based on bacteriochlorin macrocyclic structure (figure 1) has been investigated. In order to estimate the light harvesting efficiency (LHE) of the corresponding molecule [1], the excited states were obtained through the time-dependence density functional theory (TD-DFT) at M06-2X/6-311++G(d,p) level of theory [2]. According to the calculated spectroscopic properties, the studied molecule covers a wide range of sunlight. It is favorable to extend different designs of sensitizers derived from its structure to apply in the dye-sensitized solar cells (DSSCs) [3]. LS-00 can absorb the wavelengths from 287 to 648 nm. LS-00 has two maximum peaks, which one of them appears in the UV area ($\varepsilon=9*10^4$) and another peak in the visible area ($\varepsilon=1*10^4$). Also, it has the highest ability to harvest the wavelengths of 334.6 and 647.1 nm. Moreover, to find which electronic transfer is determinative for the spectroscopic properties, major electronic transitions in the excited states of the LS-00 structure were investigated. Results show the HOMO, HOMO -1, LUMO and LUMO -1 play key roles in the simulation of the UV-Vis spectrum. For example, in the visible area, the electronic transitions such as HOMO -1→ LUMO +1 and HOMO → LUMO are important, while in the UV area, the electronic transitions of HOMO -1→ LUMO and HOMO → LUMO +1 are outstanding.

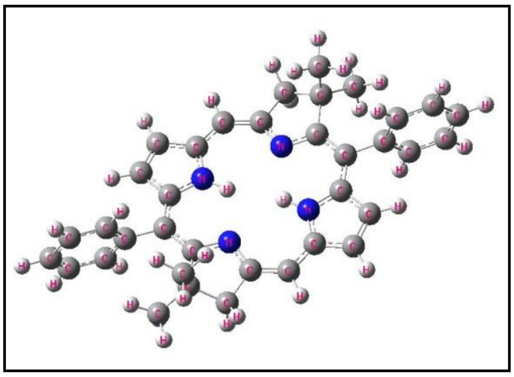

Fig. 1 The optimized molecular structure of the diphenylbacteriochlorin, LS-00.

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Paper code: 240

A bacteriochlorin-based structure with a good planarity in charge transfer in DSSCs

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A dye molecule based on the bacteriochlorin (Bacteriochlorins are planar, highly conjugated macrocyclic molecules [1]), LS-01, as a sensitizer in the dye-sensitized solar cells (DSSCs) has been investigated. This molecule has a D-π-A architecture (bacteriochlorin as donor, ethynyl-phenyl as π spacer and carboxylic acid as anchoring/acceptor group) that via an anchoring group is connected to the TiO_2 surface. In this work, a possible relationship between the dye structure and the performance of the DSSC has been investigated. The dye was optimized at the DFT/M06-2X/6-31G(d,p) level of theory [2]. Excited state calculations were done by using the TD-DFT/M06-2X/6-311++G (d,p) level of theory. The dihedral angle of dye between anchored group and π spacer, π spacer and donor moiety are ~ 0.13° and ~ 0.7° respectively. Therefore, this good planarity can increase the π-conjugation and facilitates the injection of photoexcited electrons into the TiO_2 semiconductor. The results of the DFT and TD-DFT calculations show the negative values for $\Delta G_{ing.}$ (-1.690 eV), which means that the electron injection process from the excited dye to the TiO_2 is spontaneous. This result is accordance with the structural planarity mentioned above.

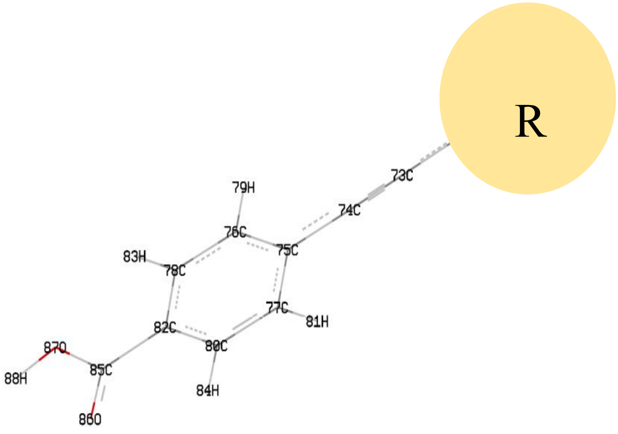

Fig. 1. The optimized molecular structure of the LS-01 dye (R= bacteriochlorin ring).

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Paper code: 244

The I–V Characteristics of dimethyl 3,5-heptane dione Nano-Molecular Wire Induced by Hydrogen Transfer

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In recent years, with the advancement of techniques for manipulating individual molecules, electronic devices based on single molecules have been considered one of the most promising candidates for today's silicon-based devices both for their novel physical properties and potential for device applications [1,2], such as negative differential resistance (NDR), switches, latches and rectifiers. β-Dicarbonyl compounds, with at least one α-hydrogen, are capable to display a keto–enol tautomerism as illustrated in Fig. 1. The cis-enol forms of β-dicarbonyl compounds are engaged in an IHB system and stabilized in a six-membered chelated ring [3].

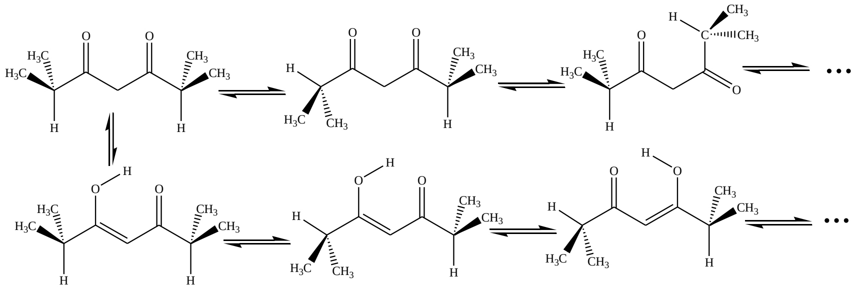

Fig. 1 Tautomery in dimethyl 3,5-heptane

Using nonequilibrium Green's function formalism combined first-principles density functional theory; we study the transport properties of dimethyl 3,5-heptane as a molecular switch. The I–V characteristics, differential conductance, *on-off* ratio, electronic transmission coefficients, HOMO–LUMO gaps and effect of electrode materials Y (Y=Au, Ag, and Pt) on electronic transport corresponding to the keto and enol forms through the molecular devices are discussed in detail. It was found that the best switching behavior performance happens in the gold electrode. Based on data when the enol form transforms to the keto form, there is a switch from *on* state to the *off* state (low resistance switches to high resistance).

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Paper code: 248

On the study of CO/H_2 potential interactions with HKUST-1 MOFs using ab initio calculations

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DFT calculations are employed to study the metal–dihydrogen and metal-carbon monoxide interactions in order to CO/H_2 gas separation, making use of a non-periodic model system (M_2 paddle wheel with M=Cu), which is representative for many copper-containing MOFs [1,2]. All-electron DFT calculations were carried out with the Orca 3.0.3 program package. A geometry optimization of the isolated $Cu_2(bmc)_4$ paddle wheel (bmc = benzene-monocarboxylate) with three different orientations of the hydrogen molecule and one orientation for carbon monoxide molecule were considered: (a) side-on orientation I, H–H bond oriented along one O–Cu–O axis; (b) side-on orientation II, H–H bond bisecting the right angle between the O–Cu–O axes; (c) end-on orientation for H_2 and CO. Single point calculations were employed to obtain a potential energy surface for H_2 and CO with Cu atoms; all geometries were finally optimized. The resulting binding energies as a function of the distance were calculated and the results show that the separation of the binary gas mixture of H_2/CO is possible.

Fig. 1 $Cu_2(bmc)_4$ paddle wheel with one H_2 molecules adsorbed (side-on orientation) in left side and one CO molecule adsorbed (end on orientation) in right side. Two central atoms (Cu), red ones (O), pink ones (C) and blue ones (H).

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Paper code: 259

Micellization parameters of a novel cationic urethane gemini surfactant in the presence of insulin: Conductivity measurements

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Gemini surfactants are newly developed amphiphilic molecules that have two hydrophilic head groups and two hydrophobic tails linked by a spacer [1]. Depending on the characteristics of the head moieties, gemini surfactants are classified in four groups: anionic, cationic, non-ionic and zwitterionic. Gemini surfactants feature interesting properties with respect to conventional surfactants, such as lower toxicity, higher degrees of biodegradability, optimal activity at extreme conditions of temperature, pH levels and salinity, etc. Therefore, they have attracted a great attention of the scientific and industrial communities [2].

Studies of protein-surfactant interactions are significant in the fields of detergents, cosmetics, biosciences, foods and pharmaceutics [3]. Therefore, the aim of this work is to study the thermodynamic characteristics of cationic urethane gemini surfactant nano-micelles having the spacer length of 6 methylene units, in protein solution at neutral pH. The electrical conductivity method was used to determine the important system parameters, such as critical aggregation concentration (CAC), protein saturation point (PSP), the ionization degree of protein-surfactant complexes (α_1) and ionization degree of free micelles (α2). The CAC is lower than the critical micelle concentration (CMC), which is determined in the absence of protein. The α_1 is determined by the ratio of the slopes of the linear parts of the graph above and below the CAC, while the ratio of the slopes below the CAC and above the PSP is attributed to α_2 [4]. The standard Gibbs energy for the surfactant-protein association process (ΔG^0_{agg}) as well as the standard Gibbs energy for the transfer of 1 mole of surfactant molecules from unperturbed micelles to protein-bound micelles (ΔG^0_{ps}) was also calculated.

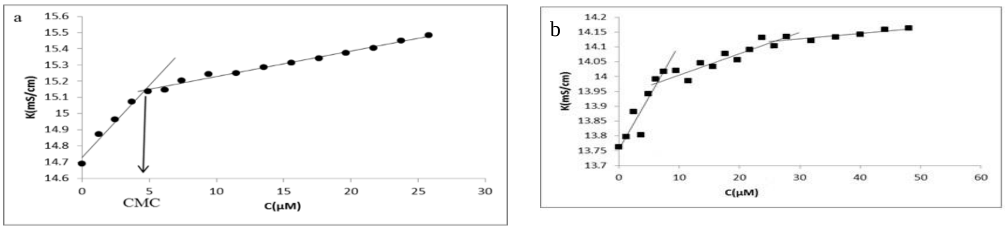

Fig. 1 Conductivity measurements of (a) a gemini surfactant solution in PBS buffer and (b) the protein solution against gemini surfactant concentration.

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Volumetric and Acoustic Studies of L-valine in Polyethylene Glycol Aqueous Solutions

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The density and sound velocity measurements were carried out on L-valine in pure water and in aqueous solutions of 0.02 w/w of PEG400, PEG2000 and PEG6000 at T = (298.15, 308.15 and 318.15) K at atmospheric pressure. From these experimental data, the values of the apparent molar volume, isentropic compressibility and apparent molar isentropic compressibility were evaluated and fitted to the Redlich – Mayer equation from which the apparent molar volume and apparent molar isentropic compressibility of the solutions at infinite dilution were calculated at each temperature. Furthermore, the effect of molar mass PEG and temperature on the volumetric and comperssibility properties of the mentioned systems have been studied. The results show that molar mass of the polymer don't affect on the values of apparent molar volume, isentropic compressibility and apparent molar isentropic compressibility.

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Paper code: 271

Investigation of the quantum molecular descriptors in reactivity of Carmustine drug with boron nitride nanotube by DFT approach

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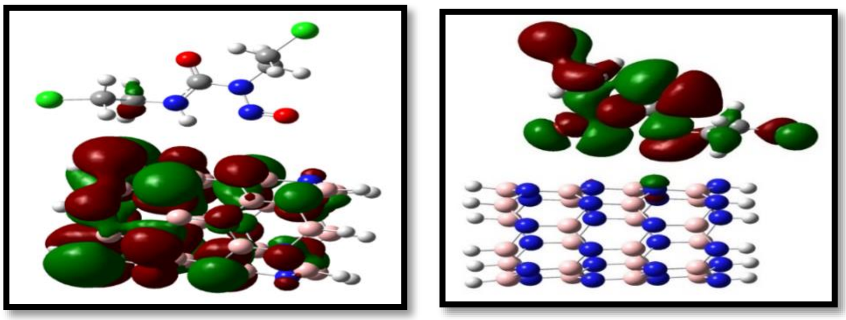
In this study, a quantum mechanical study for the interaction of the Carmustine (BCNU) with the (6, 0) zigzag single-wall boron nitride nanotube (SWBNNT) is studied by means of density functional theory (DFT) calculations at the B3LYP/6-31G* level of theory. Carmustine is an effective drug for the treatment of brain tumors which is used in chemotherapeutic [1]. It is well known that boron nitride nanotubes are more appropriate nanotubes for biomedical applications [2]. The difference between E_{HOMO} and E_{LUMO} for drug molecule and nanotube is calculated and the value of $|E_{HOMO\ (SWBNNT)}-E_{LUMO\ (BCNU)}|$ and $|E_{HOMO\ (BCNU)}-E_{LUMO\ (SWBNNT)}|$ energies are obtained 4.270 eV and 5.497 eV, respectively. The obtained results reveal that the electron density transfer can be performed between the HOMO of nanotube and the LUMO of Carmustine. Also, the HOMO and LUMO orbitals for BCNU/SWBNNT complex are shown in Fig. 1. As can be seen from Fig. 1, the HOMO is mainly localized at nitrogen atoms of the nanotube (panel (a)) while the LUMO is on the BCNU (panel (b)) in BCNU/SWBNNT complex. Also, the values of E_g and η decrease in complex by the adsorption of drug molecule on the nanotube surface ($E_{g\ SWBNNT}$ =4.88 ev $E_{g\ BCNU/SWBNNT}$ =4.59 ev, η_{BNNT} = 2.44 ev and $\eta_{BCNU/SWBNNT}$ = 2.29 ev). The lowering of energy gap and global hardness indicates that the reactivity of the system is increased. Electronegativity (χ) and electronic chemical potential ($\chi = -\mu$) identify the direction of electron flow. When the BCNU molecule and SWBNNT are brought together, electrons will flow from that of higher μ (μ_{SWBNNT}= -4.23 ev) to that of lower μ (μ_{BCNU}=-4.84 ev).



(a) **(b)**

Fig 1. Frontier molecular orbitals a) HOMO and b) LUMO localizaed on BCNU/SWBNNT.

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Paper code: 272

Electronic effects on normal and abnormal acyclic, cyclic-saturated and cyclic-unsaturated diaminocarbenes at DFT

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Carbenes are sextet neutral divalent carbon species. The two nonbonding-unpaired electrons of a triplet carbene have parallel spins with a linear or bent geometry, while those of a closed shell singlet carbene appear anti-parallel in an σ or $2p_\pi$ orbital. Carbenes are an important class of reactive intermediates. Diaminocarbenes are carbenes with two nitrogen atoms in neighboring of carbene center (acyclic or cyclic forms) [1,2]. Before, we studied on steric effects on normal and abnormal acyclic, cyclic-saturated and cyclic-unsaturated diaminocarbenes at DFT.

We used DFT calculations (M06/6-311++G** level) to attain electronic effects on the multiplicity, stability, and reactivity of normal and abnormal 2,4-disubstituted diaminocarbenes with acyclic, cyclic-saturated and cyclic-unsaturated structures (1_R, $1'_R$; 2_R, $2'_R$; and 3_R, $3'_R$; respectively), (R = NH_2, OH, OMe, SH, Ph, CN, CF_3, NO_2). All optimized structures are stable singlet ground states. In both electron withdrawing and releasing substituents, going from acyclic to cyclic structure, because of cyclization and aromatization, singlet-triplet energy gap ($\Delta E_{S\text{-}T}$), HOMO-LUMO energy gap ($\Delta E_{H\text{-}L}$), and proton affinity (PA) increase (except $3'_R$). Going from acyclic to cyclic and unsaturated structures, Nucleophilicity (N) decreases, and Electrophilicity (ω) increases.

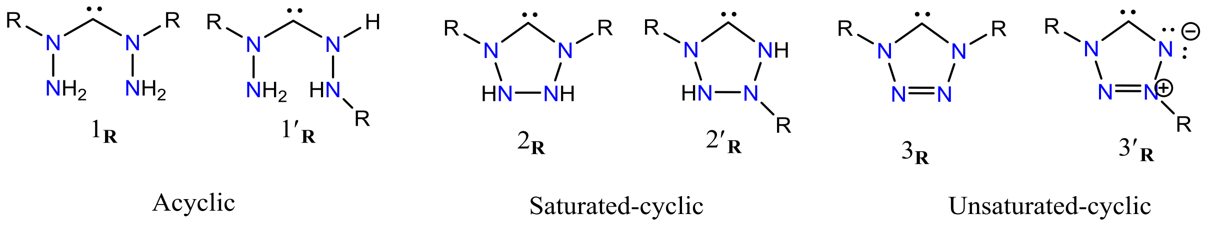

Fig. 1 Theoretically scrutinized normal and abnormal diaminocarbenes: acyclic (**1_R** and **$1'_R$**); cyclic-saturated (**2_R** and **$2'_R$**); and cyclic-unsaturated (**3_R** and **$3'_R$**) for R = OH, NH_2, OMe, SH, Ph, CF_3, CN, and NO_2.

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Paper code: 276

Cytotoxicity of Zinc Oxide Nanoparticles Synthesized in the Presence and Absence of Ultrasound on Saos-2 Cancer Cell Line

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The application of zinc oxide nanoparticles (ZnO NPs) in cancer therapy is increasing rapidly. The anticancer activity of ZnO is related to the physicochemical properties of nanoparticle such as particle size, surface charge and crystalline structure [1]. Synthesis method of nanomaterials can affect the mentioned properties of nanoparticles and under correct conditions resulting in their cytotoxicity against cancer cells [2].

In this work, the cytotoxicity of ZnO NPs synthesized in the presence and absence of ultrasonic irradiation was investigated on Saos-2 cell line. The sono-synthesized samples were prepared under direct and indirect sonication. The prepared ZnO NPs were characterized by scanning electron microscopy (SEM) (see Figure 1), X-ray diffraction (XRD) and zeta potential measurements. The cytotoxicity of resulting nanoparticles was evaluated by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-tetrazolium bromide (MTT) assay. Based on the results of MTT assay, the sono-synthesized ZnO NPs were more cytotoxic to Saos-2 cells than those obtained without sonication.

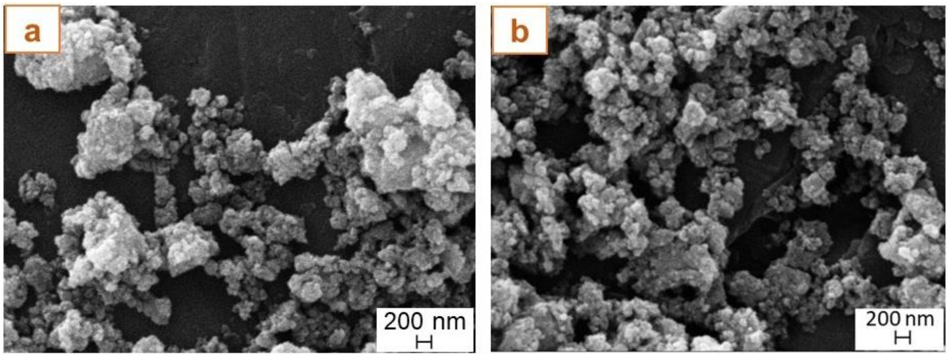

Fig. 1 SEM images of ZnO NPs prepared: a) without ultrasound and b) with ultrasonic bath.

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Paper code: 282

Adsorption of Cr and Pd transition metal atoms on the pristine Zinc oxide nanotube: a DFT Study

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The adsorption properties of a single transition metal atom; Cr and Pd on the top of the ZnONT is studied with hybrid density functional B3LYP as implemented in the GAUSSIAN 09 program. It is known that doping is an important and effective method for improving the sensing properties of metal oxide semiconductors [1]. The split-valence basis set 6-31G* is applied to O and H atoms while the effective-core-potential LANL2DZ basis set is used for transition metal atoms. The intermolecular distances between oxygen atom of the ZnONT and the transition metal atoms are 1.835 and 2.105 Å with the binding energies of -7.413 eV and -5.730 eV for Cr and Pd atoms, respectively. Based on the obtained results, it is found that the binding energy of Cr adsorption is higher than that for Pd atom; furthermore, Cr atom could be stably adsorbed on the similar site with respect to Pd atom. Moreover, the natural bond orbital (NBO) analysis has been employed to evaluate the direction of donor–acceptor interactions. The difference between the highest occupied molecular orbital (E_{HOMO}) and the lowest unoccupied molecular orbital (E_{LUMO}) for transition metal atoms and ZnONT are calculated and the value of $|E_{HOMO\ (ZnONT)}-E_{LUMO\ (Cr)}|$, $|E_{HOMO\ (ZnONT)}-E_{LUMO\ (Pd)}|$, $|E_{HOMO\ (Cr)}-E_{LUMO\ (ZnONT)}|$ and $|E_{HOMO\ (Pd)}-E_{LUMO\ (ZnONT)}|$ energies are obtained 0.895, 1.937, 1.599 and 0.669 eV, respectively. The obtained results reveal that the electron density transfer can be performed between the HOMO orbital of Zinc oxide nanotube and the LUMO orbital of Cr transition metal for the adsorption Cr atom on the pristine nanotube and there is a reverse result for the adsorption of Pd atom on the nanotube surface.

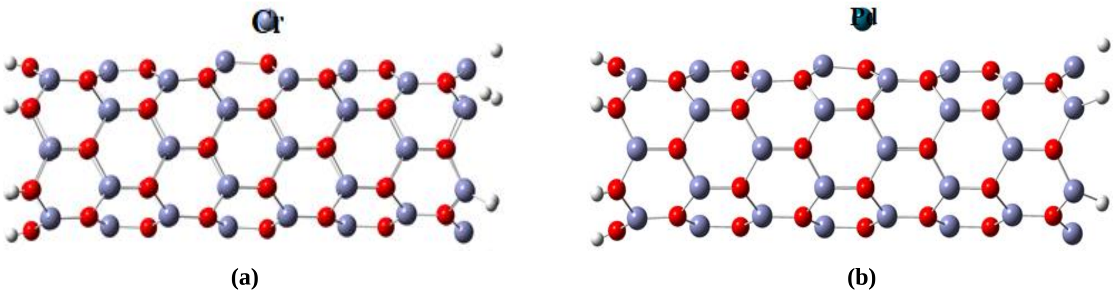

Fig. 1 The optimized structures for the adsorption of (a) Cr and (b) Pd atoms on the pristine ZnONTs.

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Paper code: 284

System toward the anticancer drug molecules

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Single-walled carbon nanotubes (SWNTs) are the novel emerging nanomaterials often considered as an ideal material in a variety of applications due to their potential biocompatibility in pharmaceutical drug delivery systems and capacity to penetrate into cells to promote the cellular uptake of therapeutic agents. Tegafur (TG) is a depot form of 5-Fluorouracil (5-FU) consisting of a new class of oral chemotherapeutic agents belonging to the group of nucleoside analogues. TG is a very effective drug in the treatment of a wide variety of solid malignancies, including head, neck, breast, and colon cancers. In this work, the molecular dynamics simulation is applied to predict the competitive adsorption behavior of 5-FU and TG drug molecules on the surface of the (10, 0) SWCNT. Initially, SWCNTs have been located in the center of boxes; then, ten molecules of each studied drug are randomly added to the simulation boxes. In the next step, all simulation systems are fully hydrated by water molecules using the simple point-charge TIP3P model [1]. All simulations are carried out in the NPT ensemble using the GROMACS 4.5.4 software package [2] for 14 ns using the all-atom CHARMM27 force field [3]. It is noted that due to zero partial charges of SWCNT atoms, the electrostatic component is zero and only the van der Waals (vdW) energy contributes in the interaction of the adsorbed drug molecules on the nanotubes surface. Analysis of the obtained MD simulation results shows that by approaching more number of TG molecules towards the surface of SWCNT, the number of contacts between these fragments is increased and the vdW interaction energy becomes more negative, suggesting an enhanced favorability toward TG molecule binding to carbon nanotube surface with respect to 5-FU drug molecule. Such results provide valuable information on the potential applications of carbon nanotubes in the fields of drug delivery within biological systems.

