1st Iranian Catalyst Conference (ICC)

1-2 September 2018

University of Zanjan

کتابچه مقالات

اولین کنفرانس کاتالیست انجمن شیمی ایران

۱۰ و ۱۱ شهریور ۱۳۹۷

دانشگاه زنجان

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۱۰ و ۱۱ شهریور ۱۳۹۷
دانشگاه زنجان

جمهوری اسلامی ایران
وزارت علوم، تحقیقات و فناوری

دانشگاه زنجان

انجمن شیمی ایران
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1st Iranian Catalyst Conference
1-2 September 2018, University of Zanjan, Zanjan, Iran

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محورهای کنفرانس

- نانو کاتالیست
- کاتالیست‌های همگن و ناهمگن
- بیوکاتالیست
- الکترو کاتالیست
- آنزیم‌های مصنوعی و کاتالیست‌های آنزیمی
- کاتالیست‌های مایع یونی
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- تصفیه هوا
- صنعت هوا و فضا
- سایر زمینه‌های مرتبط با کاتالیست

آدرس دبیرخانه: زنجان، دانشگاه زنجان، دانشکده علوم، گروه شیمی، دبیرخانه اولین کنفرانس کاتالیست ایران

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بسم الله الرحمن الرحیم

قال الله تعالی: یرفع الله الذین آمنوا منکم و الذین أوتوا العلم درجات

دانشجویان عزیز ، شرکت کنندگان محترم و اساتید گرامی سلام علیکم و رحمة الله.

تشریف فرمایی شما به دانشگاه زنجان به منظور شرکت در اولین کنفرانس کاتالیست انجمن شیمی ایران را خوش آمد می‌گوییم و برای همه شما سرانجامی نیک آرزو داریم. از اینکه دانشگاه زنجان در روزهای بسیار مبارک ماه پر برکت ذی الحجه و در آستانه ورود به ماه محرم میزبان شما دانش پژوهان گرامی در اولین کنفرانس کاتالیست انجمن شیمی ایران است، بسیار خرسندیم و امیدواریم حق تعالی در این ماه های عزیز توفیق طاعت و عبادت، تزکیه و تهذیب نفس را نصیب همگان نماید. امروزه رویکرد اصلی دانشگاه‌ها، تولید علم، آگاهی، فناوری، ارزش آفرینی و کارآفرینی است و دانشگاه‌ها کانون‌های اصلی تولید علوم، فناوری، ارزش آفرینی و کارآفرینی محسوب می شوند. نبض پیشرفت و توسعه جامعه بدست اساتید برجسته و فرهیخته و دانشجویان آگاه و سخت کوشی رقم می‌خورد که با پشتکار و جدیت، زمینه عزت، ترقی و پیشرفت کشور را فراهم می‌سازند و این مهم زمانی امکان‌پذیر است که دانشجویان عزیز با بهره‌گیری از خلاقیت، نوآوری و استعداد خود و تعامل، همراهی و سعه صدر مسئولین و استفاده از رهنمودهای اساتید دلسوز، توانایی‌ها و امکانات دانشگاهی را برای ارتقای منزلت دانشجو و کیان دانشگاه و اعتلای علمی، آموزشی، پژوهشی، فناوری، ارزش آفرینی و کار آفرینی بکار بندند. تولید علم و آگاهی در دانشگاهها و مراکز پژوهشی باید به گونه ای باشد که علاوه بر گسترش مرزهای دانش، بتواند در جهت ارتقای زندگی مردم، تولید ثروت، پیشگیری از خام فروشی و ایجاد اشتغال، مفید واقع شود. با توجه به وجود استعدادهای فراوان انسانی و منابع سرشار خدادادی در کشورمان، لازم است اساتید، دانشگاهیان و پژوهشگران و فناوران بیش از گذشته به پژوهشهای کاربردی در جهت رفع نیازهای جامعه، پیشگیری از خام فروشی، استقلال و خودکفایی بپردازند. امیدواریم برگزاری اولین کنفرانس کاتالیست انجمن شیمی ایران در دانشگاه زنجان به تبادل تجربیات و ایجاد انگیزه های بیشتر در جهت ارتقای علمی، صنعتی، کارآفرینی و ارزش آفرینی کشورمان کمک موثری نماید.

همت بلند دار که مردان روزگار   از همت بلند به جائی رسیده‌اند.

پیروزی و عزت از آن خدا و رسول و مومنان است. پیروز و سربلند باشید انشاء الله تعالی

پروفسور علی رمضانی

دبیر اولین کنفرانس کاتالیست انجمن شیمی ایران

بسمه تعالی

دوستان ارجمند، اساتید گرامی، پژوهشگران، صنعتگران و دانشجویان عزیز سلام علیکم:
افتخاری برای ما بود که در قالب "اولین کنفرانس کاتالیست ایران"، در دانشگاه زنجان، در خدمت شما بودیم. در این کنفرانس ملی که به همت گروه شیمی دانشگاه زنجان و همکاری وزارت علوم تحقیقات و فناوری، پایگاه استنادی علوم جهان اسلام، مرکز منطقه ای اطلاع رسانی علوم و فناوری و انجمن شیمی ایران در روزهای۱۰ و ۱۱ شهریور ماه ۱۳۹۷ برگزار گردید، از میان ۵۲۲ مقاله ارسالی به دبیرخانه کنفرانس تعداد ۴۰۰ مقاله توسط کمیته علمی کنفرانس پذیرفته شد. که از این تعداد ۱۰ مقاله به صورت سخنرانی و ۳۹۰ مقاله به صورت پوستر ارائه گردید. همچنین از دیگر برنامه های علمی تدارک دیده در اولین کنفرانس کاتالیست ایران دعوت از دوازده تن از برجسته ترین اساتید شیمی کشور به عنوان سخنران کلیدی (جناب آقای پروفسور عیسی یاوری و جناب آقای پروفسور علی مرسلی) و سخنران مدعو (جناب آقای پروفسور یعقوب منصوری، جناب آقای پروفسور مهراورنگ قائدی، جناب آقای پروفسور مصطفی قلی زاده، جناب آقای دکتر محمد مهدی نجف پور، جناب آقای دکتر سعید زکوی، جناب آقای دکتر صادق رستم نیا، جناب آقای دکتر محمود نصرالله زاده، جناب آقای دکتر علی ملکی، جناب آقای دکتر روزبه جواد کلباسی و جناب آقای دکتر مهدی محمدی) در زمینه های متنوع علوم کاتالیست بود، که در طی روز های برگزاری کنفرانس به سمع و نظر شما بزرگواران رسید. از دیگر برنامه های جنبی این کنفرانس، برگزاری نمایشگاه دستاوردها و توانمندی های شرکت های دانش بنیان خصوصی، برگزاری گارگاه های آموزشی، و تورهای استان‌گردی را می توان نام برد. در پایان وظیفه خود میدانیم که از یکایک شما عزیزان، دانشجویان گرامی و اساتید فرهیخته که رنج سفر را تحمل نموده و در این کنفرانس ملی شرکت کرده بودید تقدیر و تشکر نماییم. امید آن داریم اندوخته های علمی لازم را کسب نموده و توشه راه خود کرده باشید. همچنین از همه عزیزانی که در برگزاری این کنفرانس ما را یاری کردند تقدیر و تشکر می نماییم. از اعضای کمیته علمی و کمیته داوران کنفرانس، انجمن شیمی ایران، حوزه های مختلف دانشگاه زنجان، اعضای کمیته اجرایی شامل کارکنان و دانشجویان گروه شیمی که ما را در هر چه پر بار برگزار شدن این کنفرانس علمی یاری نموده اند تقدیر و تشکر می نماییم.