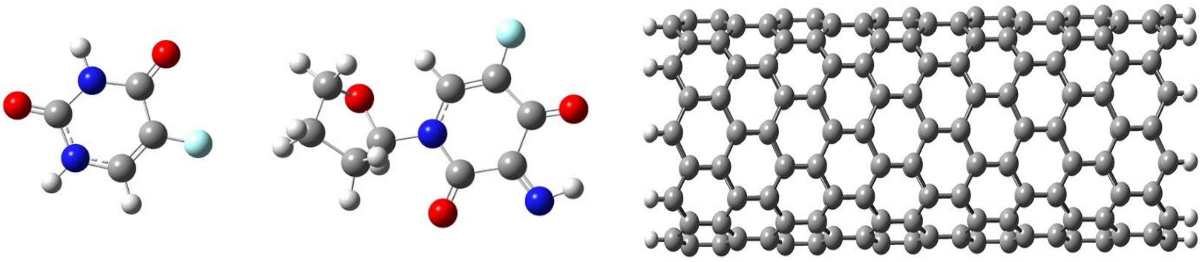

Fig. 1 uctures for the 5-FU, TG and S

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Paper code: 285

A computational study on the electronic properties of single walled boron nitride nanotube as carrier for Carmustine molecule by DFT

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In this research, the adsorption of Carmustine (BCNU) on the single wall (6, 0) boron nitride nanotube (SWBNNT) are studied using DFT method at the B3LYP/6-31G* level of theory for investigating the effect of BCNU molecule adsorption on the electronic structure properties of SWBNNT(Fig. 1). The interaction of BCNU drug and the pristine SWBNNT on the basis of five reactivity descriptors such as the $\Delta E_{SE\ (AB)}$, $\Delta E_{A\ (B)}$, $\Delta E_{B\ (A)}$, ΔN and $\Delta\omega$ have been explained [1]. According to our theoretical results, we concluded that the pristine SWBNNT is B (i.e., donor) and the BCNU drug is A (i.e., acceptor). The calculated values of $\Delta E_{SE\ (AB)}$, $\Delta E_{A\ (B)}$ and $\Delta E_{B\ (A)}$ within the reacting BCNU and SWBNNT are -0.039, -0.589 and 0.550 ev, respectively. In the present study, $\Delta E_{SE(AB)}$ and $\Delta E_{A(B)}$ are exploited to understand the thermodynamic stability of interaction between the SWBNNT and BCNU molecule. The value of $\Delta E_{A\ (B)}$ is negative, which shows that the complex [AB] is more stable than the two individual species; so, BCNU/SWBNNT is more stable than the pristine SWBNNT and BCNU molecule. Also, the amount of ΔN is calculated 0.126. This descriptor help to determine the direction of spontaneous electron flow in the process of interaction. The positive values of ΔN and $\Delta E_{B(A)}$ indicate that the donor and the acceptor species have been chosen properly.

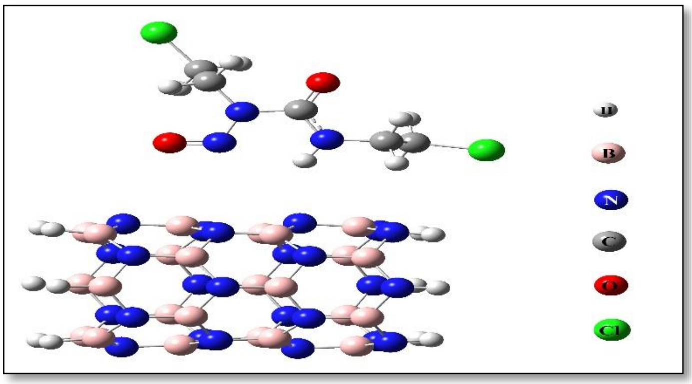

Fig. 1 The optimized geometries of BCNU /SWBNNT in the studied model (complex [AB]).

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Paper code: 330

Interactions between water and dye atoms in the adsorption process of Acid Red-88 on graphene nanosheet: A molecular dynamics simulation

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Water purification is one of the most important environmental concerns because water is directly related to public health, energy production, economic and industrial development Since dyes are one of the most common environmental pollutants, and are usually toxic, their separation from water resources is very important [1]. This paper contains the results of the adsorption of acid red 88 as a dye from an aqueous solution on graphene nanosurface using molecular dynamics simulation at 298 K by DL_POLY 2.17 software [2].

In this study, the water-dye interactions by use of radial distribution function is analyzed to distinguish which atom of acid red 88 has a stronger interaction with the hydrogen atoms of water molecules and tend to be more hydrophilic. As shown in Figure 1, the greatest interaction between the dye molecule and water hydrogen atoms is from the oxygen side of the sulfite group. In other words, this oxygen atom is more saturated by water molecules than the other atoms which seems to be due to the accumulation of negative loads of oxygen atoms in the part of the dye molecule and increases adsorption of hydrogen atoms by dye. Due to the greater spatial oxygen movement than the dye atoms as well as their number and location, this result is observed.

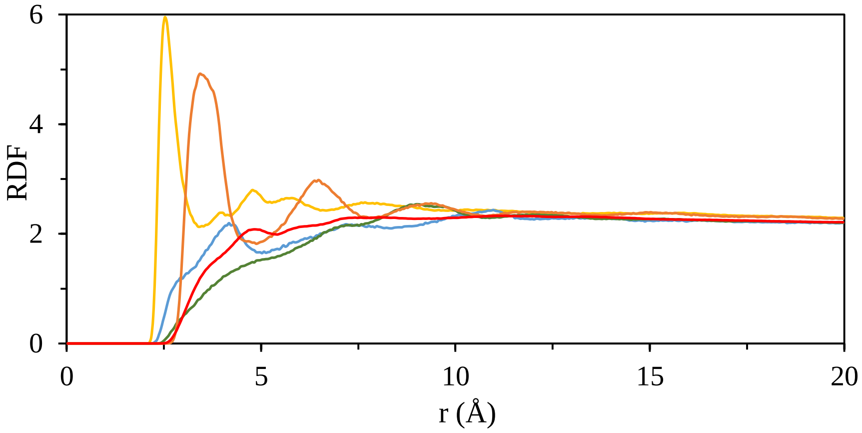

Fig. 1 The RDF plot of dye-water, yellow: oxygen atoms of sulfite group, orange: sulfur atom, blue: oxygen atom of hydroxyl group, green: nitrogen atom, and red: carbon atom.

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Paper code: 350

Thermodynamic investigation of the ternary ([BMIm]Br + LiBr + H_2O) system using potentiometric measurements

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During recent years, ionic liquids (ILs) due to their unique physical and chemical properties have attracted great interest [1-2]. ILs have been widely used in various fields of application. The presence of ionic liquids in a process needs a deeper knowledge about the thermodynamic behavior of the mixture. In this work, thermodynamic study of the aqueous electrolyte system containing 1-buthyle-3-methyl imidazolium bromide ([BMIm]Br) and lithium bromide (LiBr) was carried out on the galvanic cell of the type: [BMIm] -ISE│ [BMIm] Br (m_1), LiBr (m_2), H_2O │Br-ISE on total ionic strengths from 0.01 to 2.80 mol.kg^{-1}. Various series of the salt molal ratios (r= m_{LiBr} / $m_{[BMIm]Br}$ = 10, 7.5, 5) were used at T= 298.2 K and P = 0.1 MPa. The experimental mean activity coefficients of [BMIm]Br in the aqueous solution were determined using the emf measurements in according to Nernst equation. The plot of mean activity coefficients of [BMIm]Br at various total ionic strengths for various series of salt molal ratios at T= 298.2K were shown in Figure1. The Pitzer ion-interaction model was used to analyze the studied system. The Pitzer mixing interaction parameters were evaluated for the mixed electrolyte system. The obtained parameters were used to calculate the mean activity coefficients of the solute species, the osmotic coefficients and excess Gibbs free energies for the whole series of the mixed electrolyte system.

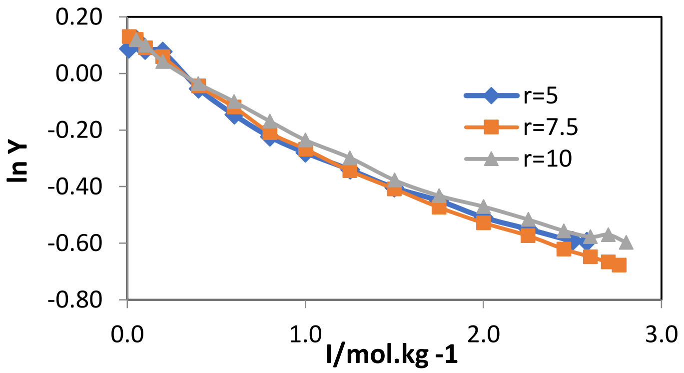

Fig. 1 The plot of mean activity coefficients of [BMIm]Br at various total ionic strengths for various series

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Paper code: 353

Molecular Dynamic Simulation of Nitrate Adsorption from Drinking water using graphene and Comparison with Experimental Data

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Environmental pollutions due to human activities is a serious risk for drinking water resources. Many of water resources are infected by nitrate at the moment. Too many different adsorbents have been studied extensively for removal of nitrate from drinking water. Molecular dynamic simulation could be used as a strong instrument in forecasting of adsorption of pollutants from drinking water and in addition to the time and cost saving, it provides better understanding of the adsorption process. In this article, adsorption of nitrate from drinking water by graphene is first investigated by molecular dynamic simulation and then the results are compared with experimental data that shows a good consistency. We first applied an NVT ensemble to fix the temperature around 300 K. Then for getting to stable conditions of pressure, we used 3 sequential runs on an NPT ensemble. The final NVE run investigated for adsorption analysis parameters such as mean square displacement of nitrate ions, density distribution before and after adsorption and g(r) function. The results showed decrease in MD amount after adsorption indication decrease in movement on nitrate ion and its adsorption. Density distribution of nitrate ions and g(r) function shows distribution of nitrate ions on both sides of graphene sheet. A Fortran code was used to count the number of nitrate ions at the distance of 5 Å of the sheet (these nitrate ions considered as adsorbed ions). The experimental data of adsorption of nitrate on graphene performed at 300 K. the amount of adsorbed nitrate (about 60 percent) was in Consistency with the results of MD simulation.

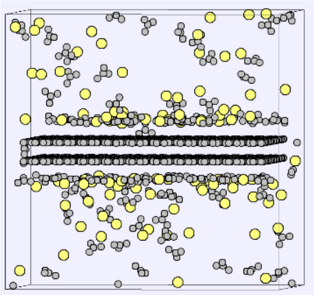

Fig. 1 adsorption of nitrate by graphene sheet of a final NVE run

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Paper code: 355

The Thermophysical Properties of Imidazolium Based Ionic Liquids from Tao- Mason Equation of state and Artificial Neural Network

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Ionic liquids (ILs) have been the focus of attention for many of their properties as potential substitutes for classic organic solvents in many different applications.

In recent years, extensive studies have been done on the thermophysical properties of ionic liquids, such as density. Equations of state provide a way to predict density of these compounds. In addition, artificial neural networks (ANN) [1] have several unique characteristics and advantages for applications such as the prediction of physicochemical properties of ILs.

In this study, first, synthesis of five imidazolium based ionic liquids have been done. Then improved Tao-Mason (TM) equation of state (EoS) [2] were applied to calculate density of ILs over a broad range of temperatures and pressures. Moreover, artificial neural network model was developed to predict density of ionic liquids. The weights and biases were randomly selected and hidden layers were regulated by tansig and purelin function. The multi-layer perceptron ANN with three layers was developed by random initial weights and biases. Also two activation functions were selected to regulating output of the network's layers and the Levenberge-Marquardt algorithm was used to optimize the weights and bias of the layers. In this work, the parameters of temperature (in Kelvin), the pressure (in bulk), molecular mass and boiling temperature (in Kelvin) as the input of the artificial neural network and the ionic liquid density parameter as the objective of the ANN are considered. In this study 404 experimental data were used including:

70% of the data (including 282 data) in the training set, 15% of the data (including 61 data) in the test set to examine the performance of the final network, 15% of the data (including 61 data) was used in the set to determine the validity of the network. To achieve the desired architecture, several networks were evaluated with different architectures. The performance of each network was evaluated by calculating its error in the training, evaluation and training stages.

The density was estimated for 404 data from proposed TM EoS and ANN model for five imidazolium based ionic liquids over the range of the temperature (283.15 - 393.15 K) and a pressure range (1-1000 bar). The predicted results from Tao-Mason EoS and ANN were compared with experimental values. The overall average absolute deviation percent (AAD %) of five ionic liquids obtained 0.2% and 0.005% from Tao-Mason EoS and ANN respectively. The results show that the obtained densities from ANN model are in excellent agreement with the experimental data at various temperature and pressures.

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Paper code: 359

2D&3D-QSAR studies on β-di keto Acids Derivatives of Pyridinones as anti-HIV drugs

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Quantitative structure studies 2D&3D, linear and nonlinear activity have been developed to estimate and predict the biological activity of the combinations of β-di keto Acids Derivatives of Pyridinones as anti-HIV drug inhibition inhibitors. The model of the relationship between descriptors and pEC_{50} values of the selected molecules is described in two steps. In the first step, the 2D-QSAR method was used by selecting the descriptors using genetic algorithm and multiple linear regression, step by step, and linear models related to it. By examining the mean effects of the descriptors, it was realized that MATS7m and HATS6p have the most effect on the bioavailability of the studied compounds. Using the descriptors element, we constructed SW-MLR and GA-MLR linear models and ANN and ANFIS nonlinear models. In the second step, using the SYBYL-X software, 3D-QSAR studies were conducted to construct three-dimensional models; in the CoMFA model, the effects of spatial and electrostatic fields are taken into account, and the results are ($Q^2 = 0.748, R^2 = 0.906$); and in relation to CoMSIA model, in which, in addition to the previous effects, hydrophilic effects, and hydrogen bond effects are taken into account and the best results are ($Q^2 = 0.752, R^2 = 0.923$). The results indicated that the CoMSIA method is more acceptable than the CoMFA method. Finally, by studying the results of the two CoMFA and CoMSIA models, the structure of some β-diketo Acids Derivatives of Pyridinones compounds has been suggested for further biological inhibitory activity.

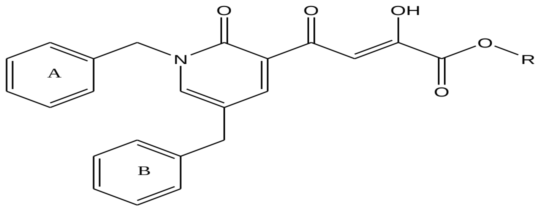

Fig. 1 The structure of β-di keto acid pyridinone derivatives

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Paper code: 368

Revealing substituent effects on π-π stacking and halogen bond interactions. A Theoretical study

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In this study, the MP2 level of theory was employed to explore the mutual influence between π-π stacking and halogen bonds interactions. Cooperativity effect was observed in X-ben||pyr···Cl-F complexes (X = CN, F, Cl, Br, CH_3 , OH and H where || and ··· denote π-π stacking and halogen bonds interactions). This effect was analyzed in details in terms of the energetic, geometrical parameters, and charge transfer properties of the complexes. It was shown that the trend of binding energies of X-ben||pyr···Cl-F complexes was as follows: H < OH < CH_3 < F < Cl < Br < CN. In addition, the quantum theory of atoms in molecules (QTAIM) and natural bond orbital (NBO) were also employed to characterize the interactions and to examine the strengthening of the interactions. The results indicate the cooperativity of π-π stacking and halogen bonds interactions in X-ben||pyr···Cl-F complexes.

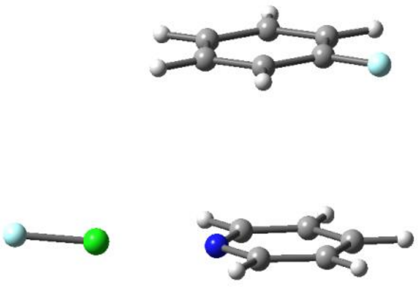

Fig. Cooperativity of π-π stacking and halogen bonding interactions in X-ben||pyr…Cl-F complexes (X = CN, F, Cl, Br, H, CH_3 and OH substituents).

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Paper code: 377

In silico study on the effects of Glucosamine group on Thermal Stability of Yarrowia lipolytica Lip2 lipase

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High secretion levels of *Yarrowia lipolytica* developed it to a potential host for proteins production is one of the main enzymes which plays a significant role with various applications, including detergent, food, cosmetic, pharmaceutical and environmental industries [1]. Lip2, the only extracellular lipase of this yeast, is a glycosylated protein with 301 amino acids have several disulfide bonds. The crystal structure confirmed the two glycosylation sites at N113 and N134. Lip2 could have activities at low temperatures about 5°C and is rapidly deactivated over 50°C, with an optimal temperature of 37°C. Therefore, here for determining the effect of sugar moieties on Lip2 thermodynamic undergo scrutiny a comprehensive explanation the entire protein structure with its glycoside groups was assigned. In this study, MD simulations were performed by GROMACS software, version 5.1.4 [2], with the CHARMM 36M force field, in three functional temperatures of 300, 310, and 333 k for 20 ns long as production run. Regarding to the results of analyses, protein with N-glucosamine groups has more temperature dependence structure. By increasing temperature, the deglycosylation formed a thermostable folding. Thus, glycosylation not only implies its impact on localized residues near the glycosylated sites necessarily, but also propagated to other regions of the protein and increase residues fluctuations and consequently the proteins' radius of gyration (Fig. 1). Root mean square displacement (RMSD) analysis also confirm radius of gyration results, too. We also computed number hydrogen bond, and their lifetimes in mutated and glycosylated forms of Lip2 lipase. These results indicate that by increasing temperature, the non-glycosylated protein folding and number of H-bonds increased. In this regard, the enzyme overall stability decreases rather than the WT with an anonymous molecular mechanism. Due to *in silico* research into thermo-stability of this protein in aqueous solution, more information about the efficacy of each compartment is provides. As the missing chain, independent presence of glucosamine group is going to be analyzed to recognize the problematic factors.

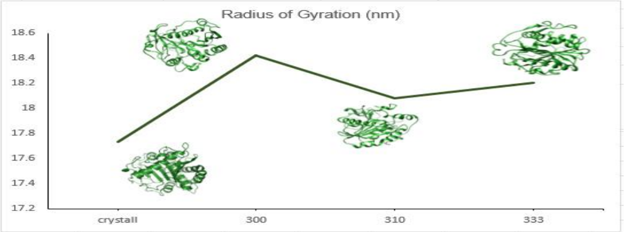

Fig. 1 Radius of gyration of the Lip2 lipase Yarrowia lipolytica versus the temperature.

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Paper code: 444

Theoretical study of solvent effect on NLO property in (η6-C6H6)Cr(CO)3 complex

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In this work, the solvent effect on non-linear optical (NLO) property in (η^6-C_6H_6)Cr(CO)$_3$ complex, was investigated with MPW1PW91 method. The calculations of systems contain main group elements described by the standard 6-311G(d,p) basis set. For Cr element standard Def2-TZVPPD basis set was used. The acceptable nature of the stationary points was ensured by performing frequency calculations. In order to investigate the solvation effects a self-consistent reaction field (SCRF) approach, polarizable continuum model (PCM), was adopted to reoptimize all the structures in the solution. These calculations show that total hyperpolarizability values (β_{tot}) values increase in solution phase in compared to gas phase. The solvent polarity effect β_{tot} values was calculated and correlated with the Kirkwood–Bauer–Magat equation (KBM):

$$\frac{\Delta\beta_{tot}}{\beta_{gas}} = 9.806\frac{\varepsilon\text{-}1}{2\varepsilon+1}\text{-}2.968;\ R^2 = 0.999$$

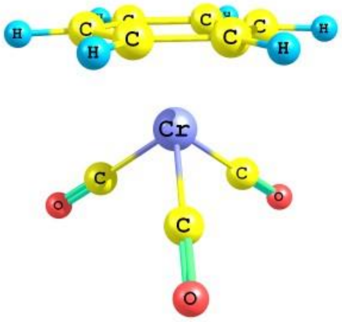

Fig. 1 The structure of (η^6-C_6H_6)Cr(CO)$_3$ complex..

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Paper code: 467

Is there any correlation between some theoretical and experimental parameters at similar and dissimilar beta-diketone complexes?.

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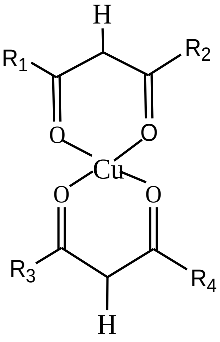
The most interesting thing in metal complexes of β-diketones comes up from their applications in science and industry. These compounds are frequently used in preparation of supported catalysts as precursors of heterogeneous catalysts. They have also been extensively applied in medicine as active pharmaceutical ingredients, antiasthmatic and lung disease drugs, and antidiabetic agents [1,2]. Furthermore, these complexes are also used as fuel additives [3]. This study presents our view of any correlation between theoretical and experimental parameters for conventional (metal-ligand) and unconventional (dihydrogen bond) strength of some similar and dissimilar beta-diketone complexes, such as bond length, vibrational frequency, total electronic density (ρ_{BCP}), and Laplacian of total electronic density in critical points, by using density functional theory (DFT) and Atoms In Molecules (AIM) calculations. So, the selected compounds classified in three categories. In the first category, the copper(II) acetylacetonate, $Cu(acac)_2$, participates with copper(II) benzoylacetonato, $Cu(bzac)_2$, and copper(II) dibenzoylmethane $Cu(dbm)_2$, by one and two phenyl groups instead of methyl groups in $Cu(acac)_2$, and in the other ones, 5,5-dimethyl hexane-2,4-dionato, $Cu(dmhd)_2$, 2,2,6,6-tetramethyl-3,5-heptanedionato, $Cu(tmhd)_2$ with one and two *t*-butyl groups have been substituted by methyl groups of $Cu(acac)_2$, respectively. The last class that have been investigated include a molecule with different β substitutions, which are named: 4,4,4-trifluoro-1-phenyl-1,3-butanedione $Cu(tfba)_2$ (with CF_3 and phenyl groups) (Fig.1). By investigating the effect of replacing one or two similar substitutions by CH_3 in the values of mentioned compounds, a linear correlation has been obtained for the titled similar β-diketone complexes (Fig.2). This conclusion also achieved for $Cu(tfba)_2$ with different groups in beta positions. AIM results indicate that the unconventional hydrogen bonds occur in the β-diketone complexes including phenyl groups, which the strength of unconventional hydrogen bond is very weak and there is a linear correlation between them.



$R1=R2=R3=R4=CH_3$	$Cu(acac)_2$
$R1=R3=CH_3$, R2=R4=Phenyl	$Cu(bzac)_2$
R1=R2=R3=R4=Phenyl	$Cu(dbm)_2$
$R1=R3=CH_3$, R2=R4=*t*-butyl	$Cu(dmhd)_2$
R1=R2=R3=R4=*t*-butyl	$Cu(tmhd)_2$
$R1=R3=CF_3$, R2=R4=Phenyl	$Cu(tfba)_2$

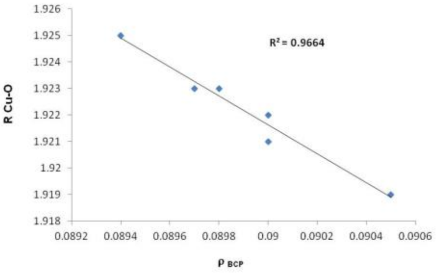


Fig. 1. The structure of titled complexes.

Fig. 2. The correlation between Cu-O bond length and total electronic density in critical points.

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Paper code: 468

DFT studies on the structure and intramolecular hydrogen bond strength in 1, 2-dibenzoylcyclopentadiene

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The β-diketones compounds that named 1,2-diacylcyclopentadiene just create in the enol form, characterized by a seven-membered ring, which can be used in determination of trace metals and also play important role in enzymatic processes [1, 2]. The simplest member of this class of compounds is Diformylcyclopentadiene (DFCP). All computations in the present study have been carried out with Gaussian 09 (B3LYP/6-311++G** level), NBO 5.0 and AIM 2000 software packages. From the theoretical point of view, with respect to the dihedral angle between phenyl and chelated ring of 1, 2-dibenzoylcyclopentadiene (DBCP), one conformer can be obtained for that (Fig.1). In order to understanding of substitutional effect of methyl group and hydrogen with phenyl group on the strength of hydrogen bond and structure, the geometrical parameters compared with those of DFCP and Diacethylcyclopentadiene (DACP). According to calculation, in DBCP, the averaged values of O···O and O···H distances decrease, while the OHO bond angle and O-H bond length increase in comparison with those of DFCP and DACP. The wiberg bond order calculated by NBO software are in agreement with the bond lengths of titled compounds. The AIM results also show that the energy of hydrogen bond (E_{HB}), the averaged density (ρ), and the Laplacian of charge density ($\nabla^2\rho$) at the O···H bond critical point of DBCP is higher than those in other compounds. These results show stronger hydrogen bonding in DBCP. According to these conclusions, the following trend could be obtained for the strength of hydrogen bond in the mentioned compounds: S_{HB}: DBCP> DACP> DFCP

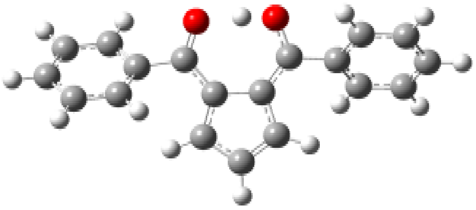

Fig. 1 The cis-enol form of DBCP.

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Paper code: 469

Dielectric Study and molecular interaction of (1,3-propanediol + 2-butanone) binary liquid mixtures at different temperatures

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Relative permittivity of a material is an intrinsic property that plays an important role in characterizing molecular structure, molecular interactions (homo- and hetero-) and molecular ordering in liquid solutions [1]. In general, type of solvent, solution constituent, concentration and temperature are the most important factors, which influence dielectric properties and dipole moments of liquids [2]. Propanediols are three carbon diols that have many industrial and biological applications [5]. Due to the presence of two –OH groups in the molecule, the dielectric behavior of this group of the organic compounds is strongly influenced by intermolecular and intramolecular hydrogen bond formation [3].

This study determined the experimental relative permittivity data for the (1,3-propanediol + 2-butanone) binary system as a function of composition at T = (298.2 and 308.2) K. In this work, the excess parameters such as the excess permittivity and the excess Helmholtz energy were calculated. The results are discussed in terms of homo and hetero interactions and structure of the studied binary mixtures.