دکتر سید جمال طباطبائی رضائی

دبیر اجرایی اولین کنفرانس کاتالیست انجمن شیمی ایران

برنامه اولین کنفرانس کاتالیست انجمن شیمی ایران

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اولین کنفرانس کاتالیست انجمن شیمی ایران

۱۰-۱۱ شهریور ۱۳۹۷، دانشکده علوم، دانشگاه زنجان

روز جمعه ۹ شهریور

ساعت برنامه	برنامه جمعه(۱۳۹۷/۰٦/۰۹)		مدت برنامه
۱٦:۳۰–۲۱	**پذیرش**	پذیرش شرکت کنندگان محترم	۲۷۰ دقیقه
۲۰:۳۰–۲۲:۳۰	**استراحت**	شام	۱۲۰ دقیقه

اولین کنفرانس کاتالیست انجمن شیمی ایران

۱۰-۱۱ شهریور ۱۳۹۷، دانشکده علوم، دانشگاه زنجان

روز شنبه ۱۰ شهریور

ساعت برنامه	برنامه روز اول کنفرانس (شنبه ۱۳۹۷/۰٦/۱۰)		مدت برنامه
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سالن الغدیر

۸:۱۵–۹:۲۰	افتتاحیه	تلاوت قرآن، سرود ملی، خیر مقدم معاونت پژوهشی و فناوری دانشگاه، سخنرانی و گزارش دبیر کنفرانس، سخنرانی عضو شورای عالی انجمن شیمی، تجلیل از حامیان کنفرانس	۷۵ دقیقه
۹:۲۰–۱۰:۰۵	سخنرانی کلیدی	**سخنران: پروفسور عیسی یاوری** In the Realm of Catalysis	۴۵ دقیقه
۱۰:۰۵–۱۰:۳۵	استراحت	پذیرایی و بازدید از نمایشگاه کنفرانس	۳۰ دقیقه
۱۰:۳۵–۱۱:۱۰	سخنرانی مدعو	**سخنران: پروفسور مهر اورنگ قائدی** Application of Various Nanostructured Photocatalysts for Degradation of Pollutants	۳۵ دقیقه
۱۱:۱۰–۱۱:۴۵	سخنرانی مدعو	**سخنران: دکتر محمد مهدی نجف پور** True catalysts	۳۵ دقیقه
۱۱:۴۵–۱۲:۲۰	سخنرانی مدعو	**سخنران: دکتر صادق رستم نیا** Nano-Sponge Microporous & Mesoporous Surfaces as a Good Place for Organic and Inorganic Species Grows/Assembling	۳۵ دقیقه

سالن سهروردی

۱۲:۲۰–۱۲:۳۵	سخنرانی	**سخنران: دکتر مهری سلیمی** Cobalt nano-particles supported on ethylenediaminefunctionalized magnetic cellulose nanofibers as a novel andefficient catalyst for oxidation of alcoholes	۱۵ دقیقه

سالن الغدیر

١٢:٢٠–١٢:٣٥	سخنرانی	**سخنران: دکتر حبیب اله زلفی خانی** تخمین و برآورد اندازه و فواصل ذرات بر اساس مشخصات الکتریکی و مغناطیسی در کاربردهای نانوکاتالیست ها	١٥ دقیقه

رستوران دانشگاه

١٢:٣٠–١٤	استراحت	نماز–ناهار	٩٠ دقیقه

سالن سهروردی

١٢:٥٠–١٤	کارگاه	کارگاه آموزشی کاربرد نرم افزار EndnoteX$_7$ درمدیریت منابع و استنادهای علمی **مدرس کارگاه: دکتر سعید تقوی فردود**	٧٠ دقیقه

سالن پوستر

١٤–١٤:٤٥	ارائه پوستر	ارائه مقالات پذیرفته شده به صورت پوستر (بخش اول)	٤٥ دقیقه

سالن الغدیر

١٤:٤٠–١٤:٥٥	سخنرانی	**سخنران: دکتر سعدی صمدی** The Synthesis of C_2-symmetric Chiral *S*, *S*-bis (Bidentate Oxazoline Benzamide-Cu (II) Complexes) and Their Applications in Oxidation of Allylic C–H Bonds of Cyclic Olefins	١٥ دقیقه

سالن سهروردی

١٤:٤٠–١٤:٥٥	سخنرانی	**سخنران: دکتر مظفر شاکری** Synthesis of Efficient TS-1 Zeolite for Selective Oxidation Reactions	١٥ دقیقه

سالن الغدیر

١٥–١٥:٣٥	**سخنرانی مدعو**	**سخنران: پروفسور یعقوب منصوری** Supported Metal Complexes on Fe_3O_4@Silica@SBA-15: Magnetically Retrievable Catalysts for Cross Coupling Reactions	٣٥ دقیقه
١٥:٣٥–١٦:١٠	**سخنرانی مدعو**	**سخنران: دکتر محمود نصراله زاده** Recent Progresses in Catalytic Transformations: A Bridge toward Eco-Nanotechnology	٣٥ دقیقه
١٦:١٠–١٦:٤٠	**استراحت**	پذیرایی و بازدید از نمایشگاه کنفرانس	٣٠ دقیقه
١٦:٤٠–١٧:١٥	**سخنرانی مدعو**	**سخنران: دکتر علی ملکی** Green Chemistry through Nanocatalysts in Organic Reactions	٣٥ دقیقه

سلطانیه

١٧:٢٠–٢١:٣٠	**گردشگری**	گردشگری سلطانیه	٢٥٠ دقیقه

رستوران دانشگاه

٢٠:٣٠–٢٢	**استراحت**	شام	٩٠ دقیقه

اولین کنفرانس کاتالیست انجمن شیمی ایران

۱۰-۱۱ شهریور ۱۳۹۷، دانشکده علوم، دانشگاه زنجان

روز یکشنبه ۱۱ شهریور

ساعت برنامه	برنامه روز دوم کنفرانس (یکشنبه ۱۳۹۷/۰٦/۱۱)	مدت برنامه
		رستوران دانشگاه
۷–۸:۱۵	**استراحت** صبحانه	۷۵ دقیقه
		سالن الغدیر
۸:٤٥–۹	**سخنرانی** سخنران: دکتر هدی نصیرا سینتیک هضم لیپید توسط آنزیم لیپاز تثبیت شده بر سطح نانوکامپوزیت گرافن	۱۵ دقیقه
		سالن سهروردی
۹–۹:۱۵	**سخنرانی** سخنران: دکتر فاطمه نوروزی Creating Catalyst Niches, a Breakthrough of Technological development via Uni-Indu collaboration	۱۵ دقیقه
		سالن الغدیر
۹–۹:۱۵	**سخنرانی** سخنران: دکتر سجاد کشی پور Cellulose and Chitosan Supported Catalysts	۱۵ دقیقه

سالن سهروردی

٩:١٥–٩:٣٠	**سخنرانی**	**سخنران: دکتر سیاوش کاظمی موحد** Palladium nanoparticles supported on Fe_3O_4@nitrogen doped carbon cubes as a highly efficient catalyst for the organic reactions	١٥ دقیقه

سالن الغدیر

٩:١٥–٩:٣٠	**سخنرانی**	**سخنران: دکتر سعید تقوی فردود** Green synthesis of magnetic $NiFe_2O_4$@CuO nanocomposite using tragacanth gel and its use as an efficient catalyst for the solvent free synthesis of tetrahydrobenzo[b]pyran derivatives	١٥ دقیقه

سالن پوستر

٩:٣٠–١٠:١٥	**ارائه پوستر**	ارائه مقالات پذیرفته شده به صورت پوستر (بخش دوم)	٤٥ دقیقه
١٠:١٥–١٠:٣٥	**استراحت**	پذیرایی و بازدید از نمایشگاه کنفرانس	٣٠ دقیقه

سالن الغدیر

١٠:٣٥–١١:٢٠	**سخنرانی کلیدی**	**سخنران: پروفسور علی مرسلی** Metal–Organic Frameworks as Platforms for Catalytic Applications	٤٥ دقیقه
١١:٢٠–١١:٥٥	**سخنرانی مدعو**	**سخنران: پروفسور مصطفی قلی‌زاده** The Process of Chemical Reactions in the Magnetized Solvents	٣٥ دقیقه

سالن پوستر

١٢–١٢:٤٥	**ارائه پوستر**	ارائه مقالات پذیرفته شده به صورت پوستر (بخش سوم)	٤٥ دقیقه

رستوران دانشگاه

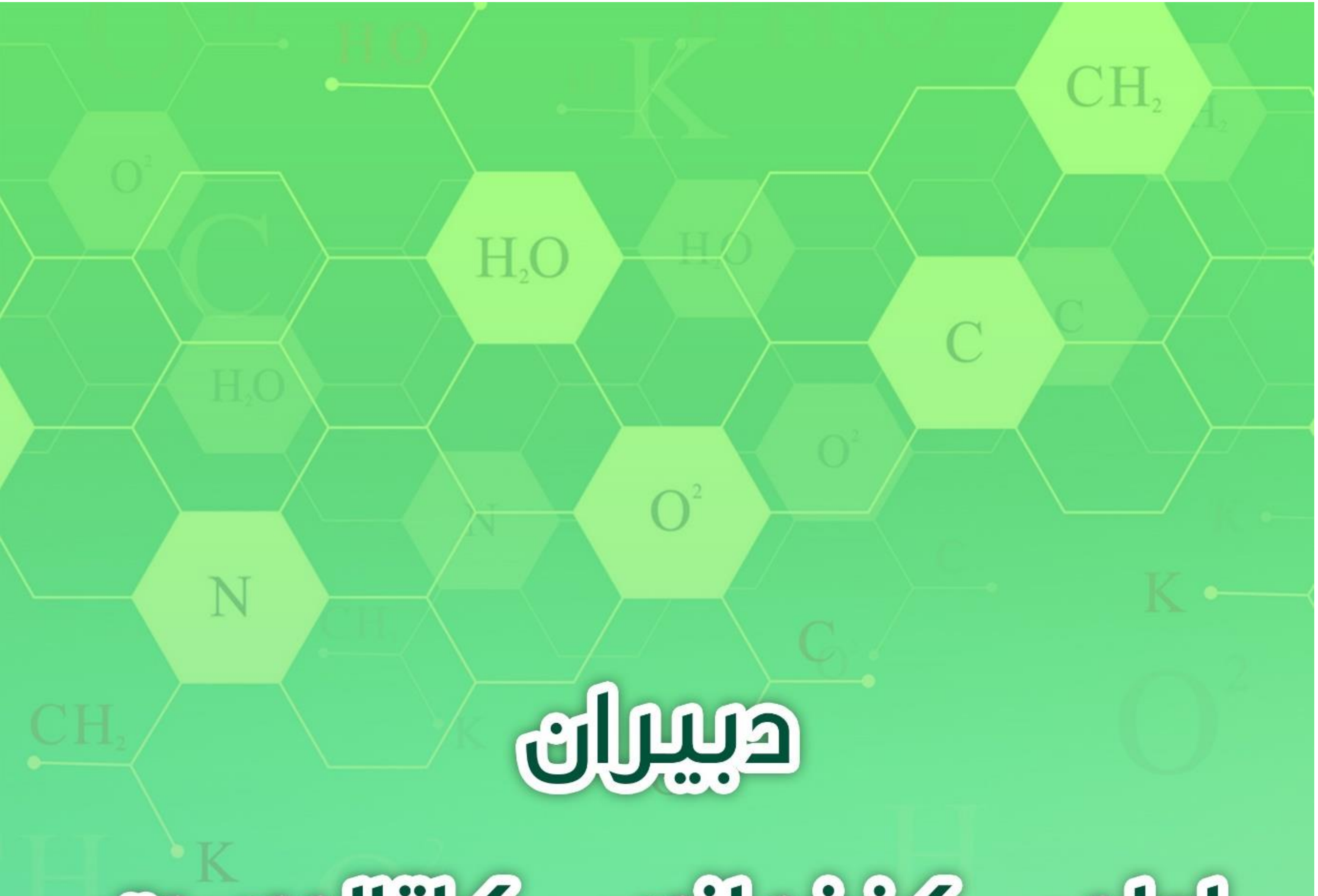
١٢:٣٠–١٤	استراحت	نماز–ناهار	٩٠ دقیقه

سالن سهروردی

١٣:١٥–١٤:٣٠	کارگاه	کارگاه تخصصی آموزش تفسیر XRD با استفاده از نرم افزار X'Pert HighScore **مدرس کارگاه: دکتر سعید تقوی فردود**	٧٥ دقیقه