In this binary system, the excess permittivity values were negative over the whole composition range, which indicates the formation of multimer structures as a consequence of intermolecular interactions between the components. The interaction is mainly through hydrogen bonding between the 1,3-propanediol and 2-butanone molecules.

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Paper code: 470

Dielectric data of binary mixtures of Isoamyl alcohol with 2-butanone at T= 298.2 K

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Studies of the dielectric and thermodynamic properties of binary mixtures including alcohols are important and desirable in deep understanding the nature of intermolecular interactions and consequence structure in the mixture due to the hydrogen bonding and other electrostatic interactions [1]. The heterogeneous and homogeneous interactions in binary mixtures using dielectric measurements have been studied and reported by several investigators [2]. Ketones are carbonyl-containing compounds that have a large range of applications in various industries. They are used as solvents or chemicals in the manufacture of gums, wax, glues, paraffin, resins, textile, and plastic [3]. These organic compounds belong to dipolar aprotic solvent groups, which are well hydrogen-bond acceptors.

This paper reports the role of hydrogen bonding and other electrostatic interactions on the dielectric behaviour, excess parameters, and structure properties of the binary system (Isoamyl alcohol + 2-butanone).

Relative permittivity measurements were made on binary mixtures of (Isoamyl alcohol + 2-butanone) for various concentrations at T = 298.2 K. In order to obtain valuable information about heterogeneous interaction (interactions between the unlike molecules), the Kirkwood correlation factor, the Bruggeman dielectric factor and the excess permittivity were calculated.

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Paper code: 485

A computational study of all di-fluoroazulenes

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The electrochemical polymerization of heterocyclic monomers to yield electronically conducting and redox electroactive polymers is well documented [1]. Electrically conducting polymers have been considered for numerous applications including charge dissipation coatings, organic thin-film transistors, and conducting textiles. The use of electrically conducting polymers in electrochromic devices, as materials that possess the ability to reversibly change color by altering redox state, has emerged. Many conjugated polymers are colored in the neutral state since the energy difference between the σ-bonding orbitals and the σ* antibonding orbitals (valence band) lies within the visible region [2]. All of the possible of di-fluoroazulenes studied in this work are presented in Fig. 1.

1:	K=L=M=Q=W=X=Y=Z=H	Azulene
2:	K=L=M=Q=W=X=H,Y=Z=F	1,2-difluoroazulene
3:	K=L=M=Q=W=Y=H,X=Z=F	2,4-difluoroazulene
4:	K=L=M=Q=X=Y=H,W=Z=F	2,5-difluoroazulene
5:	K=L=M=W=X=Y=H,Q=Z=F	2,6-difluoroazulene
6:	K=L=M=Q=W=Z=H,X=Y=F	1,8-difluoroazulene
7:	K=L=M=Q=X=Z=H,W=Y=F	1,7-difluoroazulene
8:	K=L=M=W=X=Z=H,Q=Y=F	1,6-difluoroazulene
9:	K=L=Q=W=X=Z=H,M=Y=F	1,5-difluoroazulene
10:	K=M=Q=W=X=Z=H,L=Y=F	1,4-difluoroazulene
11:	L=M=Q=W=X=Z=H,K=Y=F	1,3-difluoroazulene
12:	K=L=M=Q=Y=Z=H,W=X=F	4,5-difluoroazulene
13:	K=L=M=W=Y=Z=H,Q=X=F	4,6-difluoroazulene
14:	K=L=Q=W=Y=Z=H,M=X=F	4,7-difluoroazulene
15:	K=M=Q=W=Y=Z=H,L=X=F	4,8-difluoroazulene
16:	K=L=M=X=Y=Z=H,Q=W=F	5,6-difluoroazulene
17:	K=L=Q=X=Y=Z=H,M=W=F	5,7-difluoroazulene

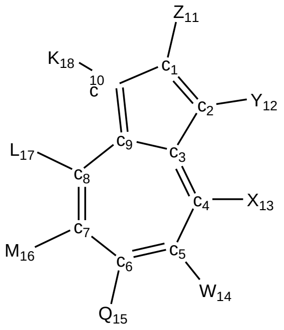

Fig. 1 All di-fluoroazulenes studied in this work

The structural and electrical properties of all di-fluoroazulenes have been studied using B3LYP method with 6-311+G* basis set. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, “the gap between HOMO and LUMO”(HLG) and size of dipole moment vector, total electrical energies, Enthalpies, Entropies, Electronic, Gibbs and Zero-Point vibrational energies, IR and NMR spectra have been calculated and studied as well. The analysis of these data showed that the 1,2-difluoroazulene has the highest value of the dipole moment. The electrochemical stability of 4,8-difluoroazulene is greater than other compounds and also the zero-point energy for this molecule is greater than other molecules. The analysis of data showed that the double bonds in 4,5-difluoroazulene is more delocalized.

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Paper code: 488

Theoretical study of the molecular carbon monoxide adsorption on the Ni_4Sc and Ni_4Mo clusters

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Transition metal (Mo, Sc) doped nickel clusters and the adsorption behavior of carbon monoxide on the Ni_4Sc and Ni_4Mo clusters surfaces have been investigated by means of density functional theory calculations (DFT) (1-3).
In this work, we report the optimization of adsorption characteristics, minimum distance, dipole moment, bond length and vibrational frequency. For systems containing carbon and oxygen atoms, the calculations was performed using B3PW91 and the standard 6-311+G* basis sets. The basis sets employed for description of clusters was the standard LANL2DZ.
Calculations show that, the stability of the clusters increased by doping of Mo and Sc elements. Our DFT calculations of CO adsorbed on the clusters reveal that the CO adsorption on the Ni_4Sc and Ni_4Mo clusters are highly dependent on the availability of adsorption sites. In this relation, the effect of molecular orientation phenomena on the adsorption process are investigated in details. Interactions between carbon and nickel happened and the surface-adsorbed CO implies its suitability as a good catalyst.

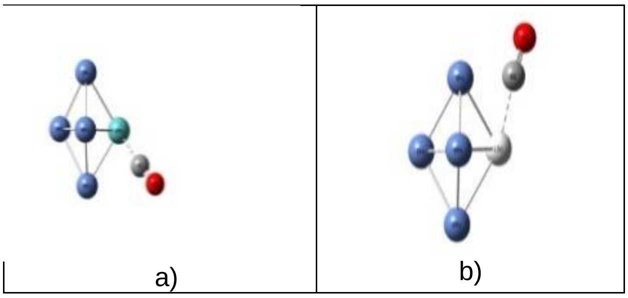

Fig. 1) The CO adsorption on the, a) Ni_4Mo and b) Ni_4Sc clusters

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Paper code: 491

Application of Hammett equation to intramolecular hydrogen bond strength in para-substituted phenyl ring in some β-diketones and schiff bases

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The stability of stable cis-enol forms in three categories of β-diketones, including para-substituted of benzoylacetone (X-BA), trifluorobenzoylacetone (X-TFBA) and 1-aryl-1,3-diketone malonates (X-ADM), and 2-(((1 phenylethyl)imino)methyl)phenol (X-PIMP), as a Schiff base with chiral carbon, has three conformers that, X=H, NO_2, OCH_3, CH_3, OH, CF_3, F, Cl, and NH_2, have been obtained by theoretical methods. According to the theoretical results, the energy difference between the mentioned stable chelated enol forms for the titled compounds is negligible. In addition, the effect of electronic different substitutions on the intramolecular hydrogen bond (IHB) has been evaluated. The correlation between experimental Hammett's para function, (σ_p) with the theoretical and experimental parameters related to the strength of hydrogen bond in p-X-BA, p-X-TFBA, p-X-ADM and p-X-PIMP molecules also investigated by means of DFT calculations at B3LYP/6-311++G(d,p) level of theory. The electronic effects of para-substitutions on the IHB strength were determined by NMR and IR data related to IHB strength, geometry, NBO results, and topological parameters. These parameters were correlated with the Hammett para-substituent constants, σ_p [1-3]. Good linear correlations between σ_p and the several parameters, related to the hydrogen bond strength, were obtained and showed in Table 1, to our knowledge as (Parameters=$\rho\sigma_p$+ const.), equation.

Table 1: The R square values between some parameters related to IHB strength *vs.* σ_p.

	X-TFBA			X-ADM			X-BA			X-PIMP		
	2	4	Avg.	2	4	Avg.	2	4	Avg.	1	2	3
R O…O/ R N…O	0.970	0.882	0.943	0.970	0.927	0.944	0.968	0.914	0.941	0.954	0.929	0.918
R O…H/ R N…H	0.971	0.925	0.970	0.989	0.883	0.955	0.979	0.930	0.962	0.926	0.916	0.913
<OHO/ < OHN	0.970	0.950	0.984	0.987	0.931	0.973	0.983	0.967	0.978	0.823	0.869	0.858
E_{HB}	0.968	0.901	0.964	0.983	0.860	0.927	0.937	0.930	0.904	0.914	0.919	0.910
δ OH	0.625	0.747	0.750	0.892	0.833	0.900	0.795	0.923	0.933	0.854	0.768	0.879
ν OH	0.965	0.934	0.979	0.982	0.827	0.975	0.959	0.933	0.965	0.911	0.903	0.832
γ OH	0.962	0.834	0.966	0.972	0.960	0.981	0.229	0.597	0.512	0.869	0.915	0.898
$\sum$LP (1), LP (2) O $\rightarrow\sigma^*$O-H	0.982	0.938	0.984	0.968	0.843	0.926	0.964	0.928	0.959	0.931	0.927	0.910
Charge Hydrogen on bridge	0.982	0.973	0.979	0.979	0.879	0.943	0.960	0.974	0.969	0.958	0.951	0.903

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Paper code: 492

Tautomeric Equilibria Studies by UV-Vis Spectroscopy in β-diketones

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In general, β-dicarbonyl compounds may exist in several tautomeric forms. It is well known that the cis-enol form of β-diketones is characterized by a strong intramolecular hydrogen bond. Benzoylacetone (BA) and trifluorobenzoylacetone (TFBA) can be considered as representative examples of chemically asymmetric β-diketone with different substitution at β positions. We study the theoretical and experimental UV absorption spectra to understand the absorption bands for tautomerism study in the absorption spectra to these molecules. The absorption spectrum are analyzed by (TD-DFT) at B3LYP/6-311++G(d,p) level of theory in normal hexane (ε =1.88) as solvent, using PCM method, where they are compared with regard to experimental Spectra. For both cis-enol-2 and cis-enol-4 forms of the target compounds, wavelength (l), oscillator strength (f), major contributions of the calculated transitions and the theoretical and experimental enol-enol equilibrium constants with the experimental wavelength are given in Table 1. According to figure 1, three experimental bands are observed for these compounds, at about 325-330, 295-300, and 255-265 nm, as strong, shoulder, and weak band, respectively. According to the theoretical results, the strong and shoulder bands at about 325-330 and 295-300 nm (see Fig. 1) have been attributed to the cis-enol-4 and cis-enol-2 forms, respectively, the weak band at about 255-265 nm has been attributed to both cis-enol-2 and cis-enol-4 forms. These equilibrium constants have been obtained theoretically as ratio of oscillator strengths, and experimentally as ratio of absorbance as strong and shoulder bands. Therefore, consistent with the previous report [1-3], both cis-enol-2 and cis-enol-4 forms are present and coexist in the samples.

Table 1: The experimental and B3LYP/6-311++G** calculatedλ, oscillator strengths (f), major contributions, and enol-enol equilibrium constants for stable cis-enol forms of BA and TFBA.

	Tautomer 2				Tautomer 4				K_{eq}	
	λ_{calc}	f	Major contribution >15%	λ_{exp}	λ_{calc}	f	Major contribution >15%	λ_{exp}	K_{calc}	K_{exp}
TFBA	300	0.0360	H-1→L(76%), H→L(17%)	-	319	0.6495	H→L(95%)	327	1.13	1.09 (1.12) [a]
	295	0.5746	H→L(81%), H-1→L(17%)	297	316	0.0249	H-2→L(92%)	-		
	264	0.0276	H-2→L(91%)	-	301	0.0439	H-1→L(93%)	-		
	244	0.0238	H-1→L+1(47%), H→L+2(23%)	253	251	0.0310	H→L+1(75%)	253		
BA	297	0.5230	H→L(70%)	288	308	0.6595	H→L(70%)	٣٠٧	1.26	1.25 (1.24) [b]
	256	0.1118	H-3→L(47%)	-	277	0.0270	H-2→L(56%), H-1→L(34%)	-		
	247	0.0467	H→L+1(67%)	245	246	0.0563	H-3→L(66%)	245		
	226	0.0679	H→L+1(41%), H→L+3(23%)	-	244	0.0714	H→L+1(64%), H-2→L(16%)	-		

[a] Data from Ref.[2], [b] Data from Ref.[3]

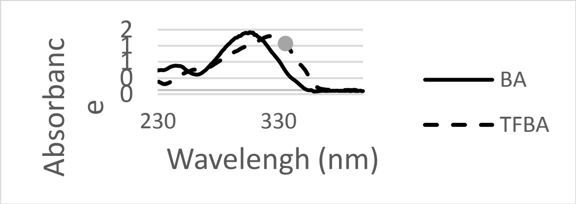

Fig. 1: the experimental UV-Vis spectra of TFBA and BA in n-hexane.

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Paper code: 510

The effect of Al atom doped and SO_2 adsorption on the electrical and structural parameters boron nitride nanotube: A quantum approach

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In this, research the effects of adsorption SO_2 molecule and Al-doped on the electrical and structural parameters of BNNTs at various configurations. From optimized structures, the NBO, AIM, HOMO-LUMO orbital and other quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), and electronegativity (χ) of the nanotubes are calculated by using DFT theory. The results indicate that the adsorption energy of all models is negative and is favourable in view of thermodynamic approach. The calculated results demonstrate that Al doping increase the sensivity of BNNTs to adsorb of SO_2 gas.The optimized geometrical structures show (Fig. 1) that the bond length and bond angle of nanotube after adsorption SO_2 molecule alter slightly from pristine state. Adsorption of SO_2 molecule at all models is exothermic in thermodynamic approach. The calculated results confirm that Al doped increase the sensivity of nanotube to adsorbing SO_2 gas.

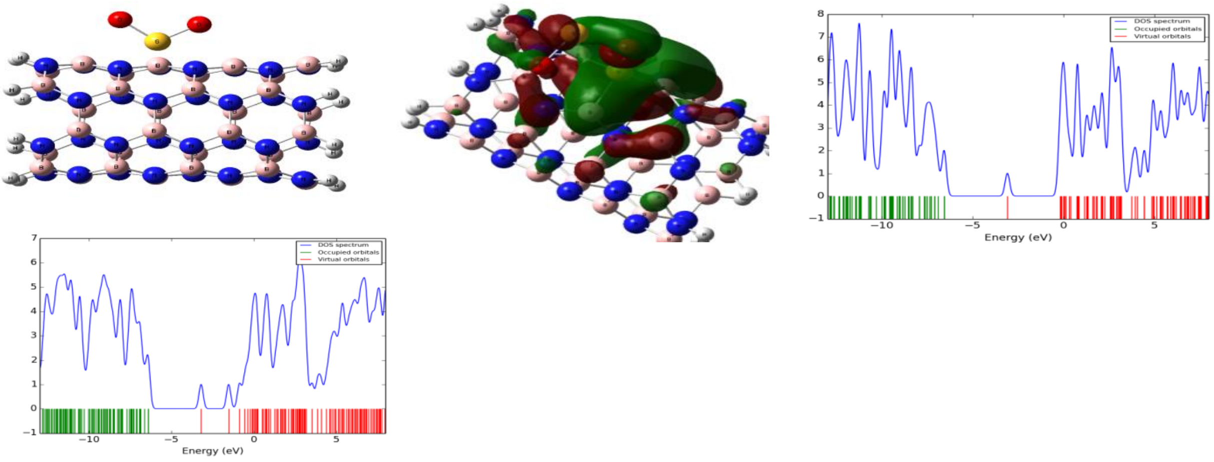

Fig. 1 2D structures , HOMO-LUMO orbital and DOS plots of SO_2 adsorption on the surface of pristine and Al doped BNNTs.

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Paper code: 517

Canonical Monte Carlo Simulation Study of Noble Gas Adsorption onto the SiNT

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Canonical Monte Carlo simulations were performed to systematically study the adsorption and separation of noble gases such as helium (He) and argon (Ar) on single wall silicon nanotube (SWSiNT). Pure noble gases, as well as binary mixtures, were simulated in silicon nanotube (SiNT) under various conditions. Adsorption data was collected at 273 K over a wide range of pressures. Based on obtain data, the adsorption isotherms for pure and an equimolar mixture of He and Ar have a Langmuir shape and no capillary condensation occur. Results show that the amount adsorbed of He and Ar increase with increasing gas pressure. To compare adsorptive selectivity of He and Ar from He/Ar mixture, separation factor were calculated. It revealed that the SiNT could be separated Ar easily from He gas which means that the SiNT is suitable candidate for this purpose. Furthermore, the potential energy curves of gas adsorption onto the SiNT were obtained from MPW1PW91/3-21G level of theory and these curves were fitted with LJ potentials. Based on obtained data, it can be seen that there is a good agreement between obtained results from calculated LJ parameters and literature's LJ parameters.

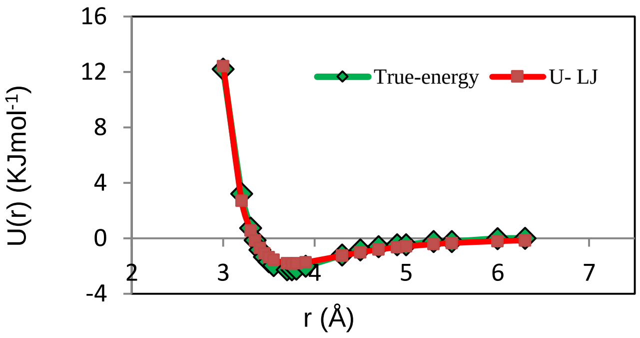

Fig. 1 Calculated corrected potential energy curves of He and Ar adsorbed onto the SiNT

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Paper code: 518

A DFT study of interaction Cd^{+2} ions with the pristine, 3Al-doped on (6,0) zigzag Boron nitride nanotube

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Abstract: In the present project we study the effects of adsorption Cd^{+2} ion on the surface pristine and 3Al atoms doped (6,0) zigzag BNNTs. From optimized structures, the adsorption energy, HOMO-LUMO orbital and other quantum molecular descriptors: electronic chemical potential (μ), global hardness (η), electrophilicity index (ω), energy gap (E_{gap}), global softness (S), and electronegativity (χ) of the nanotubes are calculated by using DFT theory. The results indicate that the adsorption energy of all studied models is negative and is favourable in view of thermodynamic approach. The computational results indicate that the bond length and bond angle of nanotube after adsorption Cd^{+2} alter significantly from original values. On the other hand the 3Al doped decrease the values of adsorption energy. The gap energy and global hardness of Cd^{+2}&BNNTs decrease significantly from original state and so the conductivity and reactivity of system increase from original state.

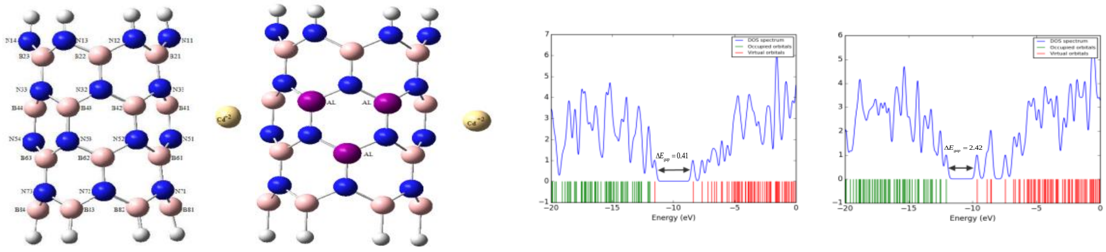

Fig. 1 The DOS, structure of optimized for Cd^{+2} adsorption on 3Al-doped BNNTs.

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Paper code: 519

The theoretical study of interaction CO gas with pristine As&N doped AlNNTs: A DFT study

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In the present project we study the effects of adsorption CO molecule and As&N-doped on the electrical and optical properties of Aluminium nitride nanotube (AlNNTs) at various configurations. From optimized structures, the adsorption energy, HOMO-LUMO orbital, quantum molecular descriptors,Density of state (DOS), MEP and RDG plots of the nanotubes are calculated at the cam-B3LYP/6-31G(d,p) level of theory. The calculated results show that the Fermi level energy of whole models is close to HOMO energy, it is probably the most important factor in determining the current and the direction of natural flow of electrons and optical properties of system. The calculated results demonstrate that As doped decreases the sensivity of AlNNTs to adsorb of CO gas. On the other hand, the adsorption energy of pristine and As&N doped of AlNNTs is in range -23.1 and -0.25 eV respectively. The negative values of adsorption energy reveal that the adsorption process is exothermic. Comparison results of The molecular electrostatic potential (MEP), The reduced density gradient (RDG) results confirm that As doped is not suitable compound for adsorbing CO gas.

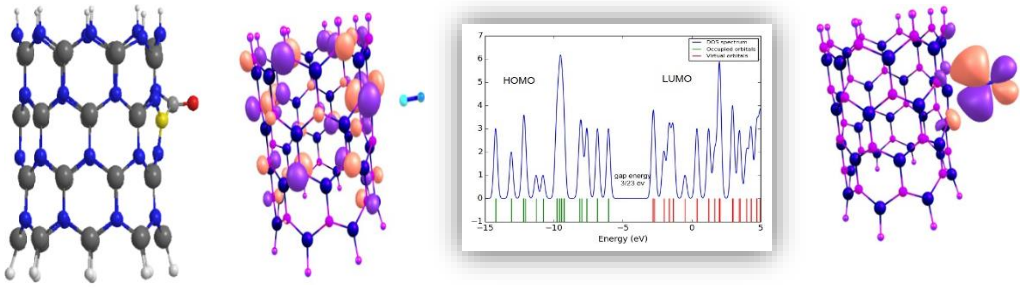

Fig. 1 2D structures and HOMO orbital of CO adsorption on the surface of pristine and As doped AlNNTs.

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Paper code: 543

The effect of slit size on stress tensor components

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The pressure that applying by particles is a mechanical quantity created by random motion of particles, which has tensor properties and has 9 components that not equal to each other, necessarily:

$$P = \begin{bmatrix} Pxx & Pxy & Pxz \\ Pyx & Pyy & Pyz \\ Pzx & Pzy & Pzz \end{bmatrix}$$

The diagonal components of tensor included normal component P_{zz} and lateral components P_{xx}, P_{yy} and the non-diagonal components are shear components (P_{ij}, i≠j, I,j=x, y, z) that are symmetrical and for this reason calculated 6 components of tensor [1].

In macroscopic system 3 diagonal components are equal and 6 non-digonal components are zero. Thermodynamic properties of a fluid confined in slit pores show deviations from those of a macroscopic fluid therefore, in slit non-diagonal components are almost zero and 3 diagonal components are not equal [2].

We performed molecular dynamics simulations of Lennard-Jones particles confined in a slit pore by using LAMMPS and investigated the effect of slits size on the value of pressure tensor components. We simulated a box with the density 0.880 and 1000 particles in temperature 1.095 and calculate the pressure tensor components. All quantities are reduced respectively to ε and σ, that is, these LJ parameters are fixed to unity.

We observed that slits with 2<h<4 have the higher vertical pressure components for both the lateral components and normal component, that means the pressure applying on these surfaces is larger but in slits size >4 approximately the value of the component is closer together. Shear components are negligible in all slits. The zz component has more oscillation than the main pressure compared to xx and yy, which are almost the same in larger sizes. (Shown in table 1).

Slit size/ pressure	**2**	**2.5**	**3**	**3.5**	**4**	**4.5**	**5**	**5.5**	**6**	**6.5**	**7**	**7.5**	**8**	**11**	**15**
$\mathbf{P_{xx}}$	18.4	24.6	11.8	13.9	8.0	9.4	4.7	5.9	5.2	5.4	3.4	6.7	3.8	5.8	5.1
$\mathbf{P_{yy}}$	18.6	24.5	11.5	14.0	7.3	9.4	5.4	5.9	5.0	5.4	4.1	6.7	4.0	5.8	5.1
$\mathbf{P_{zz}}$	20.5	5.5	11.0	4.6	8.5	3.8	7.9	6.3	5.7	5.3	5.0	6.8	4.5	5.6	5.1

Table 1: The value of pressure tensor components.

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Paper code: 548

Computational study of polycyclic unsaturated silylenes and their allenic analogs

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Computational study of silylenes, the silicon analogs of carbenes, has attracted a great attention in theoretical chemistry. Silylenes are the key intermediates in various reactions of organosilicon compounds. In this study, polycyclic unsaturated silylenes (**1**, **3**, **5**, **7**, and **9**) are compared and contrasted to their corresponding allenic isomers (**2**, **4**, **6**, **8** and **10**) with respect to their geometery optimization, zero-point vibrational energies, singlet-triplet energy gaps ($\Delta E_{s\text{-}t}$, relative stability), nucleophilicity (*N*), electrophilicity (*ω*), dipole moment (*D*), homo-lumo energy gaps ($\Delta E_{\text{Homo-Lumo}}$, band gap), geometerical parameters, changes of enthalpy (ΔH_f), Gibbs free energy (ΔG_f), natural bond orbital (NBO) and nucleous independent chemical shift (NICS) at M06/6-311++G** (considering the polarization and diffuse functions) level of theory (Pople's basis set). All calculations are carried out using the Gaussian98 software (figure 1).