سالن الغدیر

١٤:٣٠–١٥:٠٥	سخنرانی مدعو	**سخنران: دکتر روزبه جواد کلباسی** The recent studies on synthesis and characterization of hierarchical zeolites and their catalytic activities in organic reactions	٣٥ دقیقه
١٥:٠٥–١٥:٤٠	سخنرانی مدعو	**سخنران: دکتر سعید زکوی** Transition metal-based catalysts: An overview	٣٥ دقیقه
١٥:٤٠–١٦:١٥	سخنرانی مدعو	**سخنران: دکتر مهدی محمدی** Multi-component reactions for covalent immobilization of biomolecules: What is the mechanism?	٣٥ دقیقه
١٦:٢٠–١٧	هم اندیشی	**میز گرد صنعت و دانشگاه**	٤٠ دقیقه
١٧–١٧:٣٠	استراحت	پذیرایی و عکس یادگاری	٣٠ دقیقه
١٧:٣٠–١٨:١٥	اختتامیه	تجلیل از سخنران برتر، پوستر برگزیده و کادر اجرایی	٤٥ دقیقه



دبیران
اولین کنفرانس کاتالیست
انجمن شیمی ایران

پروفسور علی رمضانی

دبیر کنفرانس

دکتر محمدعلی رضوانی

دبیر علمی

دکتر سید جمال طباطبائی رضایی

دبیر اجرایی

دکتر سعید تقوی فردود

مدیر فنی

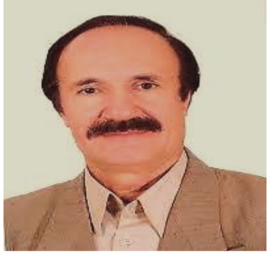
کمیته علمی
اولین کنفرانس کاتالیست
انجمن شیمی ایران

			
پروفسور علی رمضانی	**پروفسورحمید گلچوبیان**	**پروفسور فرهاد شیرینی**	**پروفسور علی مرسلی**
دانشگاه زنجان	دانشگاه مازندران	دانشگاه گیلان	دانشگاه تربیت مدرس
			
پروفسور مهر اورنگ قائدی	**پروفسور مسعود صلواتی نیاسر**	**پروفسور عبدالرضا حاجی پور**	**پروفسور علیرضا ختائی**
دانشگاه یاسوج	دانشگاه کاشان	دانشگاه اصفهان	دانشگاه تبریز
			
پروفسور عزیز حبیبی ینگجه	**پروفسور محمد علی زلفی گل**	**پروفسور ایوب بازگیر**	**پروفسور محمد جوشقانی**
دانشگاه محقق اردبیلی	دانشگاه بوعلی همدان	دانشگاه شهید بهشتی	دانشگاه رازی
			
پروفسور مصطفی قلی زاده	**پروفسور مجتبی باقر زاده**	**پروفسور علیرضا کیاست**	**پروفسور محمد قادرمزی**
دانشگاه فردوسی مشهد	دانشگاه صنعتی شریف	دانشگاه شهید چمران اهواز	دانشگاه کردستان
			
پروفسور نادر نوروزی پسیان	**پروفسور سعید رعیتی**	**پروفسور عادله مشتقی زنوز**	**پروفسور محمد مظلوم**
دانشگاه ارومیه	دانشگاه خواجه نصیرالدین طوسی	دانشگاه شهید مدنی آذربایجان	دانشگاه یزد

			
پروفسور غلامحسن ایمانزاده	**پروفسور مجید مقدم**	**پروفسور مجید تقی زاده مازندرانی**	**پروفسور احمدرضا مساح**
دانشگاه محقق اردبیلی	دانشگاه اصفهان	دانشگاه بابل	دانشگاه آزاد اسلامی واحد شهرضا
			
پروفسور حسن ولی زاده	**پروفسور داود نعمت الهی**	**پروفسور حسین نعیمی**	**پروفسور علی عموزاده**
دانشگاه شهید مدنی آذربایجان	دانشگاه بوعلی همدان	دانشگاه کاشان	دانشگاه سمنان
			
دکتر سعید زکوی	**پروفسور حسن حسینی منفرد**	**پروفسور فوآد کاظمی**	**پروفسور محمد رضا یافتیان**
دانشگاه تحصیلات تکمیلی علوم پایه - زنجان	دانشگاه زنجان	دانشگاه تحصیلات تکمیلی علوم پایه - زنجان	دانشگاه زنجان
			
دکتر فریده پیری	**پروفسور ناصر دلالی**	**پروفسور مرتضی واحدپور**	**دکتر سامی سجادی فر**
دانشگاه زنجان	دانشگاه زنجان	دانشگاه زنجان	دانشگاه پیام نور ایلام
			
دکتر علیرضا کاظمی زاده	**دکتر محمدرضا پور هروی**	**دکتر ابراهیم احمدی**	**دکتر محمد حسین رسولی فرد**
دانشگاه آزاد زنجان	دانشگاه پیام نور ابهر	دانشگاه زنجان	دانشگاه زنجان

			
دکتر روزبه جواد کلباسی	**دکتر محمد قلی نژاد**	**دکتر راضیه حبیب پور**	**دکتر محمد مهدی نجف پور**
دانشگاه خوارزمی	دانشگاه تحصیلات تکمیلی علوم پایه - زنجان	سازمان پژوهشهای علمی و صنعتی کشور	دانشگاه تحصیلات تکمیلی علوم پایه - زنجان
			
دکتر محمود زیارتی	**دکتر مهدی خوبی**	**دکتر صادق رستم نیا**	**دکتر فرهاد پناهی**
دانشگاه صنعتی مالک اشتر	دانشگاه علوم پزشکی تهران	دانشگاه مراغه	دانشگاه شیراز
			
دکتر حمزه کیانی	**دکتر محمد یوسفی**	**دکتر میر سعید سید دراجی**	**دکتر محمود نصرالله زاده بائی**
دانشگاه دامغان	پژوهشگاه پلیمر و پتروشیمی ایران	دانشگاه زنجان	دانشگاه قم
			
دکتر غلامرضا رضایی	**دکتر علی ملکی**	**دکتر نعمت الله ارشدی**	**دکتر مهدی بهزاد**
دانشگاه بین المللی قزوین	دانشگاه علم و صنعت ایران	دانشگاه زنجان	دانشگاه سمنان
			
دکتر محمدعلی رضوانی	**دکتر وحید مهدوی**	**دکتر فریبا سعادتی**	**دکتر سید جمال طباطبایی رضایی**
دانشگاه زنجان	دانشگاه اراک	دانشگاه زنجان	دانشگاه زنجان

			
دکتر مجتبی امینی	**دکتر نادر نوشیران زاده**	**دکتر فرهاد کبیری اصفهانی**	**دکتر مریم افشارپور**
دانشگاه مراغه	دانشگاه زنجان	دانشگاه زنجان	پژوهشگاه شیمی و مهندسی شیمی ایران
			
دکتر مریم شاطریان	**دکتر سعید تقوی فردود**	**دکتر حمید احمر**	**دکتر معصومه قربانلو**
دانشگاه زنجان	دانشگاه زنجان	دانشگاه زابل	دانشگاه زنجان
			
دکتر مهدی محمدی	**دکتر هدی نصیرا**	**دکتر پروانه نخستین پناهی**	**دکتر سعدی صمدی**
پژوهشگاه ملی مهندسی ژنتیک	دانشگاه زنجان	دانشگاه زنجان	دانشگاه کردستان

			
پروفسور عیسی یاوری	**پروفسور عبدالله فلاح شجاعی**	**پروفسور بابک کریمی**	**پروفسور حمید سلطانی**
دانشگاه تربیت مدرس	**دانشگاه گیلان**	**دانشگاه تحصیلات تکمیلی علوم پایه زنجان**	**دانشگاه ALU امریکا**
			
دکتر افشین سروری	**دکتر علی اکبر میران بیگی**	**دکتر فرخزاد محمدی زنوز**	**دکتر محمد رضا محمدی زاده**
دانشگاه صنعتی نوشیروانی بابل	**پژوهشگاه نفت تهران**	**دانشگاه حکیم سبزواری**	**دانشگاه خلیج فارس بوشهر**
			
دکتر علی سولدوزی	**دکتر میرزآقا بابازاده**	**دکتر سجاد کشی پور**	**دکتر حمید سعیدیان**
دانشگاه آزاد اسلامی واحد ارومیه	**دانشگاه آزاد تبریز**	**دانشگاه ارومیه**	**دانشگاه پیام نور تهران**
			
دکتر رحیم قدری	**دکتر محسن یوسفی فر**	**دکتر محمدحسن پیروی**	**دکتر عزت الله نجفی**
دانشگاه تبریز	**دانشگاه ALU امریکا**	**دانشگاه شهید بهشتی**	**دانشگاه پیام نور زنجان**

کمیته اجرایی
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دکتر سعید تقوی فردود	**دکتر سید جمال طباطبائی رضایی**	**دکتر نعمت الله ارشدی**
مدیر فنی کنفرانس	**دبیر اجرایی کنفرانس**	
		
دکتر رحمت الله پور عطا	**دکتر سهراب رحمانی**	**دکتر حسن شایانی جم**
		
دکتر هدی نصیرا	**دکتر حامد بهرامی**	**دکتر مریم شاطریان**
		
دکتر حمید ارجمندفر	**دکتر هاشم شهروس وند**	**دکتر بهمن فرجمند**

کمیته اجرایی دانشجویی اولین کنفرانس کاتالیست انجمن شیمی ایران

۱. محمدرضا معرفت سفیدان
۲. مریم احمدی
۳. رضا فروتن
۴. علی‌اصغر اسکندری
۵. وحید فرامرزی
۶. نادیا فتاحی
۷. فاطمه یکه‌زارع
۸. حدیثه اکبری
۹. زلفا افشاری
۱۰. مریم بخشعلی‌پور
۱۱. ناهید جعفری
۱۲. شادی نصیری
۱۳. سارا گنج خانلو
۱۴. لیلا عونی
۱۵. میعاد مصطفائی
۱۶. مهشید ملکی
۱۷. سحر خندان
۱۸. معصومه اقمشه
۱۹. حسن قائم‌پناه
۲۰. لیلا ظفری
۲۱. اسماعیل شامی
۲۲. فرزانه مرادنیا
۲۳. بابک پاشایی
۲۴. مهناز یارکه سلخوری
۲۵. داوود عبدالله‌نژادیان
۲۶. مجید هادی
۲۷. فاطمه پرچگانی
۲۸. شیما اصغری
۲۹. سمانه طاووسی
۳۰. زینب ایمانی
۳۱. حسین خرم‌آبادی
۳۲. مینا امیری
۳۳. پروین رحمانی
۳۴. امیر فقه‌میری
۳۵. فاطمه کلانتری
۳۶. بهنام آقاجان

حامیان کنفرانس

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پژوهشکده فناوری‌های نوین زیستی دانشگاه زنجان

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Supported Metal Complexes on Fe_3O_4@Silica@SBA-15: Magnetically Retrievable Catalysts for Cross Coupling Reactions

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Title of Lecture:

The Process of Chemical Reactions in the Magnetized Solvents

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دانشگاه قم

Title of Lecture:

Recent Progresses in Catalytic Transformations:
A Bridge toward Eco-Nanotechnology

استاد مدعو: دکتر صادق رستم نیا

دانشگاه مراغه

Title of Lecture:

Nano-Sponge Microporous & Mesoporous Surfaces as a Good Place for Organic and Inorganic Species Grows/Assembling

استاد مدعو: دکتر سعید زکوی

دانشگاه تحصیلات تکمیلی علوم پایه زنجان

Title of Lecture:

Transition metal-based catalysts: An overview

استاد مدعو: دکتر محمد مهدی نجف‌پور

دانشگاه تحصیلات تکمیلی علوم پایه زنجان

Title of Lecture:

True Catalysts

استاد مدعو: دکتر مهدی محمدی

پژوهشگاه ملی مهندسی ژنتیک و زیست‌فناوری

Title of Lecture:

Multi-component reactions for covalent immobilization of biomolecules: What is the mechanism?

مقالات سخنرانان مدعو

The Process of Chemical Reactions in the magnetized solvents

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Abstract: Performing chemical reactions at high rates is one of the purposes of chemical researchers. Therefore one of the procedures to reach this goal is doing reactions in the magnetized solvents. The solvent becomes magnetized by being passed through the Solvents Magnetizing Apparatus (SMA)(Fig.1). According to Coey et al.[2], the durability of its magnetic property is longer than 200 hours, while most chemical reactions are done in shorter than 200 hours.Some other researchers,were recommended that magnetized productivity affects the structure of hydrogen bonds among water molecules. It should be noted that both better solvation of the reactants and also decreasing the surface tension occur in this method [1, 3].

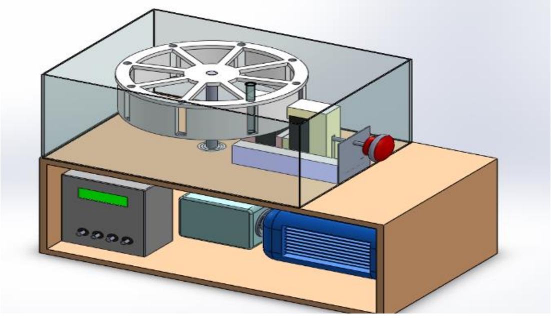

Figure 1: Solvent Magnetizing Apparatus(SMA)

***Keywords**: Magnetized Solvent, Hydrogen Bond, Surface Tension.*

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Multi-component reactions for covalent immobilization of biomolecules: What is the mechanism?