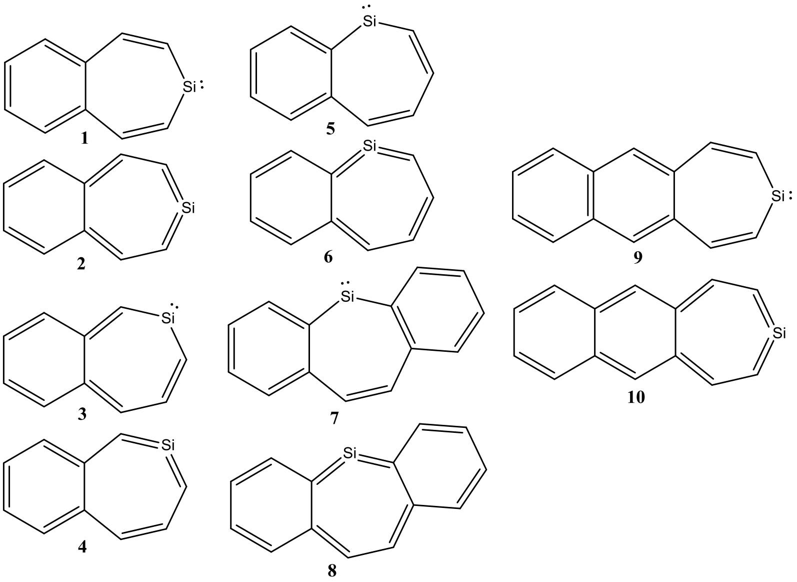

Fig 1. Two- and three-conjugated cyclic silylenes (**1**, **3**, **5**, **7** and **9**) and their allenic analogs (**2**, **4**, **6**, **8** and **10**).

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Paper code: 553

NBO analysis on all mono-fluorovinylbenzenes: A theoretical study

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The Natural Bond Orbitals analysis (NBO), and structure parameters of all mono-fluorovinylbenzenes were investigated by means B3LYP method with the 6-311++G(d,p) basis set using Gaussian 09 software. In addition, Stability of the molecule arising from hyper conjugative interactions and charge delocalization has been analyzed. Stability of the molecule arising from hyper conjugative interactions and charge delocalization has been analyzed using natural bond orbital analysis (NBO). Natural (localized) orbitals are used in computational chemistry to calculate the distribution of electron density and Natural Bond Orbitals (NBOs) include the highest possible percentage of the electron density. The results of this investigation show that among all possible mono-fluorovinylbenzenes, the electron density in 2-flourovinylbenzene molecule is more delocalized and it is the perfect monomer with high capacity of electron transfer for nano applications. The all of corresponding transitions from donor to acceptor spices are available in the Table. See inserted figure to this table for atomic numbering scheme of all mono-fluorovinylbenzenes studied in this work.

1;	H	X=Y=Z=W=L=M=N=H	Vinylbenzene
2;	X=F	Y=Z=W=L=M=N=H	2-flourovinylbenzene
3;	N=F	X=Y=Z=W=L=M=H	1-flouro-2-vinylbenzene
4;	M=F	X=Y=Z=W=L=N=H	1-flouro-3-vinylbenzene
5;	W=F	X=Y=Z=L=M=N=H	1-flouro-3-vinylbenzene
6;	Z=F	X=Y=W=L=M=N=H	1-flouro-2-vinylbenzene
7;	Y=F	X=Z=W=L=M=N=H	1-flourovinylbenzene

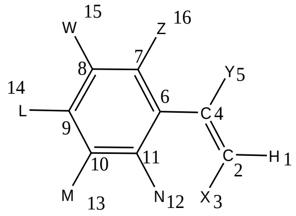

Table. B3LYP/6-311++G** *E*$_2$ values obtained of natural bond orbital (NBO) approach for all mono-fluorovinylbenzenes in kcal/mole.

Molecule	Donor → Acceptor	ΣE2 (kcal/mole)
2-flourovinylbenzene(**2**)	$\pi_{C10\text{-}C11} \rightarrow \pi^*_{C6\text{-}C4}$ (3.69), $\pi_{C11\text{-}C6} \rightarrow \pi^*_{C6\text{-}C4}$ (2.66) $\pi_{C6\text{-}C7} \rightarrow \pi^*_{C6\text{-}C4}$ (2.20), $\pi_{C6\text{-}C7} \rightarrow \pi^*_{C4\text{-}C2}$ (2.01) $\pi_{C6\text{-}C7} \rightarrow \pi^*_{C4\text{-}C2}$ (16.78), $\pi_{C6\text{-}C4} \rightarrow \pi^*_{C4\text{-}C2}$ (3.14) $\pi_{C7\text{-}C8} \rightarrow \pi^*_{C4\text{-}C2}$ (3.24), $\pi_{C4\text{-}C2} \rightarrow \pi^*_{C6\text{-}C4}$ (3.62) б$_{C4\text{-}C2}$ → б$^*_{C4\text{-}C2}$ (0.83), $\pi_{C4\text{-}C5} \rightarrow \pi^*_{C4\text{-}C2}$ (0.83) $\pi_{C2\text{-}C1} \rightarrow \pi^*_{C6\text{-}C4}$ (5.67), $\pi_{C2\text{-}C1} \rightarrow \pi^*_{C4\text{-}C2}$ (1.49)	45.16

As shown table, the 2-flourovinylbenzene with most ΣE2 energy with 45.16 kcal/mole is the best option for electropolymerization.

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Paper code: 555

A DFT and NBO study of di-fluorovinylbenzenes

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The structure parameters and Natural Bond Orbitals (NBOs) of all di-fluorovinylbenzenes were calculated by Density Functional Theories (DFT) at the 6-311++G** basis set using Gaussian 09 software. Vibration frequencies were also calculated to the structure with optimized geometry and no imaginary frequency were obtained, so the stationary point correspond to the minima of the potential energy surface. Electronic structure studies were carried out in a DFT method with a B3LYP potential, which is the most complete potential actively used in modern research and showing the best agreement to experiment in the sequence of levels. Stability of the molecule arising from hyper conjugative interactions and charge delocalization has been analyzed using natural bond orbital analysis. Addition to which E_2 energies have been calculated [1]. The calculations show that the amount these monomers the 1, 2-diflourovinylbenzene with ΣE2= 45.45 kcal/mole is the good candidate for electro polymerization. The details of donor to acceptor excitation of natural bond orbitals and for E_2 energies of them are available in Table blow.

1;	H	X=Y=Z=W=L=M=N=H	Vinyl benzene
2;	X=N=F	Y=Z=W=L=M=H	(Z)-1-fluoro-2-(2-fluorovinyl)benzene
3;	X=M=F	Y=Z=W=L=N=H	(Z)-1-fluoro-3-(2-fluorovinyl)benzene
4;	X=W=F	Y=Z=L=M=N=H	(Z´)-1-fluoro-3-(2-fluorovinyl)benzene
5;	X=Z=F	Y=W=L=M=N=H	(Z´)-1-fluoro-2-(2-fluorovinyl)benzene
6;	X=Y=F	Z=W=L=M=N=H	(E)-(1,2-diflourovinyl)benzene
7;	M=N=F	X=Y=Z=W=L=H	1,2-diflouro-3-Vinylbenzene
8;	W=N=F	X=Y=Z=L=M=H	1,4-diflouro-2-vinylbenzene
9;	Z=N=F	X=Y=W=L=M=H	1,3-diflouro-2-vinybenzene
10;	Y=N=F	Z=W=L=M=X=H	1-flouro-2-(1-flourovinyl)benzene
11;	W=M=F	X=Y=Z=L=N=H	1,3-diflouro-5-vinylbenzene
12;	Z=M=F	X=Y=W=L=N=H	1,4-difluoro-2-vinylbenzene
13;	Y=M=F	X=Z=W=L=N=H	1-fluoro-3-(1-fluorovinyl)benzene
14;	Z=W=F	X=Y=L=M=N=H	1,2-diflouro-3-Vinylbenzene
15;	Y=W=F	X=Z=L=M=N=H	1-flouro-3-(1-flourovinyl)benzene

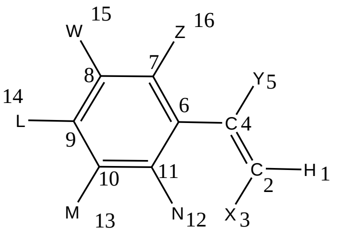

Table. B3LYP/6-311++G** E_2 values obtained of natural bond orbital (NBO) approach for all di-fluorovinylbenzenes.

Molecule	Donor → Acceptor	ΣE2
1,2-diflourovinylbenzene(**7**)	$\pi_{C10-C11} \rightarrow \pi^*_{C6-C4}$ (3.19), $\pi_{C11-C6} \rightarrow \pi^*_{C6-C4}$ (2.08), $\pi_{C6-7} \rightarrow \pi^*_{C6-C4}$ (1.89), $\pi_{C6-C7} \rightarrow \pi^*_{C4-C2}$ (1.96), $б_{C6-C7} \rightarrow б^*_{C4-C2}$ (18.31), $\pi_{C6-C4} \rightarrow \pi^*_{C4-C2}$ (3.85), $\pi_{C7-C8} \rightarrow \pi^*_{C6-C4}$ (3.02), $\pi_{C4-C2} \rightarrow \pi^*_{C6-C4}$ (4.38), $\pi_{C2-C1} \rightarrow \pi^*_{C6-C4}$ (5.43), $\pi_{C2-C1} \rightarrow \pi^*_{C4-C2}$(1.34)	45.45

Mulliken population analysis of charges and several importance of other thermodynamic properties were also performed by DFT method.

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Paper code: 556

DFT study on mono-chloroazulenes

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The active layer in organic photovoltaic bulk heterojunction devices is composed of a blend of π-conjugated, electron-donor polymers and electron-acceptor molecules [1]. Whereas the optoelectronic properties of the electron-donor polymer are primarily determined by the choice of the conjugated backbone, the solubility is predominantly determined by the position, length and makeup of the alkyl side chains. Both the polymer backbone and the alkyl side chains inchlence device efficiency and molecular packing structure, especially in donor–acceptor copolymers, which contain an ordered sequence of different subunits [2]. The objective of the present research is to study the electrical and structural properties of all mono-chloroazulenes. All of the possible of mono-chloroazulenes studied in this work are presented in Fig. 1.

1:	K=L=M=Q=W=X=Y=Z=H	Azulene
2:	K=L=M=Q=W=X=Y=H, Z=Cl	2-chloroazulene
3:	K=L=M=Q=W=X=Z=H, Y= Cl	3-chloroazulene
4:	K=L=M=Q=W=Y=Z=H, X= Cl	4-chloroazulene
5:	K=L=M=Q=X=Y=Z=H, W= Cl	5-chloroazulene
6:	K=L=M=W=X=Y=Z=H, Q= Cl	6-chloroazulene

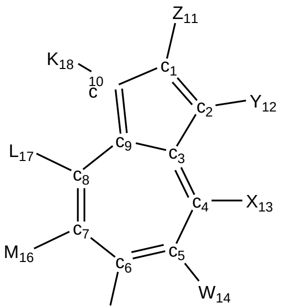

Fig. 1 All possible mono-chloroazulenes studied in this work

Structures of representative mono-chloroazulenes were optimized using B3LYP/6-311+G* levels of theory with the GAUSSIAN 09 package of programs implemented on a Pentium–PC computer with a 7300 MHz processor. The vibrational analysis showed that all structures correspond to local minima in potential energy surface. Values of dipole moment has been calculated and analyzed. The analysis of these data showed that the 2-chloroazulene has the highest value of the dipole moment (with 2.9837 Debye), and it can be suggested that this molecule has high solubility in polar solvents. The electrochemical stability of 2-chloroazulene is greater than other compounds and also the zero-point energy for this molecule is greater than other molecules. The analysis of data showed that the double bonds in 4-chloroazulene is more delocalized; accordingly, this monomer is the best candidate monomer among all mono-chloroazulenes for the synthesis of corresponding conductive polymers with modified characteristics.

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Paper code: 557

Comparative study on all di-chloroazulenes; a study of density functional theory

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The conductivity study and the electrochemical polymerization of conducting compounds (or monomers) is an interesting matter for Scientifics in the world. Electrically conducting polymers have been considered for numerous applications including charge dissipation coatings, organic thin-film transistors, and conducting textiles [1]. The use of electrically conducting polymers in electro-chromic devices, as materials that possess the ability to reversibly change color by altering redox state, has emerged. Many conjugated polymers are colored in the neutral state since the energy difference between the σ-bonding orbitals and the σ* anti-bonding orbitals (valence band) lies within the visible region [1]. All of the possible of di-chloroazulenes studied in this work are presented in Fig. 1.

1:	K=L=M=Q=W=X=Y=Z=H	Azulene
2:	K=L=M=Q=W=X=H,Y=Z=Cl	1,2-dichloroazulene
3:	K=L=M=Q=W=Y=H,X=Z= Cl	2,4-dichloroazulene
4:	K=L=M=Q=X=Y=H,W=Z= Cl	2,5-dichloroazulene
5:	K=L=M=W=X=Y=H,Q=Z= Cl	2,6-dichloroazulene
6:	K=L=M=Q=W=Z=H,X=Y= Cl	1,8-dichloroazulene
7:	K=L=M=Q=X=Z=H,W=Y= Cl	1,7-dichloroazulene
8:	K=L=M=W=X=Z=H,Q=Y= Cl	1,6-dichloroazulene
9:	K=L=Q=W=X=Z=H,M=Y= Cl	1,5-dichloroazulene
10:	K=M=Q=W=X=Z=H,L=Y= Cl	1,4-dichloroazulene
11:	L=M=Q=W=X=Z=H,K=Y= Cl	1,3-dichloroazulene
12:	K=L=M=Q=Y=Z=H,W=X= Cl	4,5-dichloroazulene
13:	K=L=M=W=Y=Z=H,Q=X= Cl	4,6-dichloroazulene
14:	K=L=Q=W=Y=Z=H,M=X= Cl	4,7-dichloroazulene
15:	K=M=Q=W=Y=Z=H,L=X= Cl	4,8-dichloroazulene
16:	K=L=M=X=Y=Z=H,Q=W= Cl	5,6-dichloroazulene
17:	K=L=Q=X=Y=Z=H,M=W= Cl	5,7-dichloroazulene

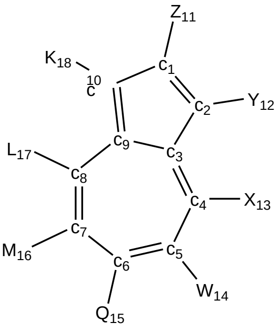

Fig. 1 All di-chloroazulenes studied in this work

The structural and electrical properties of all di-chloroazulenes have been studied using B3LYP method with 6-311+G* basis set. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, HLG (the gap between HOMO and LUMO) and size of dipole moment vector, total electrical energies, enthalpies, entropies, electronic, Gibbs and Zero-Point energies, and also IR and NMR spectra have been calculated and studied in this work. The analysis of these data showed that the 1,2-dichloroazulene (Molecule **2**) has the highest value of the dipole moment (*i.e.* 3.7735 D). The electrochemical stability of 2,6-dichloroazulene is greater than other compounds and also the zero-point energy for this molecule is greater than other molecules. The analysis of data showed that the double bonds in 4,5-dichloroazulene is more delocalized.

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Paper code: 575

Synthesis of superhydrophobic ZnO micro-rods on carbon cloth

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Carbon cloth (CC) was coated with ZnO micro-rod modified with stearic acid (SA) in order to obtain superhydrophobic properties. The prepared sample shows water contact angle (WCA) of 160°.

In recent years, solid surfaces with superhydrophobic property which display high contact angle ($\theta > 150°$) have attracted great worldwide attention [1] because of their wide applications, including self-cleaning and numerous potential applications [2].

At first the surface of carbon cloth was oxidized with $KMnO_4$ aqueous solution. The ZnO micro rods were hydrothermally deposited on the carbon cloth by dipping into the mixture composed of aqueous solution zinc nitrate, hexamethylenetetramine and NH_4OH in a Teflon lined stainless steel autoclave and then heating at 180℃ for 6h. The as prepared ZnO micro-rod on carbon cloth was immersed into an ethanol solution of stearic acid to obtain the superhydrophobic CC/ZnO/SA.

The prepared sample was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectra (FTIR), attenuated total reflectance Fourier-transform infrared spectroscopy (ATR-FTIR) and contact angle measurements.

As shown in (Fig 1a) the CC/ZnO exhibits surface hydrophobicity with water contact angle of 98°. But the sample becomes superhydrophobic after treatment with stearic acid and the contact angle increased from 98° to 160° (Fig 1b). The effect of solution pH on the wettability of CC/ZnO/SA is shown in Fig 1c. It is clear that the prepared sample is not wetted by the aqueous solutions with different pH values.

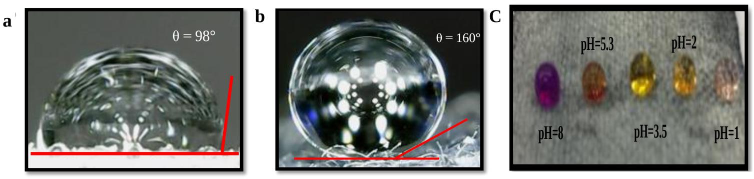

Fig. 1 Contact angle of a water droplet on a (a) CC/ZnO (b) CC/ZnO/SA (c) Optical image of water droplets (including cresol red) at different pH values on CC/ZnO/SA.

To demonstrate the self-cleaning ability of the superhydrophobic surface, the pristine carbon cloth and the fabricated superhydrophobic CC/ZnO/SA were both contaminated with soil. When water droplets dropped on the surface, they quickly penetrated in the pristine hydrophilic carbon cloth and most of the soil remain on the surface. Comparatively, most of soil powder was clearly removed with water droplets rolling off the superhydrophobic CC/ZnO/SA, exhibiting excellent self-cleaning property.

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Paper code: 581

Docking study of some novel azole-oxime ether hybrids as potential antifungal agents

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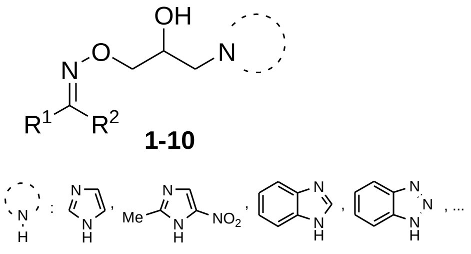
The incidence of infections caused by pathogenic fungi has increased significantly over the years. Nowadays, numerous antifungal drugs with various structures and scaffolds are known and available [1]. One of the most established antifungal azole drugs having rational versatility in structures is the miconazole family with the general structure of 1-(arylethyl)-1Himidazoles. On the other hand, oximes and oxime ether derivatives are a prominent structural motif found in numerous pharmaceutically active compounds. Many well-known drugs with various chemotherapeutic activities contain an oxime or oxime ether moiety in their structures [1].

Recently, our research group has synthesized some novel azole-oxime ether hybrids (Fig. 1) and the products were examined for their in vitro antifungal activities against *Candida albicans*, *Candida krusei*, *Aspergillus niger,* and *Trichophyton rubrum* [2]. Having realized the antifungal activities of these compounds, we were encouraged to investigate their possible interaction with the active site of cytochrome P450 14α-sterol demethylase which is a favorable target for most azole antifungal drugs. In this study, the binding properties and interaction of title compounds with *Mycobacterium* P450DM enzyme was investigated by molecular docking study. The interactions of several known antifungal drugs such as fluconazole, tebuconazole, albaconazole, and voriconazole with Mycobacterium P450DM enzyme were also investigated using molecular docking study. The Gipps-free energies (ΔG) for binding of aforementioned compounds with *Mycobacterium* P450DM enzyme have been indicated.



1-10

R^1, R^2 = aryl, alkyl

Fig. 1 The general structure of synthesized azole-oxime ether hybrids.

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Paper code: 585

The prediction of absorption and emission wavelengths in thermally activated delayed fluorescence(TADF) organic light-emitting diodes(OLEDs)

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During the last two decades, organic light-emitting diodes (OLEDs) have received a great deal of attention as a solution for high-resolution and large area flat display panels [1]. Extensive efforts have been devoted to improve their electroluminescence efficiency [2] and a lot of studies have been focused on enhancing the quantum efficiency with appropriate host and phosphorescent materials [3].

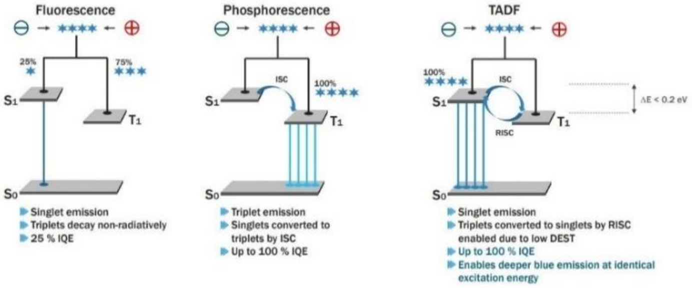
The goal of this project is to predict the absorption wavelengths and the emission of fluorescence diodes with a delayed active heat. Calculations are done using the ORCA software [4]. The first step in the calculation of the time dependent density functional of the theory (TD-DFT) is on the desired diode. In this study, According to Fig. 1 important transfers and involved orbitals are identified. In the next step, using the CASSCF/NEVPT2 calculations, the energy of the transmissions is determined. Finally, the new diodes are suggested by adding different substitutes and studying the absorption and emission wavelengths. It should be noted that the three essential requirements for an OLED-TADF are as follows [5,6]:

(A) There is a small energy gap between the excited states S1 and T1 (less than 0.2 electron volts)
(B) Small Exchange Integral between HOMO and LUMO orbital
(C) The separation and centralization of HOMO or LUMO orbital

The mechanism of action in TADF is that:

As stated in the mandatory clause of a TADF, the difference in energy between the lower energy level T1 and the higher energy level S1 shall be sufficiently small to permit reverse intersection system (RISC) to be carried out at ambient temperature (T1 → S1). The energy difference between these two levels is proportional to the energy converted, which is related to the overlap integral between the two orbital ones responsible for the states of the two levels. When the energy gap between the two T1 and S1 levels is subjected to thermal energy (about 26 mV at room temperature), the reverse cross-system through heat excitation and stimulation will occur far more and the fluorescence in this case The delayed fluorescence is known to occur from the S1 level. This phenomenon is referred to as the active-delayed light-fluorescence-delayed active heat, which has a quantum yield of close to 100%, and has recently been widely studied around it [7].

In most molecules, the fluorescence signal is very weak. Most organic fluorescent molecules have high resonance coupled systems. In this way, the basic molecular framework for organic TADF molecules remains limited to azo-aromatic (such as trizines and oxidazoles), cyanobenzenes, sulfones and spiro flora derivatives [8].



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Paper code: 598

Strain and Ring Size Effects on the 1,3-dipolar Cycloaddition reactions of the Medicine Efavirenz Derivatives; A Theoretical Studies

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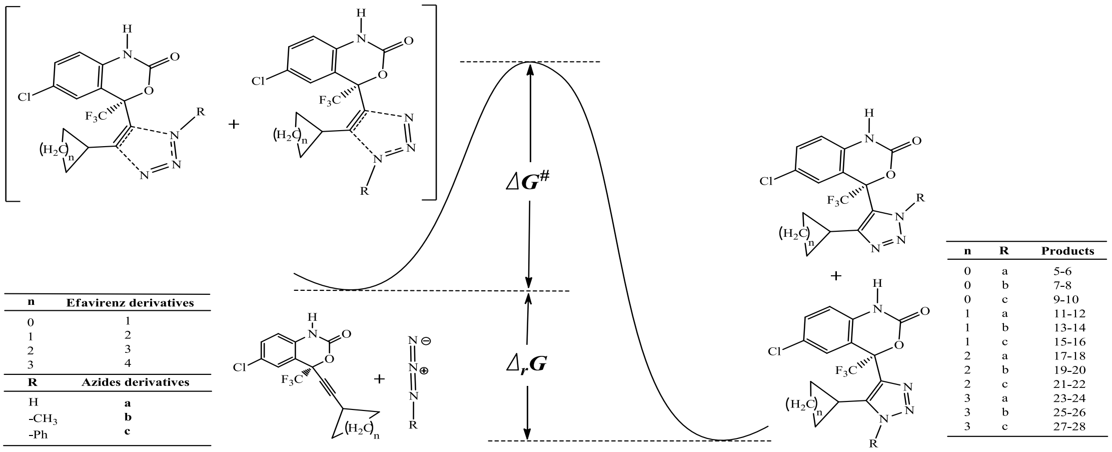
This study was focused on the theoretical and computational studies of the 1,3-dipolar cycloaddition (1,3-DC) reactions, which they have been applied in a number of diverse fields [1]. An undeniable relation between the bond angle strain around of the triple bonds in simple cycloalkynes and the kinetic of 1,3-DC reactions with azide derivatives has been proven by theoretical analysis before [2], so herein the second-order strain effect of a fused side ring on reactivity of alkyne in 1,3-DC reaction of alkynes and azides was investigated. Efavirenz as an antiretroviral medication was applied to treat and prevent HIV/AIDS [3]. The molecule of this medicine was selected as a ring closed dipolarophile. In this study, the 1,3-dipole reaction of Efavirenz analogues (**1-4**) with azide derivatives (**a-c**) were applied to produce the 1,2,3-triazole derivatives. The energy levels of the reactants, transition states (TS), products (**5-28**), the free energies (in kcal mol^{-1}) of reaction ($\Delta_r G$ and $\Delta G^{\#}$), rate constants by using *Eyring*'s equation (k and k'), structural data were calculated by DFT-B3LYP/6-31G* method.



n	Efavirenz derivatives
0	1
1	2
2	3
3	4
R	**Azides derivatives**
H	**a**
-CH_3	**b**
-Ph	**c**

n	R	Products
0	a	5-6
0	b	7-8
0	c	9-10
1	a	11-12
1	b	13-14
1	c	15-16
2	a	17-18
2	b	19-20
2	c	21-22
3	a	23-24
3	b	25-26
3	c	27-28

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Paper code: 609

3D QSAR Study of Simultaneous AT1 and ETA Antagonists as Anti-hypertensive Drugs

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Both Angiotensin (AT1) and Endothelin (ETA) antagonists cause lower blood pressure in hypertensive patients. A compound with dual AT1 and ETA receptors antagonistic function may be more efficacious antihypertensive drug. In order to understand the most important structural characteristics of AT1 and ETA inhibitors and the correlation of these features their potency, a Molecular Interaction Fields (MIF) based alignment independent three-dimensional quantitative structure-activity relationship (3D-QSAR) study was conducted. The resulted PLS model analysis indicated that the computed activities were in excellent agreement with experimentally observed values, for AT1 (R^2 = 0.89, $\mathrm{Q}^2_{\mathrm{LOO}}$ = 0.83 and $\mathrm{R}^2_{\mathrm{Pred}}$ = 0.873) and for ETA (R^2 = 0.82, $\mathrm{Q}^2_{\mathrm{LOO}}$ = 0.64 and $\mathrm{R}^2_{\mathrm{Pred}}$ = 0.778). Finally, the inhibitory activity of each AT1 and ETA inhibitor groups were predicted using the other receptor validated QSAR model and the most potent ones were selected for further studies.