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Industrial application of the free form of enzymes remains controversial because of their poor stability and prohibitive cost. Therefore, there is a great interest in methods trying to develop useful biocatalysts for industrial applications by improvement their catalytic properties such as activity, stability or recycling capacity [1]. Numerous attempts have been carried out on the preparation of immobilized enzymes, which involves a variety of immobilization techniques and new support materials [2]. Among them, irreversible covalent attachment of enzymes on a solid support is an efficient and popular method and is usually preferred when leaching of enzyme from the support is a main concern. Moreover, if the immobilization protocol is properly designed to give an intense covalent attachment, the immobilization will be a powerful way to improve the enzyme rigidity, which increases enzyme stability against any distorting agents. However covalent attachment is often time consuming, needs harsh condition (for example high pH) and generally results in reduced activity of the immobilized enzyme. Therefore, it is still a big demand for discovery of new simple strategies for the covalent binding to improve enzyme catalytic functions. Recently we have reported the interesting results of using multi-component reactions for enzyme immobilization on aldehyde, epoxy and acid functionalized supports [3-5]. High capacity of loading, simple and rapid immobilization and significant improvement in activity of the immobilized enzyme are the main advantages of this novel procedure. In this procedure the support supplies the aldehyde, epoxy or acid groups, the enzyme molecules supply the carboxylic or amine groups and the other missing component is added to the reaction medium. However this protocol offers great flexibility to use different functional groups of many supports. In fact by utilizing this method a large number of supports and functional groups can be used for immobilization of enzymes.

Keywords: *Multicomponent reactions, Biomolecules, Covalent attachment*

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Supported Metal Complexes on Fe_3O_4@Silica@SBA-15: Magnetically Retrievable Catalysts for Cross Coupling Reactions

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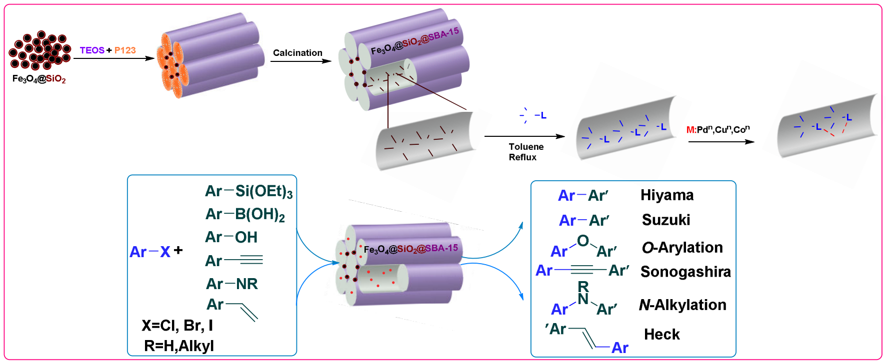
Highly ordered mesoporous silica materials have attracted a considerable deal of attention in development of different applications, such as diagnosis, drug delivery, extraction and hyperthermia. Their non-toxic nature, high surface area (700 to 1200 m^2 g^{-1}), abundant Si–OH bonds, tunable volume and pore diameter (2 to 50 nm) and potency of surface modification have represented them as an attractive candidate for coating and catalyst support purposes. For these reasons, SBA-15 has been considered for simple internal surface functionalization and release of large molecules [1]. Magnetite nanoparticles (MNPs) take advantage from nontoxicity, high dispersibility, biocompatibility, a noticeably high surface-to-volume ratio, high coercivity, superparamagnetic properties, great extraction efficiency and convenient separation [2]. In addition, MNP-supported catalysts can easily and rapidly be collected from various reaction mixtures by the means of an external magnet. Anchoring catalysts on MNPs is very exciting and it has been the topic of many research activities in recent years [3]. Combination of MNPs and mesoporous silica, e.g. SBA-15 and various kinds of MCMs, as core-shell structures provides the advantages of both high surface area and magnetic properties. These nanoparticles can be employed as magnetically retrievable catalyst supports [4].

Our current research activity has been directed toward developing of new Pd(II) complexes, e.g. NHC Pd(II), pyridine-type and other nitrogen-based ligand, supported on magnetic mesoporous core-shells of Fe_3O_4@Silica@SBA-15. The capabilities of these supported catalysts for C-C and C-N bonds formation, e.g. the reactions of halogenated hydrocarbons with, organoboron (Suzuki reactions), organosilicon (Hiyama reactions), alkenes (Heck reactions), alkynes (Sonogashira reactions), *N*-arylation and *O*-arylation are also under investigation, Scheme 1. Though magnetic silica mesoporous core-shells have been widely applied to coupling reactions, limited studies have been reported about anchoring homogeneous catalysts on magnetic silica mesoporous core-shells for coupling reactions.



Scheme 1. *Heck Reactions of Alkenes with aryl halides in the presence of Fe_3O_4@SBA-15-PPA*

Keywords: Pd(II) Supported Nanocatalysts, Coupling reactions, SBA-15, Magnetic Catalysts

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The recent studies on synthesis and characterization of hierarchical zeolites and their catalytic activities in organic reactions

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Synthesis, characterization, and application of hierarchical zeolites are becoming a subject of increasing interest among scientists. Hierarchical zeolites possessing secondary porosity at meso- and macro- scale, imposed on primary microporous structures are an original class of porous materials exhibiting both molecular sieving ability and fast mass transport [1]. These materials, due to the combination of catalytic properties of conventional zeolites with enhanced access and transport of reagents in additional meso- or micro- porosity, constitute an effective solution to the problem of mass transport. Several innovative methods have been presented to produce hierarchical zeolite, including removal of framework atoms, surfactant-assisted recrystallization method, dual templating with surfactants, zeolitization of materials, nanoparticle assembly, and template-assisted synthesis [2]. In this presentation, besides defining the concept of hierarchical zeolite, zeolitization of materials and dual templating with surfactant methods are discussed.

Keywords: *Hierarchical Zeolite, Nanoparticle assembly, Dry gel method.*

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Nano-based materials for photocatalytic degradation of organic pollutants

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Due to industrialization, population growth, and urbanization, the global environmental issues, especially the organic pollutants in industrial and household wastewater, have become a great threat to human life and environment in the recent decades [1-4]. An effective solution for confront with these problems is the use of method, which not only can relieve these problems, but also reduce the effluent discharge into the ecosystem. Among various methods that have been used for this regard, photocatalytic degradation as a cheap, available, clean and green purification technology in wastewater treatment process has always been considered. Therefore, application of nano-based materials for photocatalytic degradation of organic pollutants due to impressive properties of nanomaterial's in terms of high specific surface area, high surface free energy, sufficient reactive sites, fast dissolution, and various discontinuous properties (e.g. superparamagnetism, localized surface plasmon resonance, and quantum confinement effect) can enhance and improve the efficiency of photocatalytic degradation based methods for treatment and removal of organic pollutants from wastewater and environment [5-8].

Keywords: *Photocatalysis, Nanomaterials, Degradation of organic pollutants.*

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Nano-sponge microporous & mesoporous surfaces as a good place for organic and inorganic species grows/assembling

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Abstract

Postsynthetic functionalization/grafting precursors play an important role in tailoring nanoporous materials and and convert them to a solid hybrid catalyst nature. These kinds of solid materials contribute to sustainable and green chemistry by their heterogeneous, recyclable, and high efficiency features. Therefore, knowing the properties and reactivity of nanoporous materials as nano-sponge surface can guide us to manufacture a mesostructures compatible with reaction type and conditions.

Keywords: Nano-sponge, mesoporous materials, metal-organic frameworks (MOFs), catalysis.

Introduction

As our ongoing research interest in the development of catalytic applications of mesoporous silica materials [1-3], we recently discussed and reviewed organocatalysts which are supported inside the mesopores. Herein, we aimed to review recent advances in the catalytic applications of mesostructures in a comprehensive paper (Scheme 1).

Results and discussion

Propylsulfonic acid-based precursor

Propylsulfonic acid-based precursor (SprAP) is the earlier type of SAPs which can be obtained by functionalization of MPTS and further oxidation of it. SprAP is a most common and available precursor which is extensively used in various catalytic applications. It was first incorporated into MCM-type mesostructures by some pioneering groups in 1998. Rhijn and coworkers [3] used MCM type mesostructure as a catalyst for the synthesis of 2,2-bis(5-methylfuryl)propane which was obtained from condensation of acetone and 2-methylfuran (Figure 1).

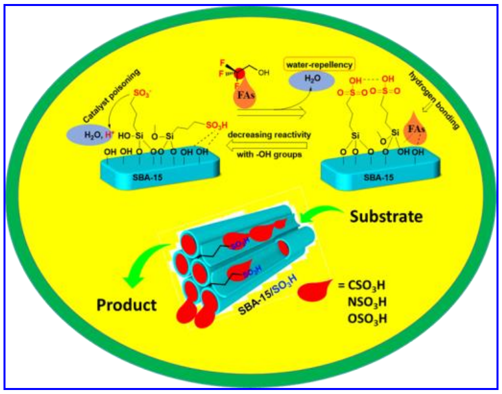


Figure 1. Mesoporous solid mateials as the catalysis of orgnic reactions.

They also applied it in the esterification of D-sorbitol with lauric acid. Then, Jacobs et al. disclosed the synthesis of monolaurin through direct esterification of glycerol with lauric acid over reusable MCM-41 and HMS-Pr-SO3H which were far more active than H-USY zeolite and even than commercial sulfonic-acid resins [3].

Metal-organic frameworks (MOFs) as the catalysis

When the subject of catalytic activities of MOFs is raised, active sites of MOFs and their corresponding interfaces become of utmost importance. Recent studies consider an intrinsic nature for MOFs' actives sites derived by the metal nodes or the organic linker. However, MOFs can be used as hosts to embed active species. On the other hand, post-modification ability of MOFs is a powerful tool to manipulate and adjust the catalytic activity of MOFs enabling them to catalyze various sorts of reactions [4]. Therefore, MOFs have attained much attention as the catalyst in some C-C, C-N or C-X bond formation reactions. Accordingly, in this review, we try to overview some of the recent developments in producing materials through C-C and C-X bond formation reactions derived by different parts of various MOFs [4]. The emphasis has been made on discussing the stability of the MOFs, their reusability and in providing a comparison of the performance of MOFs with respect to other homogeneous and heterogeneous catalysts (Figure 2).

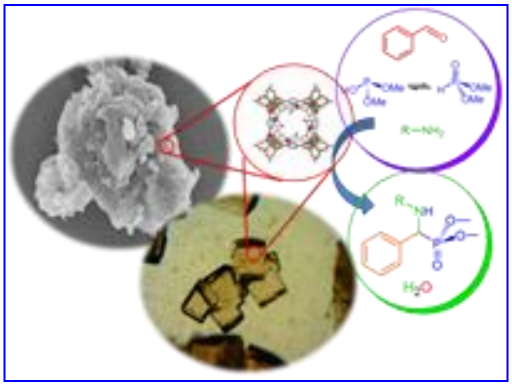
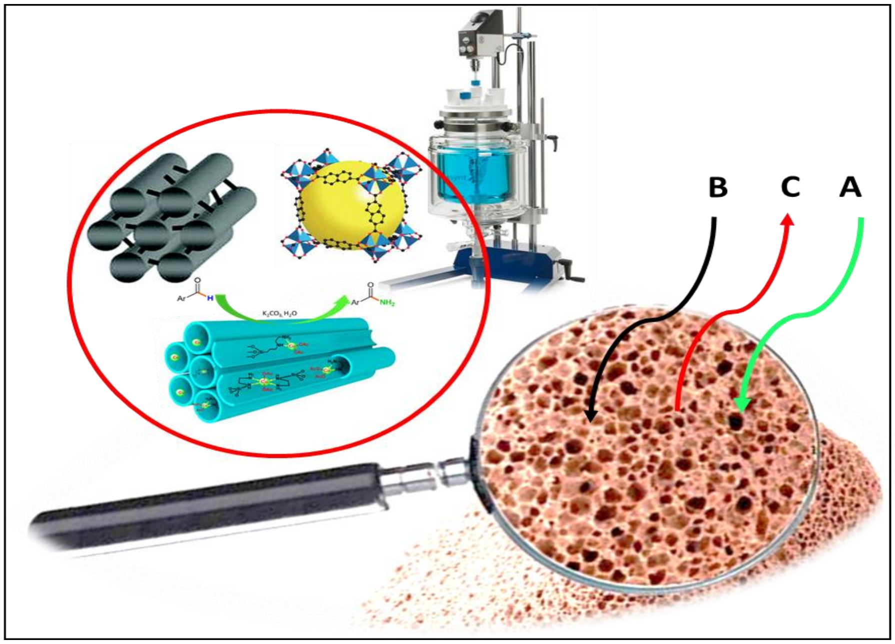


Figure 2. MOfs mateials act as the catalysis.



Scheme 1. Representation of catalytic action of nano-sponges.

Nanoporous catalytic translation of homogeneous catalysis into heterogeneous catalysis is a promising solution to green and sustainable development in the chemical industry. The use of these MOFs and mesoporous materials as heterogeneous catalysts in the liquid phase is highly desirable for the organic reaction, because the use of conventional homogeneous catalysts for those kind of reactions would lead to several problems, such as difficulty in separation and recovery and disposal of spent catalysts. reaction environments make them ideal candidates for new directions in catalyst design and application. Homochiral nanoporous also can use for enantiomeric selectivity in product formation, which is generally non-preferred in homogeneous catalysis. Although inferior to zeolites in thermal or hydrolytic stability, nano-sponge like porous materials possess extensive tunability, highly regular catalytic sites, flexibility domains in which zeolites have met limited success [3-5].