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Paper code: 622

Quantum mechanical study of interaction between phenolic compounds as inhibitor with active site of human carbonic anhydrase enzyme

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CO_2, bicarbonate and protons are an essential molecule and ions for many important physiologic processes occurring in all living organisms. However, the uncatalyzed rate of interconversion of such species is too slow to meet the physiological needs of most biochemical processes. This task is efficiently accomplished by the carbonic anhydrases. This superfamily of metals-enzymes possess within their active sites a highly nucleophilic metal hydroxide species, such as zinc(II), cadmium(II) or iron (II) hydroxide, depending on the class [1].

Phenol and its derivatives were reported to be a competitive inhibitor of human Carbonic Anhydrase II (hCA II). The phenolic moiety has an amphiphilic character. The presence of the hydrophobic planar aromatic ring is responsible for hydrophobic interactions (π-stacking), whereas at the same time the polar hydroxyl groups can participate in hydrogen bonding. This dual behavior allows these molecules to bind to the amino acid residues of several proteins, enzymes or receptors Figure 1 [2]. In the present research the mechanism of the inhibition of phenolic compounds with active form of CA (II) using DFT calculations have been investigated. The electronic structure and electronic energy of all studied compounds have been calculated in the gas phase and then in water solvent using B3LYP and split-valance6-31G* basis set.

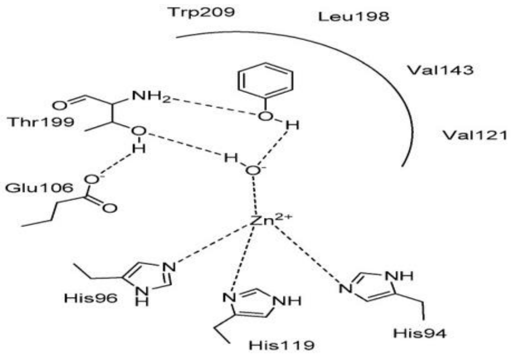

Fig. 1. Schematic representation of the binding mode of phenol within the hCA II active site

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Paper code: 644

Planar Stacking Interactions in the Binding of Type II Statins to HMG-CoA Reductase

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Statins act by inhibiting 3-hydroxy-3-methylglutaryl coenzyme A (HMG-CoA) reductase and thereby reducing cholesterol synthesis. Statins can be divided into two classes based on their structure; Type I statins (e.g., simvastatin) exhibit binding *via* a decalin ring structure, while type II statins (e.g., rosuvastatin) exhibit additional binding *via* their fluorophenyl group [1]. Statins primarily use dipole/dipole and hydrogen bonds to bind to the active site of the reductase, focusing on the portion of the active site dominated by lysine 735, arginine 590, aspartic acid 690, serine 684, lysine 691, asparagine 755, lysine 692 and glutamine 559 with minimal explicit incorporation of hydrophobic side-chain interactions [2] (1HW8, 1HW9, 1HWJ, 1HWI, 1HWK, 1HWL).

We examine potentially important enzyme-ligand interactions currently not incorporated: planar stacking interactions between type II statins and residue arginine 590 in the HMG-CoA reductase active site. We calculated electronic interaction energies between the residue and types of statins using M06/6-311++G** level in the gas phase. The results indicate the absolute binding energy for type II statins is more overall than type I statins. In addition, stacking interaction is verified through AIM calculations at MP2/6-31G(0.25)* level.

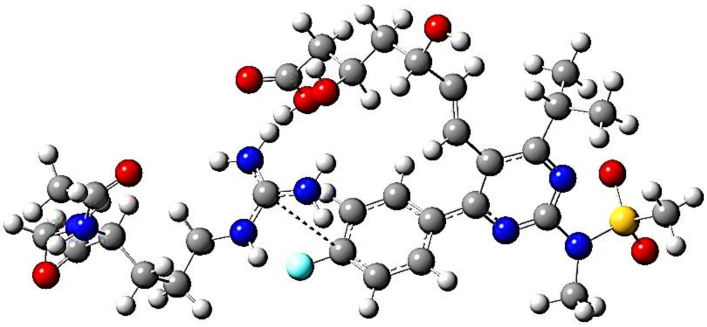

Fig. 1 Arginine/aromatic stacked interaction in rosuvastatin complex with HMG-CoA Reductase.

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Paper code: 679

Theoretical prediction of nonmetal-doping effects on the photocatalytic performance of graphite-like carbon nitrides

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Because of the importance of reducing greenhouse gases, especially CO_2, and their utilization in the generation of materials that are being used as a source of energy, the investigation of photocatalytic processes of graphite-like carbon nitrides is of great interest, from the theoretical viewpoint. In comparison to the metal-containing visible-light photocatalysts, such as oxide, sulfide and oxynitride, graphitic carbon nitride, g-C_3N_4, (Fig. 1), has been regarded as a highly potential photocatalytic material under solar light irradiation because of its low cost, unique chemical stability, environmentally benign and tunable. In this study, the effect of nonmetal, sulfur and phosphorus, doping on the structural and electronic properties of two-dimension g-C_3N_4 sheet was calculated by the first principle method. The bare and doped g-C_3N_4 structures were optimized at the B3LYP/6-31G(d) level of the theory. All calculations were implemented by using Gaussian 09 package. Our results demonstrated that the doping with nonmetal impurities increases the separation of photogenerated electron−hole pairs. Furthermore, doping with nonmetal impurities improves the photocatalytic activity of the CO_2 conversion.

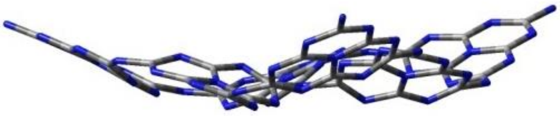

Fig. 1 The optimized structural of g-C_3N_4.

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Paper code: 694

Kinetic investigation on sonocatalytic degradation of methylene blue in the presence of La:ZnO/GO

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Degradation of organic pollutants is a potential source of water protection in the world. According to different reports, the industries in many developed and developing countries discharge about 70% of their waste products directly and without any filtration into surface water [1]. In recent decades, the use of heterogeneous catalysts in the presence of eco-friendly source such as light and ultrasound radiation as eco-friendly technology has attracted global attention [2].The degradation of pollutant by ultrasound radiation requires a lot of energy and a complete degradation is rarely done; to overcome this restriction, using a heterogeneous catalyst with ultrasound radiation, which is called the sonocatalytic process, is recommended. Lanthanum doped Zinc oxide/graphene oxide (La:ZnO/GO) heterostructures were synthesized via a simple method. The obtained (La:ZnO/GO) Composites were characterized by the XRD, FT-IR, TEM, SEM, EDS, DRS analyses. The potential of La:ZnO/GO, has been explored as an effective catalyst for the sono-degradation of Methylene blue (MB). The effects of process parameters such as, catalyst dosage, initial dye concentration and irradiation time on the extent of sono-degradation efficiency have been investigated. The results show that process matched well with the Langmuir–Hinshelwood (L–H) kinetic model.

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Paper code: 701

Tautomerism, molecular structure, intramolecular hydrogen bond, and tautomery equilibrium of α-methyl and ethyl substituted 4-amino-3-penten-2-one; A theoretical study.

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We subsisted methyl and ethyl groups in α-position of 4-amino-3-penten-2-one, APO. α,β-Unsaturated-β-ketoenamines, are capable to exist in three different tautomers at equilibrium, i.e., iminoketone, aminoketone, and iminoenol forms, see Fig. 1. The structure of all iminoketone, aminoketone, and iminoenol tautomers of 3-MeAPO, 3-EtAPO, and APO have been optimized at the B3LYP level, using 6-311++G** basis set. To confirm the relative stability of the iminoketone, aminoketone, and iminoenol forms of 3-MeAPO, 3-EtAPO, and APO, the obtained stable structures were also fully optimized at the B3LYP, using 6-31G*, 6-31G**, 6-311G**, 6-311++G**, D95** basis set, the second-order Moller-Plesset (MP2), using 6-31G* basis set, level in gas phase. Also, we optimized all iminoketone, aminoketone, and iminoenol tautomers of 3-MeAPO, 3-EtAPO, and APO at B3LYP/6-311++G** in CCl_4, C_2H_5OH, and CH_3CN solutions.

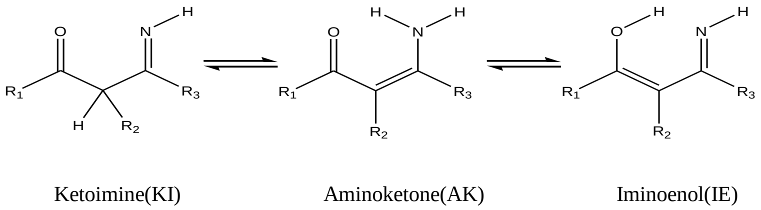

Fig.1. Tautomery in β-ketoenamines.

According to the results of our calculations and previous works [1-2], aminoketone form of 3-MeAPO, 3-EtAPO, and APO is more stable than iminoketone and iminoenol forms. upon the substitution of methyl and ethyl group in the α position and because of the larger steric effect of this group with the hydrogen atoms of methyl groups in β positions, which pushes the methyl groups toward oxygen and nitrogen atoms, this effect, causes to reduce the N…O and O…H distances decrease, while the OHN bond angle and N-H bond length increase [4]. Therefore, the IHB strength of 3-MeAPO and 3-EtAPO increases compared to that of APO. AIM results confirm that the IHB in 3-MeAPO, 3-EtAPO are stronger than APO. This result is in agreement with the E_{HB} for 3-MeAPO and 3-EtAPO molecules, which are obtained by the AIM method. The E_{HB} values are 10.85, 11.00 and 7.67 kcal/mol, in 3-MeAPO, 3-EtAPO and APO, respectively.

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Paper code: 704

Intramolecular hydrogen bond strength of 3-methyl-4-amino-3-penten-2-one, an experimental approach

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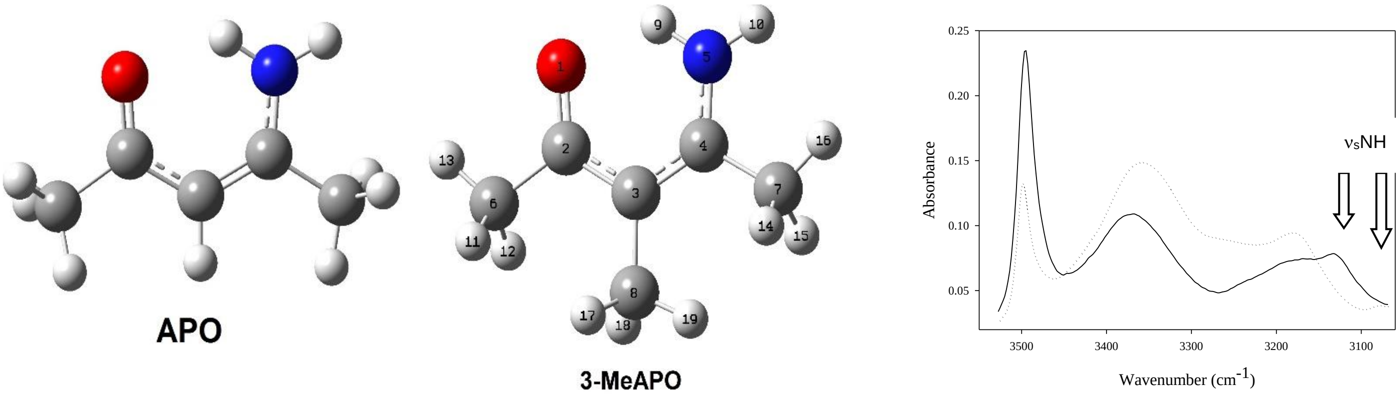
The intramolecular hydrogen bonding of 3-methyl-4-amino-3-penten-2-one, 3-MeAPO, has been investigated by experimental results, including NMR, IR, and UV spectra. According to ^{1}H-NMR spectrum, the titled molecule is as a keto-amine form. The vibrational spectra of 3-MeAPO and its deuterated analogous have been recorded. The existence of intermolecular and intramolecular hydrogen bond is also shown in both solid and solution phases. The DFT suggested a relatively medium intramolecular hydrogen bond with N···O distance at 2.597 Å for 3-MeAPO, which is in agreement with the calculated hydrogen bond energy about 10.85 kcal/mol for the mentioned molecule. In the IR spectrum of 3-MeAPO, the mode ν_sNH(NH$_{in}$) observed at 3135 cm^{-1} in the CCl_4 solution, and δNH at 10.32 ppm. The mentioned bands are in 3184 cm^{-1} [1] and 9.7 ppm [2] for 4-amino-3-penten-2-one (APO), See fig.1. The UV-Vis spectrum of 3-MeAPO was recorded in ethanol, as solvent. The UV-Vis spectra of 3-MeAPO and APO are shown a band at 319 and 299 nm [3], respectively. The theoretical calculations and spectroscopic results indicate that the intramolecular hydrogen bonding (IHB) strength of 3-MeAPO is stronger than that in 4-amino-3-penten-2-one (APO).



a)

b)

Fig.1: a) the structures of 3-MeAPO and APO molecules. b) The infrared spectra of 3-MeAPO (—) and APO (…….) in CCl_4 in the 3600–3000 cm^{-1} range (ν N-H in plane region).

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Paper code: 706

Conformational stability, molecular structure, and intramolecular hydrogen bond of 2,2-dimethyl-5-amino-4-hexen-3-one.

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We substituted the t-but group on C_β position of 4-amino-3-penten-2-one, APO. The aminoketone form of α,β-Unsaturated-β-ketoenamines are more stable than iminoketone and iminoenol forms [1-2]. From the theoretical point of view, by considering the torsion of methyl groups with respect to together and chelated ring, 4 aminoketone forms can be drawn for 2,2-dimethyl-5-amino-4-hexen-3-one, DMAHO, molecule. All the mentioned forms of DMAHO have been optimized at the B3LYP level, using 6-311++G** basis set. Some selected optimized structural parameters, related to intramolecular hydrogen bond (IHB), of DMAHO and APO are collected in Table 1. According to this table 1, the N…O and O…H distances decrease, while the OHN bond angle and N-H bond length increase. Therefore, the IHB strength of DMHAO is more than that of APO. The AIM results confirm that the IHB in DMHAO is stronger than that in APO. This result is in agreement with the E_{HB} for DMHAO molecule, which is obtained by the AIM method. The E_{HB} values are 9.20 and 7.67 kcal/mol, in DMHAO and APO, respectively.

Table 1. Some selected theoretical parameters of DMHAO and APO calculated (bond lengths and bond angles are in Å and °, respectively).

	DMAHO					APO
	AK1[a]	AK2[a]	AK3[a]	AK4[a]	Avg.	AK
N-H(in)	1.018	1.019	1.021	1.023	1.020	1.019
O-H	1.913	1.861	1.833	1.822	1.857	1.89
N...O	2.684	2.643	2.642	2.639	2.652	2.669
OHN (angle)	130.1	130.8	133.5	134.2	132.2	130.8
AIM results[b]						
ρ_{BCP}	0.032	0.034	0.036	0.037	0.035	0.031
∇^2_{BCP}	-0.029	-0.031	-0.032	-0.032	0.031	-0.028
E(HB)	8.20	8.92	9.68	10.00	9.20	7.67

[a] AK1, AK2, AK3, and AK4 are 4 conformers of aminoketone forms of DMHAO. Avg. is the average value of 4 conformers.

[b] Charge density (ρ) in $e.au^{-3}$, Laplacian of charge density ($\nabla^2\rho$) in ($e.au^{-5}$) at the bond critical point (BCP) of the O…H bond. E_{HB} is the IHB energy in kcal/mol.

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Paper code: 725

Thermodynamic study of malachite green by nanomaterial $LaMnO_3$

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Pollution of aquatic environments containing color waste from the chemical industry, such as pigment, textiles, leather and cosmetics, is harmful to humans and the environment [1,2]. In this study, $LaMnO_3$ nanoparticles were used as a suitable adsorbent for malachite green (MG) removal from aqueous solutions. Adsorption values were investigated by changing the parameters of time, pH, temperature, adsorbent amount and initial amount of dye. The thermodynamic parameters of the $LaMnO_3$ adsorption process were calculated such as Gibbs free energy (ΔG^0), enthalpy (ΔH^0) and entropy changes (ΔS^0).The results showed that, due to the negative Gibbs free energy and the positive integrity of the enthalpy, the process is spontaneous and endothermic.

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Paper code: 750

The effect of functionalizing graphene nanosheets on adsorption of Hydroxynaphtol Blue dye, A molecular dynamics simulation

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One of the most effective methods for removing many pollutants from aqueous solutions is adsorption. Removal of particles based on adsorption is accomplished by connecting dissolved pollutants in a stream towards a solid surface. In this process, choosing an adsorbent with high selectivity over the desired pollutant is very important [1]. Occasional levels of adsorption can be increased by using auxiliary groups; in other words, the adsorbent can be modified. Today, graphene nanosheets are one of the most widely used adsorbents in the field of adsorption that can also be improved with auxiliary groups [2]. In the present study, the process of adsorption of hydroxynaphtol blue (as a dye that is a water pollutant) on pure and oxidized graphene nanosurfaces is simulated at 298 K with DL_POLY_2.17 simulation package. Analyzing the radial distribution function (RDF) between the dye center of mass (COM) and the graphene nanosheets demonstrates the effect of surface modification on the adsorption. As seen in Figure 1, oxidation of graphene nano surface with the combination of hydroxy and epoxy groups enhances the adsorption of the desired dye on the surface and rises the efficiency of the adsorption process. Here, hydrogen atoms of hydroxy group possess the best contribution on adsorption process.

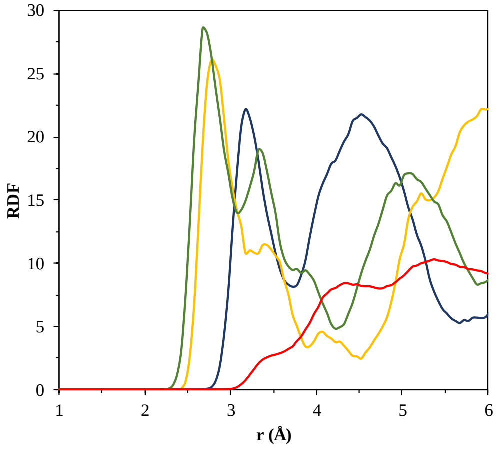

Fig. 1 RDF of dye COM and surface atoms. Green, hydrogen atom of hydroxy group; yellow, oxygen of epoxy group; blue, oxygen of hydroxy group; and red, carbon atoms of graphene nanosheet.

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Paper code: 768

Applying the Laplace transform to solve the kinetic equations of rubber vulcanization

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Sulphur vulcanization is a complicated process, since here crosslinking occurs through both series and parallel reactions [1]. So proposing a quantitative macroscopic model enabling us to predict the rubber physical properties is still a real challenge. This process involves three steps, i.e. induction, curing, and post curing. In post curing, reversion could take place quite frequently giving rise to a remarkable decrease in rubber vulcanized properties. It was found out that, this phenomenon cause a decrease in sulfur crosslinking.

In this work, the mechanism of curing and post curing will be investigated. To implement the task, Han et al. model [2, 3] was chosen as a base.

$$A \overset{k1}{\rightarrow} Vu1$$

$$A \overset{k2}{\rightarrow} Vu2 \overset{k3}{\rightarrow} D$$

Where A is sulfur available for the formation of crosslinks, Vu1 is the stable sulfur crosslinks formed during vulcanization, Vu2 is the unstable sulfur crosslinks, formed during vulcanization, D is product of the reversion reaction, and k1, k2,and k3 are rate constants. We managed to solve their three developed differential equations by using Laplace's transform (equation1).

$$\mathcal{L}Vu = \frac{k1A0}{p(p+k1+k2)} + \frac{k2\ A0}{(p+k3)(p+k1+k2)} \qquad (1)$$

Where $\mathcal{L}Vu$ is Laplace's transform of product (Vu1+Vu2), A0 is initial sulfur concentration and p is independent variable for Laplace's transform. Our analytical solution was in good agreement in comparing to literature [2, 3]. Mechanism by applying the Levenberg-Marquardt algorithm which were in consistent with experimental results obtained by the other researchers. In addition, the temperature effect on rate constants was examined and found that the rate constants follows the Arrhenius law.

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Paper code: 779

Fast removal of Methyl orange (MO) by hollow $LaMnO_3$

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In the present study, hollow $LaMnO_3$ nanoparticles have been used as a suitable adsorbent to remove methyl orange (MO) from aqueous solution. First, spherical carbon particles were prepared. Then, by using the prepared carbon, $LaMnO_3$ was prepared with a hollow permeate structure in a hydrothermal method [1-2].

Using calcination gravimetric results, the calcination was performed at 850 °C for 6 hours.

Characterizations of the resulting powders were performed by means of an X-ray diffraction (XRD) and transmission electron microscopy (TEM) (fig.1). The results of the TEM specification show that the composition is composed of hollow peroxide structures.

Then, the efficiency of the combination of LaMnO3 as a sorbent was used to remove the water soluble anionic methyl orange dye (MO) dye.

The impact of sorbent dosage, initial MO concentration and pH on MO adsorption onto hollow LaMnO3 were studied. The results showed that the adsorbent amount of 0.0056 g, the initial dye concentration of 10 mg / L and the pH value of 2.5 and the temperature of the environment of the removal efficiency of the dye increased.

The results of methyl orange removal show that removal of Methyl Orange in acidic solution was more effective and 90% of methyl orange disappear within 15 minutes.

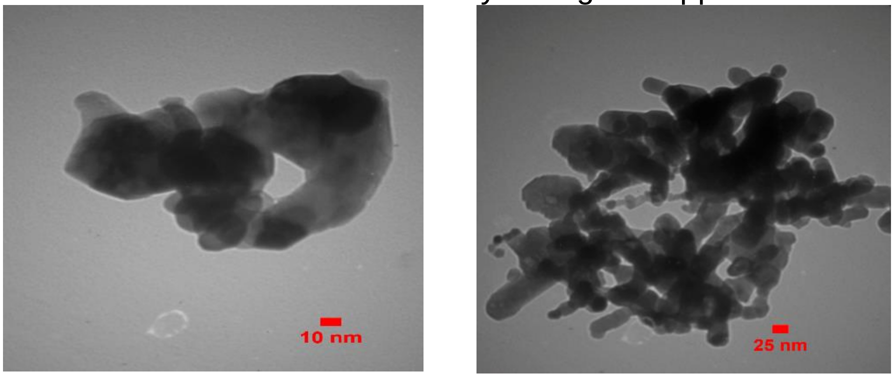

Fig. 1. TEM images

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Paper code: 782

Evaluation of Geometries, Stabilities and Optical Properties of B_n and Be©B_n (n=6-12) Clusters: Computational Assessment

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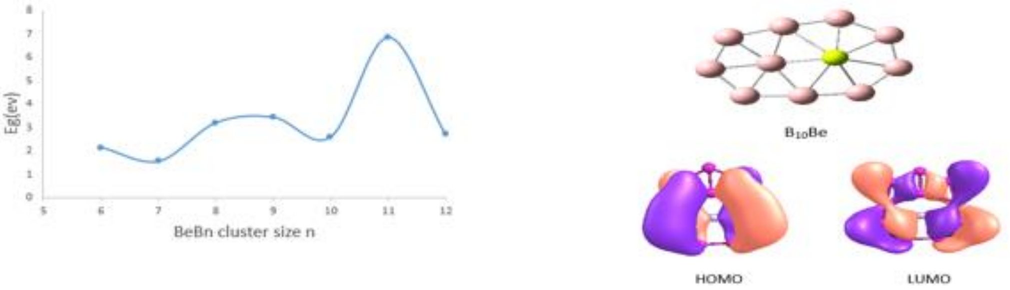
In recently computational and experimentally investigations of boron clusters have become of great scientific interest due to various shapes of boron nano-clusters which depends on the size structural and electronic properties. Small planar boron clusters can be used as novel inorganic ligands for coordination compounds. Herein, the geometries, stabilities and optical properties of B_n and Be©B_n (n=6-12) clusters were investigated via DFT calculations with B3LYP/6-311+ G(d) basis set. Furthermore, to obtain opto-electronic properties, the TD-DFT and NLO calculations were performed at cam/B3LYP/6-311+G(d) level of theory. Subsequently, more accurate single point energy calculations were performed at MP_2 method. It obtained that the Be metal atom was located in out of the ring except Be©B_6, Be©B_{11} and Be©B_{12} clusters. Relative stability as well as HOMO-LUMO energy gap of the ground-state was estimated for all clusters. It was found that Be©B_{10}, Be©B_{11} and Be©B_{12} are the most stable species, respectively. The values of HOMO-LUMO energy gap were found to be in the range of 1.5-7 eV for all studied clusters and the highest and lowest values is belonging to the Be©B_{11} and Be©B_7 clusters respectively.



(a) (b)

Fig.1. (a) Size dependence of the E_g of Be©Bn (n=6-12) and (b) the optimized structure of $B_{10}Be$ with related the HOMO and LUMO orbitals.

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Paper code: 794

Soret coefficients for binary mixtures of Helium and hydrogen isotopes: The nonadiabatic effects

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In the limit of zero density, the transport coefficients of a gas can be expressed in terms of the collision integrals, which are related to the intermolecular potential energy between two molecules. For different isotopes, the non-adiabatic effects on the potential energy surface can be affected on the collision integrals as well as transport properties of isotopic molecules. The accurate ab initio potential energy between helium/hydrogen and their isotope mixtures developed by bakr [2] have used to calculate the transport cross-sections as well as transport collision integrals. The model potential was fitted as a function of intermolecular separation and the relative orientation of the molecule as

$$V(R,\Theta) = \sum_{l=0,2,4} (A_{0l0} + A_{0l1}\,R + A_{0l2}R^2 + A_{0l2}R^3) \times e^{-\alpha_0 R} P_l(cos\theta) - \sum_{l=0,2} \sum_{n=6,8,10} f_n\,(dR)\frac{C_{n0l}}{R^n} P_l(cos\theta)$$

In this work, we first utilized a full analytical potential energy function including the non-adiabatic terms to calculate the Soret coefficients of the He-H_2 and their isotopic mixtures. The extensive comparisons with experimental data as well as with our calculations in the frame work of the classical kinetic theory demonstrate that the ab initio transport properties can be used as standard values in a wide range of scientific needs. Moreover, the density corrections to the gaseous Soret coefficients are formulated and used to calculate for the isotopic mixtures of hydrogen and helium mixtures. To the best of our knowledge, the formulations for Soret coefficients and thermal diffusion factors are new. The theory was checked with the previous works of Maghari et al. [3,4] studied by the non-equilibrium molecular dynamic simulations.

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Paper code: 797

Ultrasound assisted salting-out extraction of antioxidant phenolics from some pharmaceutical plants

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Over the last years, aqueous two-phase systems (ATPS) regained an increasing interest due to their potential in the downstream extraction and separation of antioxidants [1-3]. The extraction procedure is an important step in the separation of the antioxidants from plant materials and needs meticulous evaluation. In this work, the use of alcohol-salt-based ATPS was investigated as an alternative platform for the extraction and recovery of antioxidants from pharmaceutical plants. As a first approach, the systematic studies on the liquid−liquid equilibrium behavior of aqueous solutions were investigated. Different parameters, namely the type of alcohol and salt, the composition of the system, were evaluated regarding the salting-out coefficient, tie-line length and tie line data obtained. As a second step, the same ATPS were further used for the salting-out extraction of antioxidant phenolics from pharmaceutical plants. The results of this systematic study and the distribution of antioxidants in two phases were provided valuable information on the structure and antioxidant capacity of the active ingredients of pharmaceutical plants. In order to enhance the process, ultrasound was used to assist salting-out extraction (UA-SOE) of antioxidants from pharmaceutical plants. This procedure combines solid–liquid extraction, liquid–liquid micro-extraction and ultrasonic extraction in a single step. For example figure 1. demonstrate that this innovative and environmentally friendly technique (UA-SOE) can be successfully applied to the extraction and separation of antioxidant phenolics from pharmaceutical plants. The objective of the present research work was to characterize the partition behavior of antioxidants, on alcohol–salt ATPS in order to propose a potential strategy for the recovery and purification of these bioactive molecules. To obtain a higher partition coefficient and higher recovery of antioxidants in the ATPS, the main effective parameters (kind of salt and alcohol, concentration of salt and alcohol, sonication time, ratio solid to solvent and method of extraction) were studied.

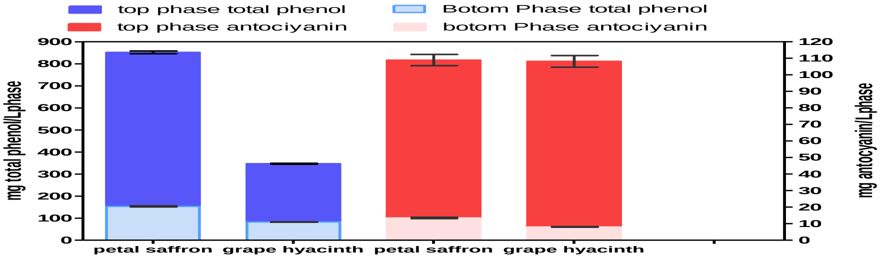

Fig. 1 UA-SOE of antioxidant phenolics from pharmaceutical plants.

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802

The effect of glycosylation on the chloroperoxidase structure: A molecular dynamic simulation analysis

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Chloroperoxidase (CPO), a heme-thiolate protein secreted by the marine fungus Caldariomyces fumago, has received much attention as the most versatile known heme enzyme. The signature function of CPO is halogenation of electron-rich organic substrates [1]. Chloroperoxidase is an extensively glycosylated monomeric enzyme with both N- and O-linked glycosyl chains [2]. Molecular dynamics (MD) simulations were performed by the GROMACS 4.5.6 package using the GROMOS96 43A1 force field [3]. In this study, the effect of glycosylation on the structure of chloroperoxidase has been investigated using MD simulation. Root mean square deviation (RMSD), root mean square fluctuation (RMSF) and protein secondary structure were evaluated before and after the removal of the carbohydrate. The results of RMSD showed that glycosylated enzyme increases stability rather than unglycosylated enzyme. RMSF values revealed that the flexibility of most residuals of enzyme reduces after removing N-linked oligosaccharides from CPO. The analysis of secondary structure showed that glycosylation on the chloroperoxidase reduces the formation of 3.10 Helix in the structure of protein. This study confirmed the experimental results of the role of N- and O-linked glycosyl chains in the structure and function of CPO.

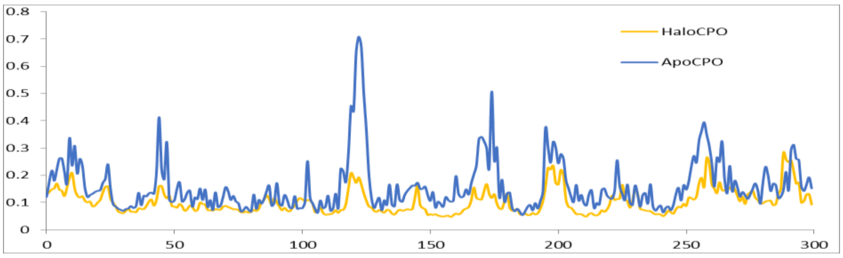

Fig. 1 RMSF gragh before and after removing carbohydrate

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Paper code: 804

A Theoretical Study on the Kinetics and Thermodynamic Parameters of Chelotropic Reactions: Dienes with Dichlorophenylphosphine

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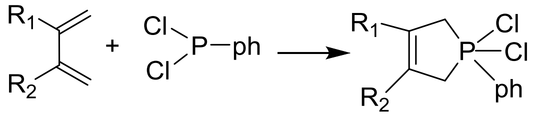
The kinetics and thermodynamic parameters of the chelotropic reactions between dichlorophenylphosphine and the conjugated hydrocarbon dienes [1] (see Fig1) have been theoretically investigated. The geometries of reactants, products, intermediates, and transition states involved in the reactions were optimized at the M062x/6–311++G (2d,2p) level of theory [2,3]. The ground and transition states were confirmed by the frequency calculations. The kinetic parameters were calculated with the transition state theory. The comparison showed that the reaction rates in the presence of dienes such as isoprene ($k = 5.88\times10^{-26} cm^3 molecule^{-1} s^{-1}$), phenoprene ($k = 6.63\times10^{-24} cm^3 molecule^{-1} s^{-1}$), and 2,3-dimethylbutadiene ($k = 3.58\times10^{-25} cm^3 molecule^{-1} s^{-1}$) were increased, while chloroprene ($k = 1.48\times10^{-26} cm^3 molecule^{-1} s^{-1}$) and 2-bromobutadiene ($k = 2.23\times10^{-26} cm^3 molecule^{-1} s^{-1}$) decreased the reaction rate. The rate constant of the butadiene was $k= 4.03\times10^{-26} cm^3 molecule^{-1} s^{-1}$.The free energies for dienes such as isoprene ($\Delta G = 26.98 kJmol^{-1}$), phenoprene ($\Delta G =19.63 kJmol^{-1}$), and 2,3-dimethylbutadiene ($\Delta G = 23.38 kJmol^{-1}$) were lower than butadiene ($\Delta G = 33.04 kJmol^{-1}$) while chloroprene ($\Delta G = 33.52 kJmol^{-1}$) and 2-bromobutadiene ($\Delta G = 35 kJmol^{-1}$) had a larger amount of free energy. As a result, dienes include butadiene, isoprene, phenoprene and 2,3-dimethylbutadiene were thermodynamically and kinetically more favorable than chloroprene and 2-bromobutadiene.



R_1=R_2=H; R_1=Cl,Br,ph,CH_3,R_2=H ;
R_1=R_2=CH_3

Fig1. Chelotropic reactions of dienes and dichlorophenylphosphine

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Paper code: 810

Investigation of accelerated sulfur vulcanization by irreversible consecutive mechanism

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The most mathematical application in chemical kinetics is to find analytical solutions for the rate equations. Rate equations describe how the rate of concentration change depends on concentrations. By solving these equations, the relationship between species concentration and time are sought. Solutions of the rate equations for single step reactions (elementary reaction) are often well known but for reactions involving several steps (complex reaction) are difficult. Since the accelerated sulfur vulcanization involves a large number of parallel and series steps [1], it is impossible to obtain a complete analytical solution, therefore, a mechanism involving several steps for this reaction is suggested. A typical schematic of the cure-curve obtained from an ODR exhibits three main regions, scorch delay, cure and postcure. The regions, cure and postcure could be modeled using a two-step consecutive mechanism as follow.

$$A \overset{k_1}{\rightarrow} B \overset{k_2}{\rightarrow} C$$

The concentration of the intermediate, *B(t)*, can be defined by the following general differential equation:

$$\frac{dB(t)}{dt} = f(t) - k_2 B(t)$$

Considering B as a product, the second stage represents a reversion in postcuring. The analytical solution derived from the above equation is dependent on f(t) and thus with the type of reaction of the first step[2]. In this research, the order of zero, one, two (two modes with identical and different materials) and three order reaction were considered as the first step and the analytical solutions of this equation were investigated. Validity of reaction behavior in the first stage was evaluated by comparing the error of fitting the equations with experimental data. The order of reaction rate in the first step was evaluated by comparing fitting the obtained equations with experimental data.

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Paper code: 822

Ab initio study of fumagillin derivatives as potent anticancer compounds

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Fumagillin is a complex biomolecule and used as antimicrobial for treatment of parasites in honey bees [1]. Furthermore, it can block blood vessel formation by binding to an enzyme named methionine aminopeptidase 2 (MetAP-2). Thus, it is investigated as an angiogenesis inhibitor in cancer treatment [2]. Fumagillin can covalently bind from reactive epoxide (connected to cyclohexane) and histidine-231 in the active site of MetAP-2 and the other epoxide ring on the side chain is dispensable [3,4]. It is suggested that the fumagillin epoxide ring can play an important role in potent angiogenic activity [5]. Unfortunately the covalent binding of *fumagillin* to MetAP-2 requires the oxygen *protonation* of the *epoxied* on the side chain [6]. Thus designing new derivatives is pioneer. Herein designing novel derivatives of fumagillin was performed and the suggested biomimics were optimized with ab initio method and 3-21g basis set.

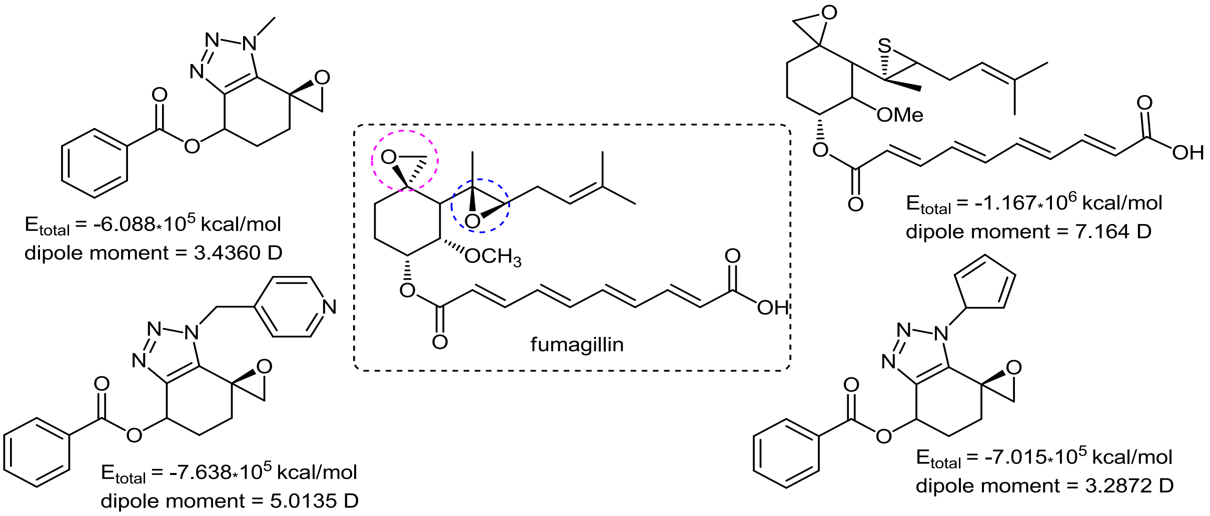

Fig. 1 chemical structures of fumagillin and some derivatives.

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Paper code: 827

Solubility of salicylic acid in ethanol, acetone and ethyl acetate solvents at temperature ranging from 298 to 313K

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In this study, the solubilities of salicylic acid in ethanol, acetone, ethyl acetate solvents at temperature ranging from 298 to 313 K were measured by gravimetrical method under atmospheric pressure. The results showed that the solubilities of salicylic acid increase with increasing temperature. The Modified Appellate equation, λh equation, Wilson equation and NRTL equation were used to correlate the solubility results [1-3]. That NRTL was the best model for correlation of the solubility data. All experimental solubility data and interaction parameters will be used as key information to chemical thermodynamic modeling and as reference in process/ product development.

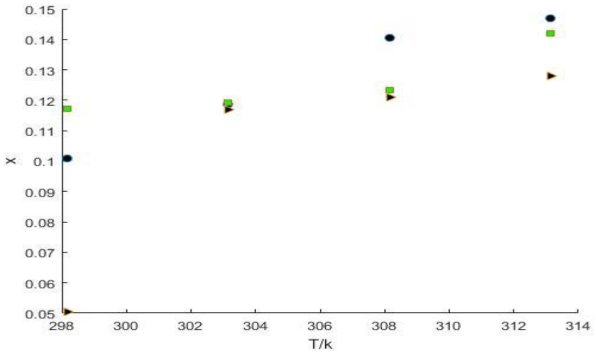

Fig.1. solubility of salicylic acid in pure solvents (●ethanol; ■ acetone; ►ethyl acetate)

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Paper code: 834

Thermodynamic modeling of the solubility of cholesteryl acetate and cholesteryl butyrate in supercritical carbon dioxide: Evaluation of cubic equation of states

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During the past 20 years, supercritical fluid (SCF) based technologies have been gaining an increasing attention through the academic and industrial communities due to its advantages. One of the most important parameter for any supercritical-based technologies is the knowledge of the solute solubility at different pressures and temperatures. But, due to several concerns e.g. time and expense, measuring the solubility of all compounds in wide ranges of temperature and pressure is not possible. The modelling of solid solubilities in supercritical fluids is usually performed by means of thermodynamic models based on cubic equations of state together with the use of correlations for estimating the solid properties .In this study, prediction of solubility of cholesteryl acetate and cholesteryl butyrate in supercritical carbon dioxide (scCO2) were performed using cubic equation of states. The Peng-Robinson equation of state (PR-EOS) with van der waals, Wong & Sandler and MHV2 mixing rules were employed to correlate the experimental data. Good correlations between the calculated and experimental solubility data were obtained. Results indicate that the combination PR equation of state with the WS mixing rule leads to more accurate results (AARD=9.95-10.55) compared with other the ones.

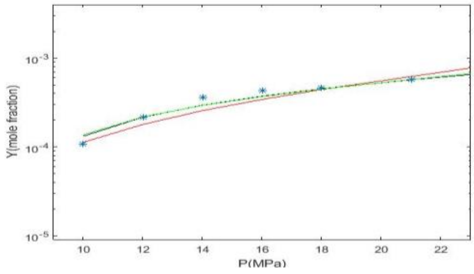

Fig.1 Cholesteryl butyrate solubility in supercritical carbon dioxide using Peng-Robinson equation of state (PR-EOS) with van der waals (red line), Wong & Sandler(green line) and MHV2 (black line) mixing rules at 308.15 K.

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Paper code: 854

Graphene Oxide Nanosheet as a Drug Delivery Vehicle For 5-Fluorouracil Anticancer Drug

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Due to the need to reduce the side effects of anticancer drugs, in the past two decades targeted drug delivery has been extensively developed. One of the most widely used anticancer drugs is 5-fluorouracil (5-FU). Because of unique properties of graphene oxide nanosheet (GONS) such as large surface area, chemical and mechanical stability, super conductivity and good biocompatibility, we investigated interaction between the drug and graphene oxide nanosheet as a drug delivery vehicle using density functional theory (DFT). Calculations were performed for 13 different configurations of adsorption 5-FU on GONS at the m05-2x/6-31G using G09 program. Interaction energies of complexes have been computed. Topologic parameters, NMR, NQR parameters and thermodynamic properties were evaluated for all of configurations. All the interaction energies were negative, revealing that the adsorption of the drug molecule was exothermic and energetically favorable. Bader's theory and Natural Bond Orbital (NBO) methods were also applied. Electronic density (ρ) and laplacian field ($\nabla^2\rho$) were obtained that values describe the strength and characteristic of a bond, respectively. The partially covalent adsorption of 5-FU was thermodynamically favoured onto the nanosheet. The overall stability of the most stable configuration contributed to the formation of more number of hydrogen bonds between the adsorbed drug molecule and the functional groups of nanosheet. The frontier molecular orbital analysis such as the highest occupied molecular orbital, the lowest unoccupied molecular orbital, energy gap (E_g) were also performed that helped to get a pictorial depiction to the charge delocalization within the nanosystems upon adsorption of 5-FU molecule. The results demonstrate GONS can be a good carrier for delivering of 5-FU through formation hydrogen bond and π–π stacking.

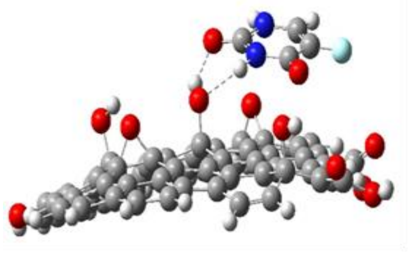

Fig. 1 One of the studied structures for different configurations of 5-FU molecule adsorbed on GONS

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Paper code: 862

Study of Structural and Electronic Properties of Doped group III (B, Al, Ga and In) on (6, 3) Chiral CNTs

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Since the discovery of carbon nanotubes (CNTs) by Iijima [1], because of their extraordinary structural, mechanical, chemical, physical, and electronic properties a great attention have been paid to them [2,3]. All DFT calculations were performed using Gaussian 98 program [4]. In the optimized structures by using B3LYP/6-31G* for the all sites. So this functional is chosen for band gap calculations. Also utilized to prepare and analyze the data and the density of states spectra are derived using Gauss sum program.

Structural and electronic properties including bond lengths, angles, dipole moments (µ), band gaps, NBO, NMR parameters of the isotropic and anisotropic chemical shielding parameters for the sites of various atoms were calculated using DFT for B, Al, Ga, In doped (6,3) Chiral CNTs . The calculations indicated that average bond lengths were as: C-In > C-Ga > C-Al > C-B. The dipole moments for B, Al, Ga, In doped (6, 3) Chiral CNTs structures show fairly large changes with respect to the pristine model, The delocalization energy corresponding to the transfer of electrons from the bonding orbital of C26 (σ) to antibonding orbital (σ*) of Al, In are lower than that of the energy corresponding to the transfer of electron from the bonding orbital of C26 (σ) to the antibonding orbital of Ga.

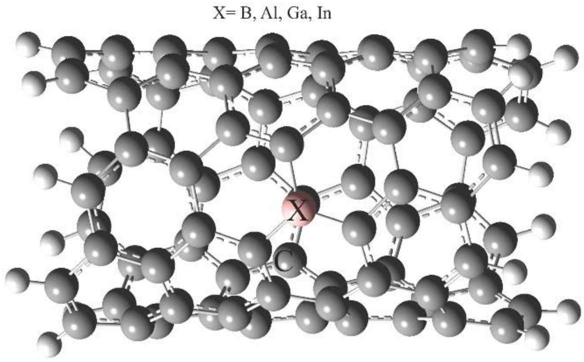

Fig. 1. Three-dimensional (3D) view of X-doped (X=B, Al, Ga, In) ON (6, 3) chiral CNTs.

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Paper code: 893

Chloropicrin sensor based on the doped-graphene: DFT studies

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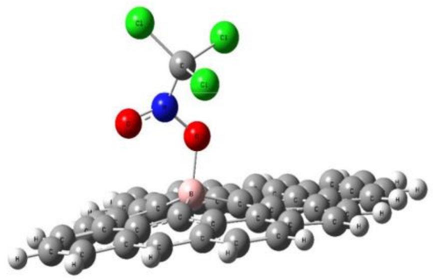
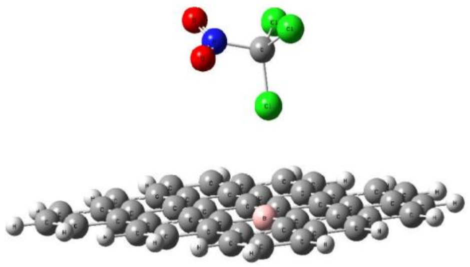
Chloropicrin (Cl_3CNO_2) one of the fumigants, is a powerful pesticide applied in agriculture to sterilize the soil [1]. It is also applied as a chemical warfare agent [2]. In the present study, the interaction between doped nano carbon and poisonous compound chloropicrin was investigated by using B3LYP method with Basis Set (BS) 6-31G (d) and Gaussian (09) software. The interaction between chloropicrin and nanoparticle can be carried out from different directions. At first different probabilites of chloropicrin interaction with nanoparticle were investigated. The total energy, interaction energy and bonding distance, HOMO and LUMO energy of chloropicrin on the surface of nanoparticle were explored. The obtained data was indicated that chloropicrin tends to interact from O side more than Cl side because in this case the quantity of total energy and interaction energy quantity is more stable. Also, the recovery time of these complexes was studied which indicated that interaction between born-doped nanosheet and chloropicrin can be the best sensor.





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Paper code: 900

The study of anaerobic reaction kinetics by comparing the removal of BOD and the production of biogas in the ECSB anaerobic reactor

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External Circulation Sludge Bed Anaerobic digesters convert Zar grain refinery waste (Effluent from High fructose corn syrup) into energy in the form of biogas. Most reactions that take place in ECSB reactor are slow and the consideration of the kinetics is important. ECSB reactor is a process of degradation of an organic matter in the absence of oxygen. There are four basic steps of ECSB reactor such as Hydrolysis, Acidogenesis, Acetogenesis and Methanogenesis. Important Parameters that Influence biogas Production is Temperature, pH, residence time, BOD loading and internal Circulation flow rate. The reaction rate r is the term used to represent between the reaction rate, concentration of the reagent and the order of reaction is given by the expression: $r=kC^n$ .In this paper, we study the reaction kinetics of anaerobic reactor and compare the production of biogas with removal BOD was investigated.

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Paper code: 931

Gold nanoparticles supported on magnetic Metal Organic Framework: kinetics and mechanism of alkenes oxidation by dioxygen

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Gold nanoparticles deposited on cubic metal organic framework (MOF) surface by homogeneous deposition precipitation method. For characterization of nanocatalysts several methods applied. XRD, SEM, TEM and TGA used for determination of morphology, texture properties, specific surface area and thermal stability. Au@MOF composites demonstrated high stability and six-time reusability was observed. TEM images showed that gold nanoparticles have proper dispersity on support surface. Metal organic framework provided high surface area for deposition of gold particles homogenously. The catalysts demonstrated high catalytic activity in aerobic oxidation of alkenes by oxygen under mild condition. Alkene oxides are the main product with more than 92% selectivity. The origin of catalytic activity of gold is not completely understood, but we think that the mail reason is interaction between the gold and support. Langmuir Hinshelwood mechanism is preferred according to concentration monitoring and kinetics investigation. Molecular oxygen adsorbed on surface radically and each oxygen radical play an effective role epoxide production.

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Paper code: 1016

Theoretical studies of 2,4,6-triarylpyridines, 1,8-dioxo-decahydroacridines and pyrido[2,3-d]-pyrimidine *via* an anomeric based oxidation

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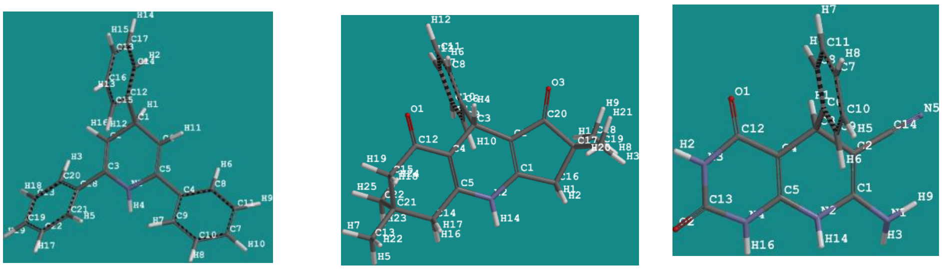
After introducing of anomeric effect (The Edward-Lemieux effect) by J.T. Edward in 1955 for the first time. Development of the topic of anomeric effect has a great attractive for chemists and biochemists [1]. A computational studies in the synthesis of 2,4,6-triarylpyridines, 1,8-dioxo-decahydroacridines and pyrido[2,3-d]-pyrimidine using $Fe_3O_4@TiO_2@O_2PO_2(CH_2)_2NHSO_3H$ and $[Fe_3O_4@SiO_2] (CH_2)_3S\text{-}SO_3H$ respectively as catalysts under solvent free conditions were occurred (Figure 1). The modeling and the appropriate calculations on the structures of the precursors, the transition states (TS) of the reactions, intermediates and the products have undertaken by DFT-B3LYP/6-31G* method [2]. The suggested anomeric based oxidation mechanism was supported by theoretical evidences. The theoretical study shows that the unpaired electron of the nitrogen atom within the 1,8-dioxo-decahydroacridines and pyrido[2,3-d]-pyrimid structures, showed favor resonance interaction toward electron withdrawing carbonyl groups. This phenomena do not allows the lone pair of the nitrogen atom to interact with the anti-bonding orbital of C-H bond in the 1,4- dihydropyridine moiety of 1,8-dioxo-decahydroacridine and pyrido[2,3-d]-pyrimidine. Therefore, the unaromatized 1,8- dioxo-decahydroacridines and pyrido[2,3-d]-pyrimid are the preferred structures than their corresponding aromatized products.



A *B* *C*

Fig. 1 The Structural of 2,4,6-triarylpyridines (A), 1,8-dioxo-decahydroacridines (B) pyrido[2,3-d]-pyrimidine (C).

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Paper code: 1027

Determination of the Stable Structures and Phase Transitions of Adamantane Nanoclusters by Molecular Dynamics Simulation

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Adamantane (C6H12) is the smallest possible of diamondoids with a highly symmetric and point group symmetry, *Td*. A cage like structure is formed with six CH2 and four CH groups giving rise to a molecular structure with four cyclohexane rings in chair form. Due to their six or more linking groups, they have found major applications as templates and as molecular building blocks in nanotechnology, drug delivery, drug targeting [1-3]. This report is aimed at studying the stable structure and phase transition behaviors of adamantane nanoclusters for further understanding of their structures and possibly building molecular devices with them. Applying ab initio calculation and molecular dynamics simulation method, we have been calculated and predicting the stable structure and phase transition of adamantane nanoclusters. We have chosen a large number of nanocluster systems consisting of 5, 10, 13, 15, 20, 25, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 85, 90, 95, 100, 105, 110, 115, 120, 125, 130, 135, 140 and 147 molecules of adamantane. We first performed (DFT) calculation to optimize initial geometric structure of adamantane. In order to find the equilibrium configurations and phase transition of the mentioned collections of the 5-147 molecules at every given temperature we performed MD simulation for these systems until they were equilibrated, and to gain phase transition of these nanoclusters we used the simulated-annealing procedure. Then their phase transitions have been obtained via ploting of diagram of the lindemann index versus temperature. As shown in Fig.1 (a) Increasing the number of particles does not increase the phase transition temperature regularly, and the higher phase transition temperatures are related to the symmetric structures of icosahedral belong to 13, 55,135 and 147 nanoclusters. Because the structures proceed by increasing the particles toward the formation of an icosahedral stable structure, hence some of the structures relative to their close family is more unstable and less phase transition point. In fact, this process is similar to the increase of electrons in a period of the periodic table, which evolve until the formation of the closed shell of noble gaseous. Fig.1 (b) and Fig.1(c) show the icosahedral stable structure for 13 and 55 nanoclusters.

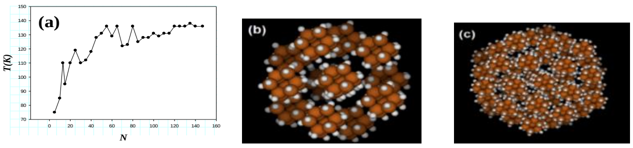

Fig.1. (a) Phase transition point versus the number of particles of nanoclusters. Icosahedral stable structure of (b) 13 and (c) 55 adamantane nanocluster

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Paper code: 1031

3D-QSAR Study of Human DHFR Inhibitors Based on GRIND Descriptors and Designing of New Inhibitors

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Dihydrofolate reductase (DHFR), an indispensable enzyme in the folate metabolism, converts dihydrofolate (DHF) to tetrahydrofolate (THF) in the presence of NADPH found in all organisms and regulates the level of THF in the cell. DHFR has been a validated drug target for the development of therapeutics for human cancer for decades [1]. Hence, there is an urgent need to identify and develop new inhibitors with high potency and selectivity relative to a specific species of DHFR. In this regard, 3D-QSAR modeling is one of the powerful computational methods employed in medicinal chemistry for deciding about the structure-activity relationship of new chemical compounds. In the present study, we studied a data set including 2, 4-diaminopyrimidine scaffold with the acetylenic linker to another substituted aryl ring with human DHFR receptor for 3D-QSAR modeling.

Moreover, we implemented a 3D-QSAR model based on GRIND descriptors on a series of 36 dihydrofolate reductase inhibitors. Genetic algorithm (GA) variable selection technique was applied to reduce the number of the molecular descriptors. The correlation between molecular descriptors and biological activity was established using PLS regression method. To assess the quality of the model, internal and external validations were implemented by different statistical procedures [2]. The results show that all the calculated external/internal validation parameters are in good agreement with acceptance criteria. New ligands were designed based on results of 3D-QSAR studies. Designed compounds were evaluated by docking and their biological activities were predicted by the 3D-QSAR model. Finally, ADME/Tox parameters of new ligands were predicted.

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Paper code: 1046

Theoretical Studies of the Electrostatic Attraction of the Regiochemical outcome on the 1,3-DC Reactions to the Medicine Ethisterone

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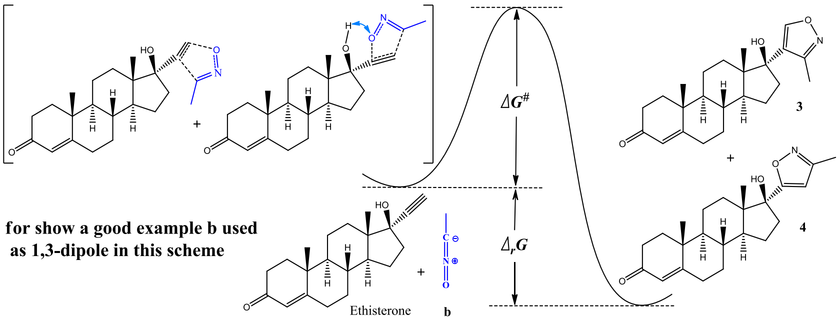
The different types of 1,3-dipolar cycloaddition (1,3-DC) reactions have been widely used in various fields. Based on the recent researches, Stereochemistry of these reactions is spotlight [1]. In this study, the theoretical aspects of the electrostatic attraction effect on the regioselectivity of the 1,3-DC reactions to Ethisterone was assessed which it is a progestin medication [2] as a dipolarophile white Nitrile imine, Nitrile oxide and Azide (**a-c**) as 1,3-dipoles. Cycloaddition of Ethisterone to each of **a**, **b** and **c** can lead to regioselective five-membered heteroaromatic rings, the 4- and/or 5-substituted, due to secondary effect between the hetro atom of 1,3-dipoles and the hydroxy group in Ethisterone. These heteroaromatic rings were widely used as an important role in various biochemical processes [3]. In this study, the (1,3-DC) reaction of Ethisterone with **a**, **b** and **c** were utilized to produce the five-membered aromatic heterocyclic rings, i.e. pyrazole, isoxazole and triazole derivatives. The whole 1,3-dipole showed rewarding results for regioselectivity to produce **2**, **4** & **6** but the selectivity was clearly more obvious for **a** & **b.** Data were calculated and obtained by DFT-B3LYP/6-31G* method.



for show a good example b used as 1,3-dipole in this scheme

Structur & name of 1,3-dipoles				1,3-dipoles	Products
$Ph—C≡\overset{\oplus}{N}—\overset{\ominus}{N}—Ph$	$\longleftrightarrow$	$Ph—\overset{\ominus}{C}=\overset{\oplus}{N}=N—Ph$	Nitrile imine	a	4- & 5-substituted pyrazole derivatives; **1 , 2**
$—C≡\overset{\oplus}{N}—\overset{\ominus}{O}$	$\longleftrightarrow$	$—\overset{\ominus}{C}=\overset{\oplus}{N}=O$	Nitrile oxide	b	4- & 5-substituted isoxazole derivatives; **3 , 4**
$N≡\overset{\oplus}{N}—\overset{\ominus}{N}—$	$\longleftrightarrow$	$\overset{\ominus}{N}=\overset{\oplus}{N}=N—$	Azide	c	4- & 5-substituted triazole derivatives; **5 , 6**

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Paper code: 1049

VX gas sensor based on the doped-nano cage: DFT studies

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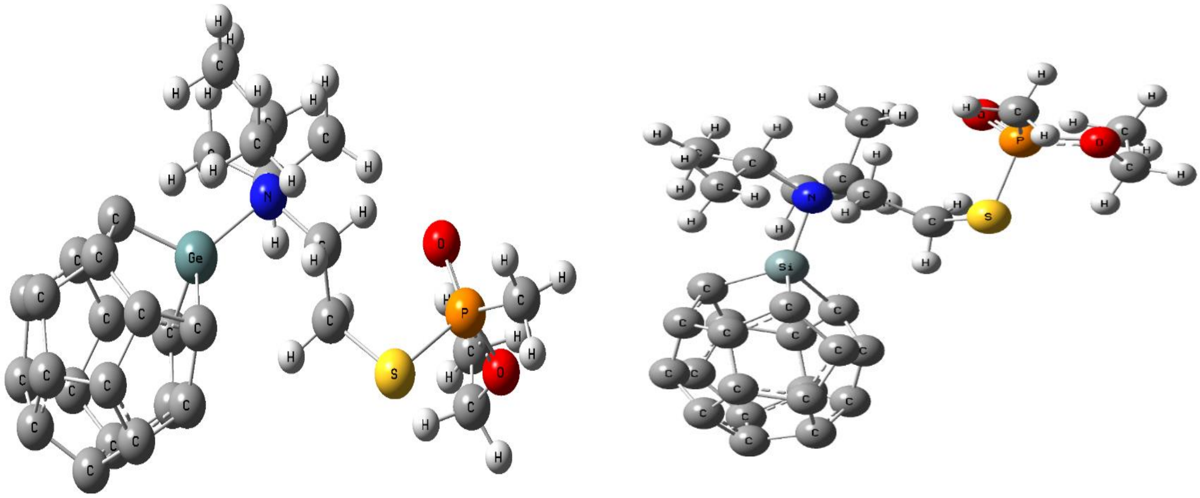
In the present study, the interaction between doped carbon nano cage and VX gas was investigated by using B3LYP method with basis set 6-31G* and Gaussian (09) software. The interaction between VX gas and nanocage can be carried out from different directions. At first, different probabilites of VX gas interaction with nanocage was investigated. The total energy, interaction energy and bonding distance, HOMO and LUMO energy of complex (VX- nanocage) was obtained. The obtained data was indicated that VX gas tends to interaction from oxygen atom more than sulfur side and nitrogen side because in this case total energy and interaction energy quantity are more negative. Also, the recovery time of these complexes were studied and discussed.



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Paper code: 1053

Mechanical Properties of Graphene, Silicen, Germanen and mixtures of them

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The mechanical properties of graphene and similar structures i.e. silicone and germanium nanosheets have been studied in this article. All calculations were performed with Quantum Espresso Code. The ultrasoft pseudo potential based on PBE functional was employed to calculate the properties of structures. All structures were optimized and the energy of structures as function of extered stress was calculated. The Yang modulus of all structures were calculated and it was shown that the graphene (C-C structure) and germanene (Ge-Ge structure) have higher and lower Yang modulus respectively. Other structures had values between these two cases. It was seen that the Yang modulus reduced by increasing the volume of unit cell. In Figure 1, the Yang modulus is plotted as function of unit cell volume.

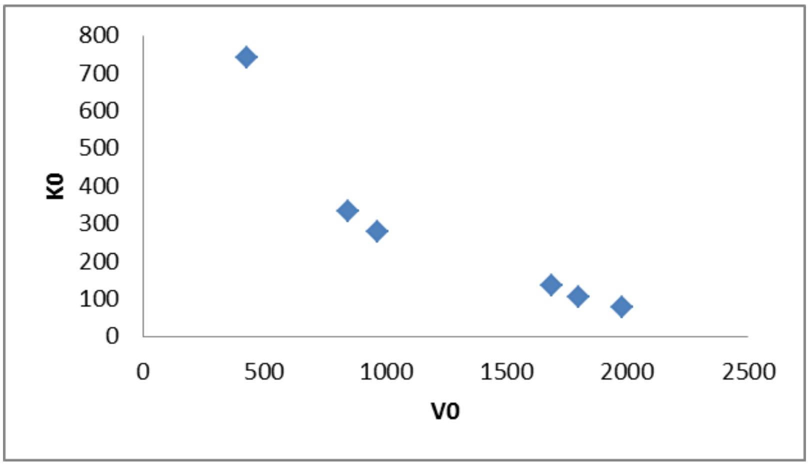

Figure1. The calculated Yang modulus as function of unit cell volume

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Paper code: 1062

Effect of alkyl chain length on aggregation behavior of amino acid ionic liquid surfactant by molecular dynamics simulation

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Amino acid ionic liquids (AAILs) with the amino acids as anion or cation have attracted a considerable attention in green chemistry and environmental engineering. The ion pairs possess good biodegradability and biocompatibility that may shed light on the synthesis of specialized solvents for medical, biological, and pharmaceutical sciences [1]. The effect of alkyl chain length on the structure of cation aggregation in $[C_nH_{2n+2}NO_2][C_4H_6NO_3]$ AAIL was studied by molecular dynamics (MD) simulation at different alkyl chain lengths (n= 8, 12, and 16) at 300 K. The anion is N-acyl glycinate and the cation is n-alkyl betaine.

The radial distribution functions (RDFs) of cation-cation, cation-anion and anion-anion demonstrated that the position of RDF for three alkyl chain lengths is almost similar because of the same interactions in spite of different heights due to the interaction strength. In addition, the root-mean-square deviation (RMSD) was studied. Figure 1 indicates RMSD for micelles. As the figure shows the AAILs follow n8 > n16 > n12 trend that demonstrates dodecyl betaine N-acyl glycinate is the most stable micelle while octyl betaine N-acyl glycinate is the least stable [2].

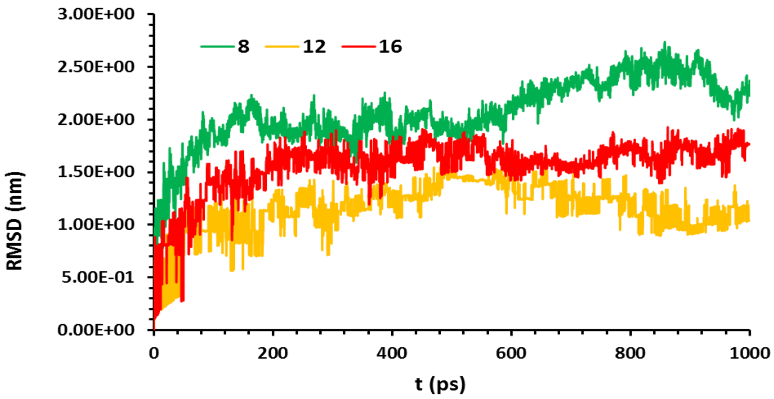

Figure 1: RMSD compare for octyl (green), dodecyl (yellow), and hexyldecyl (red) betaine N-acyl glycinate AAILs.

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Paper code: 1071

Theoretical studies of pyramidality of nitrogen in (2-Cyclohexyl-vinyl)-methyl-amine, (2-Cyclopentyl-vinyl)-methyl-amine, (2-Cyclobutyl-vinyl)-methyl-amine and (2-Cyclopropyl-vinyl)-methyl-amine

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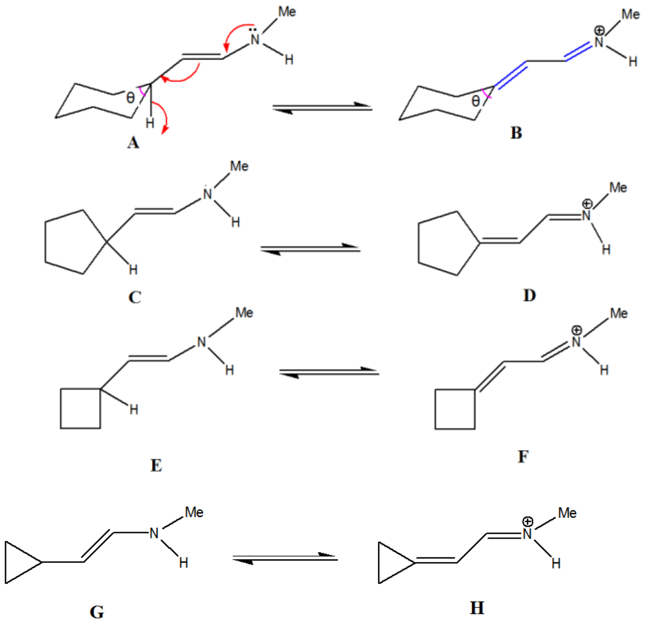
The structures **A-H** were optimized at the DFT-B3LYP/6-31G* theory level.[1] All the calculations were carried out using the *Spartan '10* package.[3] Pramidality of nitrogen, the energetic and geometric parameters (bond length (Å), bond angle (°) and torsional angle (°)) of the structures were undertaken using a DFT-B3LYP/6-31G* method. Theatrical study of ^{1}HNMR and IR spectral have calculated. In Figure 1 the stability and bond angle have compared. In (2-Cyclopentyl-vinyl)-methyl-amine (C) high tendency of resonance nitrogen has seen.



Stable stracture	bond angle
A	$\theta_B > \theta_A$
D	$\theta_D > \theta_C$
E	$\theta_F > \theta_E$
G	$\theta_G > \theta_H$

Fig. 1 The structures **A-H,** the stability and bond angle have compared

References

[1] All of the calculations were performed by: *Spatran '10*-Quantum Mechanics Program: (PC/x86) 1.1.0v4. **2011**, Wavefunction Inc., USA.

Paper code: 1079

Corrosion inhibition behavior of collidine on aluminium in hydrochloric acid solution

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Corrosion is the destructive attack of a metal or alloy chemically or electrochemically by its environment which leads to loss of useful properties of materials [1,2]. Inhibitors are compounds that reduce the rate of corrosion by adsorption on the metal surfaces [3].

In this research the inhibitory effect of 2,4,6-collidine on aluminum corrosion in 1M hydrochloric acid solution was studied using polarization curves. The values of potentiodynamic polarization parameters such as corrosion potential (E_{corr}), corrosion current density (i_{corr}), anodic and cathodic Tafel slopes (β_a, β_c) were obtained from the polarization curves through extrapolation method. As the results shown, the addition of collidine decrease the corrosion current density. The results show that, E_{corr} shifts to positive direction which is an indication that inhibitor molecule is more adsorbed on the anodic sites, resulting in an inhibition of the anodic reaction.

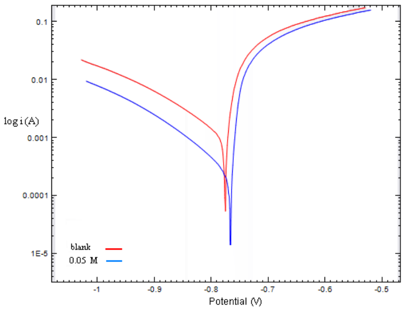

Fig. 1. Potentiodynamic polarization curves observed for pure aluminum in HCl solution in absence and presents of 2,4,6-collidine

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Paper code: 1084

A Computational Study of all mono-chlorostyrenes

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The optoelectronic properties of the electron-donor polymer are primarily determined by the choice of the conjugated backbone, the solubility is predominantly determined by the position, length and makeup of the alkyl side chains. Both the polymer backbone and the alkyl side chains device efficiency and molecular packing structure, especially in donor–acceptor copolymers, which contain an ordered sequence of different subunits [1]. The active layer in organic photovoltaic bulk heterojunction devices is composed of a blend of π-conjugated, electron-donor polymers and electron-acceptor molecules [2]. The objective of the present research is to study the electrical and structural properties of all mono-chlorostyrenes. All of the possible of mono-chlorostyrenes studied in this work are presented in Fig. 1.

1:	Z=W=X=T=R=Q=L=H	Styrene
2:	Z=W=T=R=Q=L=H,X=Cl	1-chloro-2-vinylbenzene
3:	Z=W=X=R=Q=L=H,T=Cl	(Z)-1-chloro-3-vinylbenzene
4:	Z=W=X=T=Q=L=H,R=Cl	1-chloro-4-vinylbenzene
5:	Z=W=X=T=R=L=H,Q=Cl	1-chloro-3-vinylbenzene
6:	Z=W=X=T=R=Q=H,L=Cl	(Z)-1-chloro-2-vinylbenzene
7:	Z=X=T=R=Q=L=H,W=Cl	1-(1-chlorovinyl)benzene
8:	W=X=T=R=Q=L=H,Z=Cl	(Z)-1-(2-chlorovinyl)benzene

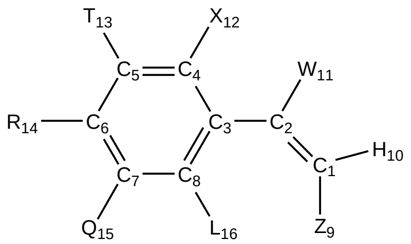

Fig. 1 All possible mono-chlorostyrene studied in this work.

Structures of representative mono-chlorostyrenes were optimized using B3LYP/6-311++G levels of theory with the G09 package of programs implemented on a Pentium–PC computer with a 7300 MHz processor [3]. The vibrational analysis showed that all structures correspond to local minima in potential energy surface. Values of dipole moment has been calculated and analyzed. The analysis of these data showed that the (Z)-1-chloro-3-vinylbenzene has the highest value of the dipole moment (with 2.4202 Debye), and it can be suggested that this molecule has high solubility in polar solvents. The (Z)-1-(2-chlorovinyl)benzene (Monomer **8**) has the lowest HOMO-LUMO gap among all monomers. The electrochemical stability of 1-chloro-3-vinylbenzene is greater than other compounds, and also the zero-point energy for this molecule is greater than other molecules. The analysis of data showed that the double bonds in the (Z)-1-(2-chlorovinyl)benzene are more delocalized.

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Paper code: 1086

Comparative analysis on all di-chlorostyrenes; a DFT-B3LYP study

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The use of electrically conducting polymers in electro-chromic devices, as materials that possess the ability to reversibly change color by altering redox state, has emerged. Many conjugated polymers are colored in the neutral state since the energy difference between the σ-bonding orbitals and the σ^* anti-bonding orbitals (valence band) lies within the visible region [1]. The conductivity study and the electrochemical polymerization of conducting compounds (or monomers) is an interesting matter for Scientifics in the world. Electrically conducting polymers have been considered for numerous applications including charge dissipation coatings, organic thin-film transistors, and conducting textiles. All of the possible of di-chlorostyrenes studied in this work are presented in Fig. 1.

1:	Z=W=X=T=R=Q=L=H	Styrene
2:	Z=W=R=Q=L=H,X=T=Cl	1,2-dichloro-3-vinylbenzene
3:	Z=W=T=Q=L=H,X=R=Cl	2,4-dichloro-1-vinylbenzene
4:	Z=W=T=R=L=H,X=Q=Cl	1,4-dichloro-2-vinylbenzene
5:	Z=W=T=R=Q=H,X=L=Cl	1,3-dichloro-2-vinylbenzene
6:	Z=W=X=T=R=H,Q=L=Cl	(Z)-1,2-dichloro-3-vinylbenzene
7:	Z=W=X=T=Q=H,L=R=Cl	(Z)-2,4-dichloro-1-vinylbenzene
8:	Z=W=X=R=Q=H,L=T=Cl	(Z)-1,4-dichloro-2-vinylbenzene
9:	Z=W=X=R=L=H,Q=T=Cl	1,3-dichloro-5-vinylbenzene
10:	Z=W=X=T=L=H,Q=R=Cl	1,2-dichloro-4-vinylbenzene
11:	Z=W=X=Q=L=H,T=R=Cl	(Z)-1,2-dichloro-4-vinylbenzene
12:	Z=T=R=Q=L=H,W=X=Cl	1-chloro-2-(1-chlorovinyl)benzene
13:	Z=X=R=Q=L=H,W=T=Cl	1-chloro-3-(1-chlorovinyl)benzene
14:	Z=X=T=Q=L=H,W=R=Cl	1-chloro-4-(1-chlorovinyl)benzene
15:	Z=X=T=R=L=H,W=Q=Cl	(Z)-1-chloro-3-(1-chlorovinyl)benzene
16:	Z=X=T=R=Q=H,W=L=Cl	(Z)-1-chloro-2-(1-chlorovinyl)benzene
17:	X=T=R=Q=L=H,W=Z=Cl	1-(1,2-dichlorovinyl)benzene
18:	W=T=R=Q=L=H,Z=X=Cl	1-chloro-2-(2-chlorovinyl)benzene
19:	W=X=R=Q=L=H,Z=T=Cl	1-chloro-3-(2-chlorovinyl)benzene
20:	W=X=T=Q=L=H,Z=R=Cl	1-chloro-4-(2-chlorovinyl)benzene
21:	W=X=T=R=L=H,Z=Q=Cl	(Z)-1-chloro-3-(2-chlorovinyl)benzene

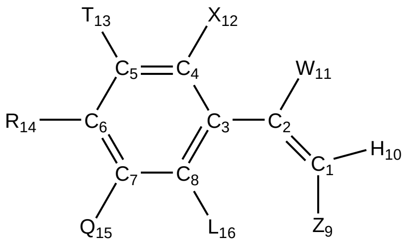

Fig. 1 All di-chlorostyrenes studied in this work.

The structural and electrical properties of all di-chlorostyrenes have been studied using B3LYP method with 6-311++G basis set. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies, HLG (the gap between HOMO and LUMO) and size of dipole moment vector, total electrical energies, enthalpies, entropies, electronic, Gibbs and Zero-Point energies, and also IR spectra have been calculated and studied in this work. The analysis of these data showed that the 1-chloro-4-(2-chlorovinyl)benzene has the highest value of the dipole moment (*i.e.* 2.9696 D). The analysis of data showed that the 1-chloro-3-(2-chlorovinyl)benzene has the lowest HLG and highest delocalization double bonds.

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Paper code: 1112

The effects of sodium dodecyl sulphate on the behaviour of glucose oxidase enzyme

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Glucose oxidase (GOx) is a flavoenzyme having applications in medical industries. GOx has found in the food industry for the glucose removal from dried eggs, for the removal of oxygen from fruit juices, for the production of gluconic acid, and as a source of hydrogen peroxide in food preservation [1]. Although it was observed that sodium dodecyl sulphate (SDS) can change the structure and function of protein, details of this interaction are not properly known yet. We treated GOx as dimer-active enzyme in the presence of various concentrations of SDS and seen that the enzyme become inactive at high concentration (25mM) of SDS. These experimental results are in agreement with recently published researches. To find a possible mechanism, simulation of the enzyme was performed in the presence of 25mM of SDS. MD simulations were carried out by GROMACS 5.0.4 with a GROMOS 43a1 forcefiled [2]. Parameters for flavin adenine dinucleotide (FAD) coezyme, which is the active center for GOx, were taken from the work of van den Berg et al [3]. RMSD values showed that the enzyme has an unstable conformation upon treatment with SDS. RMSF values demonstrated that the residue fluctuations for SDS-treated GOx were higher than those in native enzyme which such a situation is usually observed in the unstable structure. According to MD analysis, treatment of GOx with SDS may induce unfolding of the native dimeric enzyme, releasing FAD molecule from the enzyme and leading to a significant decrease in the enzyme activity. To the best of our knowledge, this is the first study that bears detailed structural mechanism about the SDS effects on multimeric macromolecule.

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Paper code: 1113

Can Prion and Aptamar Connect Stabemeter?

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Prion diseases are caused by misfolding and aggregation of the prion protein (prp). The native form of prp (denoted as prp^c) is innocuous and expressed ubiquitously in all mammalian cells. However, prp^c can misfold into prp^{sc}, which can then self-aggregate and form soluble oligomers that cause neuronal cell death. Misfolding is rare, but it can be induced by an acidic pH environment.

All mammalian prp^c structures consist of a structured C-terminal domain with three helices (HA, HB and HC), two short β-strands (S1 and S2) and a flexible N-terminal domain. Although no high resolution structure for prp^{sc} is available, low resolution experimental methods have suggested that the native prp^c converts from an α-helical rich protein (47% α-helix, 3% β-structure) to the β-sheet rich prp^{sc} (43–54% α-helix, 17–30% β-structure)(1). So, the key to the illness here is to turn the α-helix into a β-structure on the part of the Prion protein biomagnetic sensor or biosensor is the name of a group of sensors designed to react only to specific target. One of the many types of biosensors is aptamer. Aptamers are oligonucleotides of the single-stranded molecules of RNA and ssDNA, or peptide molecules, whichcan be linked to their goals with high specificity and desire (2). Depending on the mode of Prion's disease and the inability to identify this disease agent in the usual way the operating agent is the best option for diagnosis of aptarms. Prion's proprietary aptamer consists of two quadrants of G. In this study, the connection between aptamer and the part of prion has been investigated using molecular dynamics (MD) simulation. A system consisting of aptamar has RNA G-Quadruplexes G-RNA from the protein data bank and is selected with a selection of Prion proteins MD simulations were performed during 100 ns time interval by GROMACS 5.0.2 with Charmm forcefiled. The results showed that the attachment of the periotic part to the aptemer increased the intermediate surface of the two parts of the aptamer, which resulted in the stabilization of the aptemer caused by the connection of the Prion.Root mean square deviation and fluctuation calculations indicated that Aptamer binding to prion resulted in smaller prion responsible for the choice of unusual behavior .Structural changes were not observed in the structure of RNA, and only the connection of the Prion resulted in greater opacity.

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Paper code: 1116

Structure and vibrational analysis of copper (II) heptane-3,5-dione

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β-diketonates of different metals have been used in the preparation of some kinds of catalysts [1,2]. In this study, the structure and vibrational spectra of copper (II) heptane-3,5-dione, $Cu(HPD)_2$, were investigated by density functional theory (DFT) studies. The molecular equilibrium geometry and vibrational wavenumbers of this complex were calculated at the B3LYP/6-311G* level of theory. The calculated geometrical parameters and vibrational wavenumbers were compared with those observed experimentally in the complex and the ligand spectra [3]. The calculated vibrational wavenumbers are in good agreement with the experimental results. Therefore, this level of theory is adequate enough for predicting the structure and vibrational spectra of the complex.

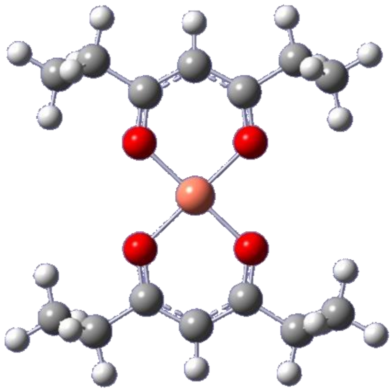

Fig. 1 The structure of $Cu(HPD)_2$

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Paper code: 1117

Electron Transport Properties of Defected Carbon Atomic Chains between Nano Capsule Electrodes

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Molecular junctions based on single molecules have attracted much attention due to the potential of molecular electronic devices such as molecular switches, memory devices, or field effects transistors. Electron transport properties of carbon atomic chains (CACs) bridged with the different defect in carbon atoms such as B and Si atoms covalently connecting to (5,5) capped carbon nanotube leads are investigated using the first-principles calculations based on non-equilibrium Green's functions conjugated with the density-functional theory. The pristine and defected CACs (with boron and Silicon atoms) with the same length of even carbon chains were considered. The I-V characteristics were calculated for junctions containing carbon chain with length six carbon atoms. As shown in Fig. 1, the higher voltage applied to the left and right electrodes, raises the current. The carbon atomic chains exhibit negative differential resistance behavior under very low biases for pristine C6 chain. Also, zero-bias transmission peaks for scattering state obtained for the C6 junction and the height of transmission peak was decreased steadily with increasing the bias.

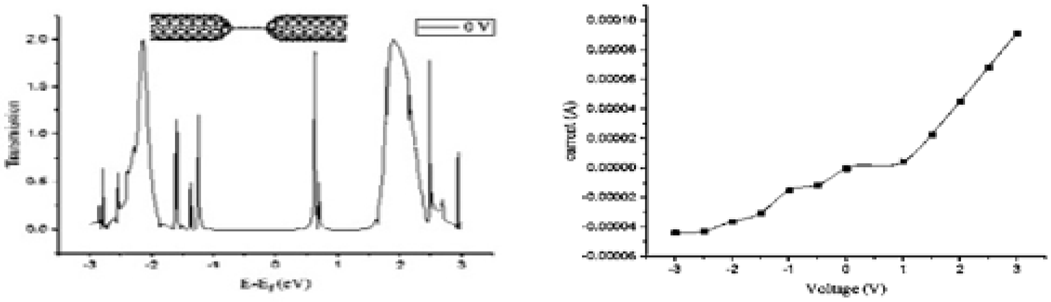

Fig. 1. Zero-bias transmission and I-V curves of studied device.

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Paper code: 1122

Synthesis, Structure and vibrational assignment of bis(3-amino-1-phenyl-2-buten-1-onato) nickel(II)

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Recently, many studies have been carried out on Cu(II) and Ni(II) β- ketoamine complexes because of the special properties and applications of these complexes [1-3]. Particularly, the Ni(II) complexes bearing N,O mixed ligands have been used for generation of petroleum and natural gas[4] and biological fluids[5, 6]. in the present article the full assignment of the vibrational spectra has been given and the calculated vibrational frequencies are compared with those observed experimentally.

The APBO ligand, 3-amino-1-phenyl-2-buten-1-one, was synthesized according to literature [7] and was added by stirring to an alcoholic solution of nickel (II) acetate. The IR spectra were recorded on a Bomem B-154 Fourier Transform spectrophotometer in the region 4000–600 cm^{-1} by averaging 20 scans with a resolution of 2 cm^{-1}. Geometrical calculations were performed using Gaussian 09 [8] program. The full geometry optimization was performed at hybrid density functional B3LYP using 6-311G basis set. The vibrational frequencies were also calculated at B3LYP/6-311G* level of theory.

The results showed that the Ni-O and Ni-N bond lengths in this complex are shorter and therefore stronger than Cu-O and Cu-N in Cu(APBO)$_2$[3] The fundamental wavenumbers were compared with the experimental ones.

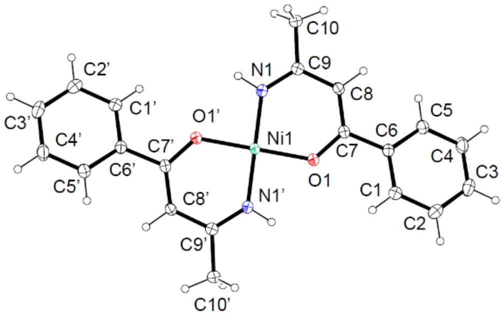

Fig. 1 The X-Ray geometries of Ni(APBO)$_2$.

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Paper code: 1129

Investigation of effective factors in separation process with ATPS and PEG 8000

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The process of liquid-liquid extraction is one of the most important separation

Investigation of malic acid ability to partition in polymer/salt aqueous two phase systems has been the main goal of this research. So, three different temperatures 27, 32 and 40ºC were chosen and three different salts with PEG8000 in each temperature were investigated. Two parameters of distribution coefficient and percentage of extraction were calculated for the distribution of malic acid. The results showed that disodium hydrogen phosphate had the highest distribution coefficient and percentage of extraction at 27℃. processes. In the last half century, researchers have focused on liquid-liquid extraction systems for the recovery and purification of biomolecules. Conventional liquid-liquid extraction methods include the use of organic solvents. For example, they are not suitable for the recovery of biomolecules, because most organic materials change their nature. Indeed, aqueous two-phase systems, which are formed by combining two incompatible polymers, or a polymer and a salt in water, are formed due to the high percentage of water in both mild environmental phases for biomolecules. Also, due to selectivity in the separation of biomolecules, stability in a wide range of non-toxicity, non-flammability, continuity of operation, high efficiency, low energy and time have become especially important in recent years. Aqueous two-phase systems, also known as one of the effective methods in the process of protein regeneration for the industrial production of drugs and proteins. The purpose of this study was to investigate the distribution of malic acid in aqueous two-phase systems.

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Paper code: 1136

The effect of temperature on cation aggregation in dodecyl betaine N-acyl glycinate amino acid ionic liquid: Molecular dynamics simulation investigation

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The effect of temperature on the cation aggregation in dodecyl betaine N-acyl glycinate amino acid ionic liquid (AAIL) surfactant was studied using molecular dynamics (MD) simulation. The structure of the AAIL is shown in Figure 1.

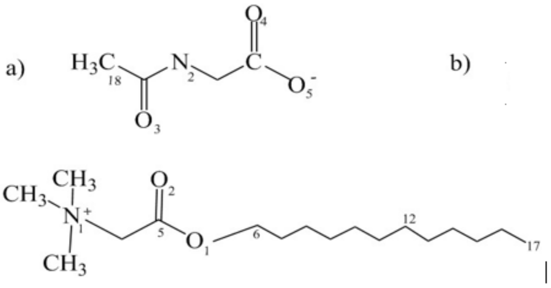

Fig. 1 Schematics of a) N-acyl glycinate anion and b) dodecyl betaine cation

Radial distribution function (RDF) for cation-cation, cation-anion, and anion-anion, mean square displacement (MSD) for cation, anion and water, root mean square displacement (RMSD) for micelle and root mean square fluctuation (RMSF) for cation and anion at three temperatures (290, 300 and, 310 K) were applied to obtain the results. RDF plots were almost the same because of similar interactions. The MSD decreases with temperature for cation, anion, and water since the mobility increases with increasing temperature. In addition, anion-water, cation-water, cation-anion, and anion-anion interactions become weak with temperature enhancement. RMSD plots for micelle at 290 and 300 K were almost the same though a significant increase is observed at 310 K indicating the micelles are less stable at 310 K according to Jana et al. results [1]. Moreover, RMSF of both cation and anion increased considerably at 310 K that confirmed the less rigidity at the highest studied temperature [2]. Based on the results, micelle stability is dependent on the temperature and the structural properties confirm the variation of the anion and cation positions.

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Paper code: 1151

Study of thermodynamic properties and intermolecular forces in the formation of aqueous aggregation of Arachidonic acid

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Arachidonic acid is a 20-carbon fatty acid with four non-conjugated cis-double bonds. This fatty acid participates in cell signaling as a secondary messenger [1,2]. The thermodynamic properties and intermolecular forces of its molecular aggregation were estimated by the GROMACS software [3] with gromos96 43a1 force field at 300 K. Arachidonic acid solvation in water occurs during two processes: 1) hydration of every molecule individually and then 2) formation of molecular aggregation.

Changes in both enthalpy and entropy are negative (Fig. 1), indicating that the formation of molecular aggregates has a dominant contribution. The formation of hydrogen bonding between the polar heads of the molecules as well as between the polar heads of the molecules and water molecules plays an important role in the formation of the micelle. The number of hydrogen bonds is seven for each molecule. In addition, polar interactions between polar heads of molecules and also van der Waals interactions between hydrophilic tails play important roles in the formation of its micelle.

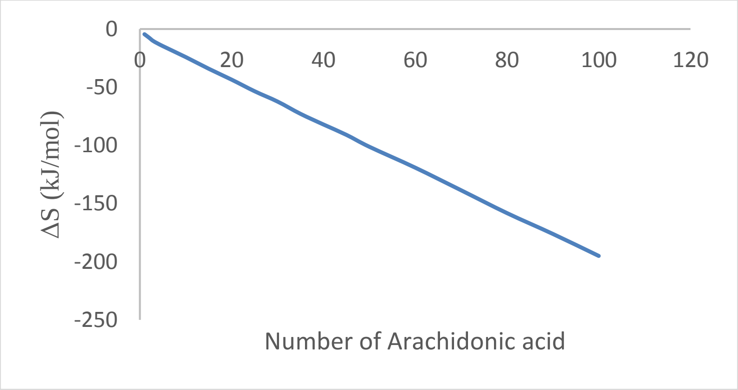

Fig. 1: Entropy changes of hydration and formation of molecular aggregation of Arachidonic acid.

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Paper code: 1154

Investigation of the Formation of Arachidonic Acid Micelle in Aqueous Medium

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Arachidonic acid is a 20-carbon fatty acid that plays the role of hormone in the human body. Due to the hydrophobicity of the nonpolar tail, it forms molecular aggregates or micelles in aqueous medium [1,2]. Using the Gromacs software [3] with the Gromos96 43A1 force field, formation of arachidonic acid aggregates was studied in aqueous medium at 300 Kelvin. This study has been conducted on molecular systems of up to 100 molecules. The shape of the molecular aggregates was analyzed by the VMD software.

In the low number, the arachidonic acid molecules are mostly dispersed and far apart, in addition to a few binary and triple complexes (Fig. 1A). By increasing the concentration of arachidonic acid, the formed micelles exhibit volumetric growth, indicating an increase in the number of arachidonic acid molecules per micelle. The system consists of a large number of small micelles up to 50 molecules. The number of micelles decreased in the presence of more than 50 molecules (up to 100 molecules) and volume of remaining micelles increased (Fig. 1B). It is indicating that smaller micelles added together and made larger micelles.

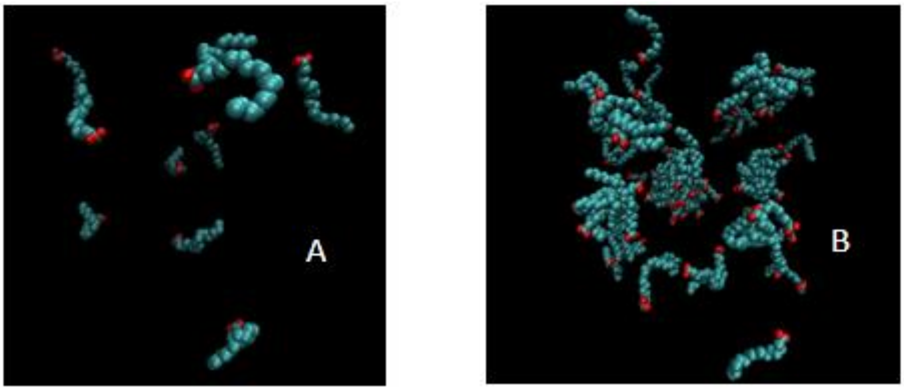

Fig. 1: The shape of Arachconic acid aggregates, 10 molecules (A) and 70 molecules (B).

References

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[3] D. Van Der Spoel, E. Lindahl, B. Hess, G. Groenho, A. E. Mark, H. J. Berendsen, *J Comput Chem*. 2005, 26, 1701.

Paper code: 1156

Study of inter- and intra- molecular interactions on conformational stability of *N*-(1,3-thiazol-2-yl) benzamide

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For many years, the eight-member hydrogen bonds [1] in two strands of DNA (responsible for the transfer of hereditary properties) have been the center of attention of chemistry and biology scientists. On the other hand, there is a structure of N- (1,3-thiazol-2-yl) Benzamide in many drugs. In the previous studies that proved the existence of a dimmer form in the crystalline structure of N-(1,3-thiazol-2-yl) Benz amide, we first succeeded in considering possible AD conformers, and then through computational methods such as B3LYP, PBEPBE and Wb97XD We examine the relative stability of the proposed conformers. In this study, the effects of dipolar-dipolar interactions and hydrogen bonds [2] were investigated and we succeeded in extending the obtained calculations to an acceptable level along the experimental results. In addition to the above factors, the presence of a non-bonded interaction between the two atoms of oxygen and sulfur in form A, which is certainly a major contributor to the stability of the A, is determined by the presence of two atomic oxygen and sulfur have electrostatic interaction. This and over the past years has repeatedly been attempting to reach the results confirming this interaction, but this important was not yet available, and we were able to prove this interaction for the first time and determine the magnitude of this interaction in terms of energy. Verification of electrostatic interaction oxygen and sulfur including ELF, QTAIM, NBO and NCI.

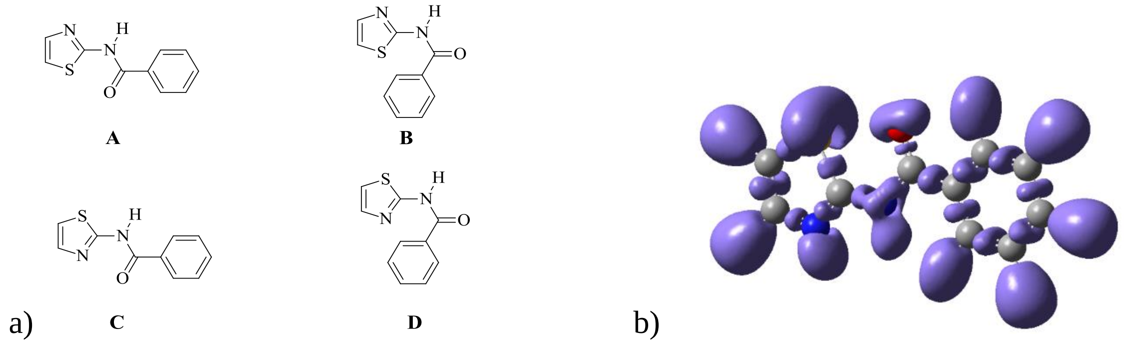

Fig. 1 On the basis of the van der Waals radius, the two oxygen and sulfur atoms should diverge each other, while you can see here on a plate. a) four possible conformers. b) ELF analysis for A conformer

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Kinetics and thermodynamics of Rhodamine B adsorption by $La_{0.7}Ca_{0.3}MnO_3$

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calcium doped lanthanum manganite (LCMO) nanostructure was synthesized via the mild hydrothermal method. Properties of synthesized material were characterized by X-ray diffraction, Fourier Transform Infrared Spectroscopy, Field Emission Scanning Electron Microscopy. The results of XRD and FTIR analyses show that the as-prepared material is composed of single-phase structure without impurity and nanorod morphology with a mean length of 126.8 nm.

The present study aims at exploring the potential of the LCMO, for the removal of cationic Rhodamine B (RhB) dye from aqueous solution [1, 2]. Impact of pH, adsorbent dosage, dye concentration and contact time have been assessed during adsorption. About 80% removal has been attained with 0.5 g/L of adsorbent over the studied system. Thermodynamic and kinetic studies, followed by second order kinetic model, directed towards the endothermic nature of adsorption. The results obtained from batch experiments were modelled using Langmuir and Freundlich isotherm and were analysed on the basis of R^2. Langmuir isotherm was found to be best fitted to the experimental data with high values of R^2. Adsorption study revealed the affinity of LCMO for the dye ions present in waste water, introducing a novel adsorbent in field of waste water treatment..

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Novel MIL-88A(Fe)@g-C_3N_4 core@shell nanocomposites: fabrication, characterization and application as a photocatalyst

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Novel MIL-88A(Fe)@g-C_3N_4 core@shell nanocomposite was successfully synthesized by a facile hydrothermal method. Photocatalytic performances of prepared samples were investigated for the degradation of Methylene Blue (MB) dye under visible light irradiation. The characterization results showed that the MIL-88A(Fe) particles were successfully dispersed on the surface of g-C_3N_4 with core@shell structure. Photocatalytic results demonstrated that the MIL-88A(Fe)@g-C_3N_4/H_2O_2 exhibited excellent visible light photocatalytic performance. Hydroxyl radicals ($^{\cdot}$OH) are generated via decomposition of H_2O_2 under visible light can significantly enhance the degradation rate of MB molecules. Meanwhile, the studies of catalytic activity indicated that the high surface area and conductive properties of MIL-88A(Fe)@g-C_3N_4 with core@shell structure as well as ROS specie formation simultaneously lead to the enhanced photocatalytic activity of MIL-88A(Fe)@g-C_3N_4 composite**.** Additionally, studies performed using radical scavengers showed the main reactive species in the photocataytic reaction for MB degradation. Photocatalytic mechanism for MB degradation over MIL-88A(Fe)@g-C_3N_4 was also proposed. Heterojunctions were formed in MIL-88A(Fe) and g-C_3N_4 exhibiting electron-hole separation and therefore improved performance for MB degradation. Moreover, the formation of hydroxyl radicals in the presence of H_2O_2 outperformed the MB degradation. The kinetic results illustrated that the MB degradation obeys the pseudo-first-order reaction model as Langmuir–Hinshelwood (L-H). The recyclability of MIL-88A(Fe)@g-C_3N_4 core@shell was examined and the results showed that this photocatalyst could be used as an effective one.

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