Conclusion

In view of the quickly increasing variety of MOFs and other soilid porus materials of nano-sponges that can be prepared, there is no doubt that the use of nanoporous solids as heterogeneous catalysts for organic reactions will grow in the near future, in which they can replace other echo-unfriendly and homogeneous catalysts.

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Graphical Abstract

Nano-sponge microporous & mesoporous surfaces as a good place for organic and inorganic species grows/assembling

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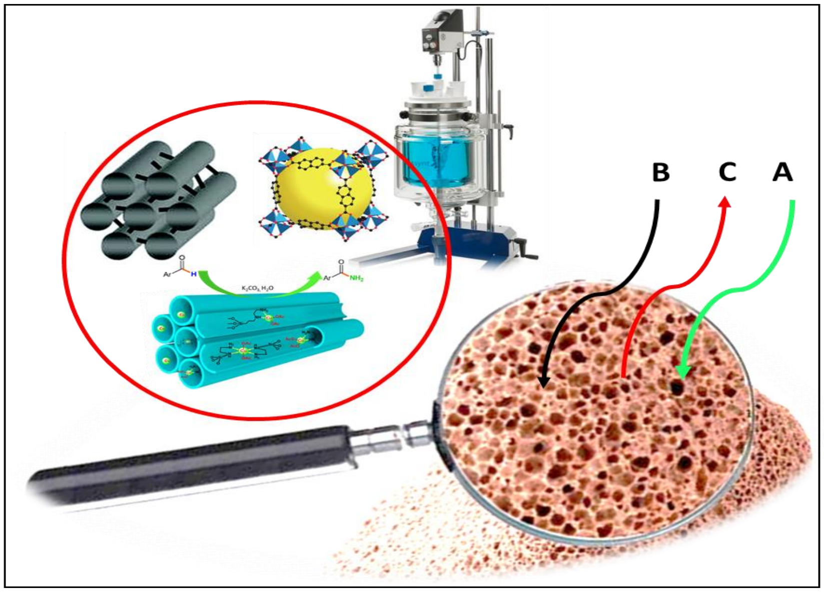

True Catalysts

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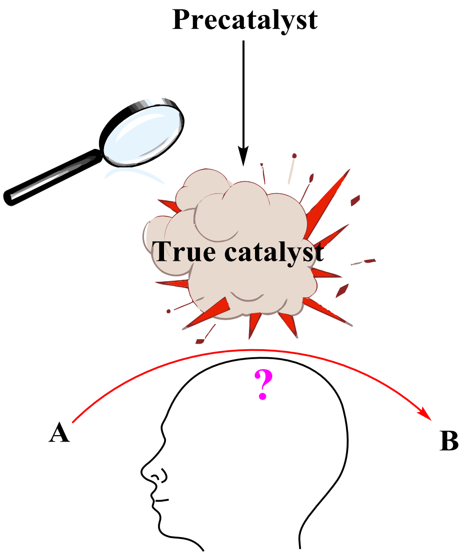
Many compounds have been used as precatalysts for different reactions in the presence of various chemical oxidants and reductants, or under electro-photochemical conditions. Currently, the advances in characterization techniques and different spectroscopic methods enable a better understanding of true catalysts and their related pathways [1-3]. In all the reactions for true catalysis studies, one of the most important points is that the kinetics, and the rate law for each species present, to unequivocally determine the true catalyst and no true catalyst can be identified without a rate law. Interestingly, recent experiments have shown that many known catalysts are the precursors to catalysts rather than true catalysts (**Scheme 1**) [1-3]. In the 21st century, it is necessary to develop the field of catalysis by seriously monitoring, without prejudice to find true catalysts. This issue is very important and relevant to the design and synthesis of efficient and stable catalysts. Herein, we focus on some true catalysts in various reactions.



***Scheme 1.** "What is true catalyst?" is an important question toward synthesis and design new and efficient catalysts.*

Keywords: *Catalyst, conversion, mechanism, metal complex, nanosized metal, nanosized metal oxide, true catalyst.*

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Recent Progresses in Catalytic Transformations: A Bridge toward Eco-Nanotechnology

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Several reports confirmed that various metals can be complexed with *N*-containing heterocyclic groups and prepared effective and remarkably catalysts for a variety of fundamentally significant transformations [1]. Among the important heterocyclic compounds, the tetrazoles chemistry, especially for using in coordination chemistry conducted us to synthesis of complex heterocyclic structures. As researches grows in order to the development of designing supported metal catalysts, it has been found that batches of tetrazoles can be coordinated with various metals to produce core-shell nanostructure composites (Figure 1). This is while, there are very few examples of using tetrazoles for the synthesis of core-shell nanostructures [2,3].

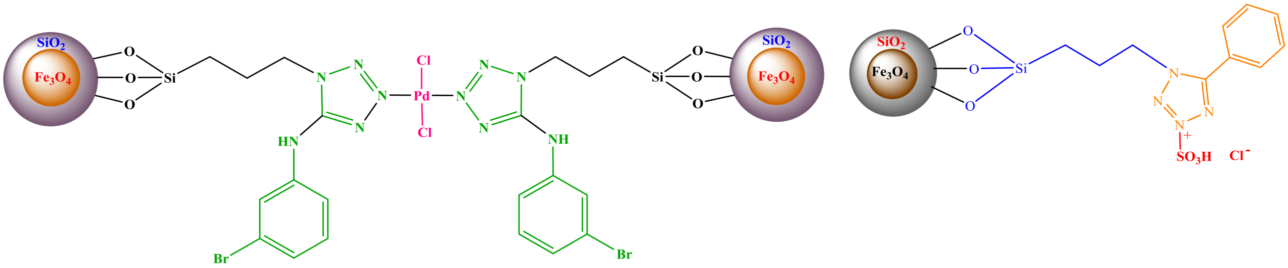

Figure 1. Proposed structure of $Fe_3O_4@SiO_2$ nanoparticles supported ionic liquid or palladium(II) complex.

It is well known that nanostructures synthesis has attracted much attention in various areas. In addition to chemical approaches to synthesize nanostructures, utility of simple and eco-friendly strategy caused to shift our study toward the green synthesis of metal nanoparticles (MNPs) by using plant extracts (Figure 2) [4,5]. In this context, employment of biological methods for bioreduction of metal ions have obtained opportunities for substituting traditional chemistry methods. Different plant parts could be remarkably valuable to biosynthesis of MNPs which do not provide process to quest for energy efficient but also can be used as an economic and extraordinary alternative for the large-scale production of MNPs. Concerning the extraordinary abilities and benefits of ecofriendly methods, we employed a distinctive and novel procedure through making a green bridge toward the eco-friendly fabrication of core-shell nanostructures using biosynthesis of $Fe_3O_4@SiO_2$ nanosubstrate.

Figure 2. Green synthesis of MNPs by using plant extracts.

Keywords: *Tetrazoles, Nanotechnology, Nanoparticles, Biosynthesis, Plant extracts.*

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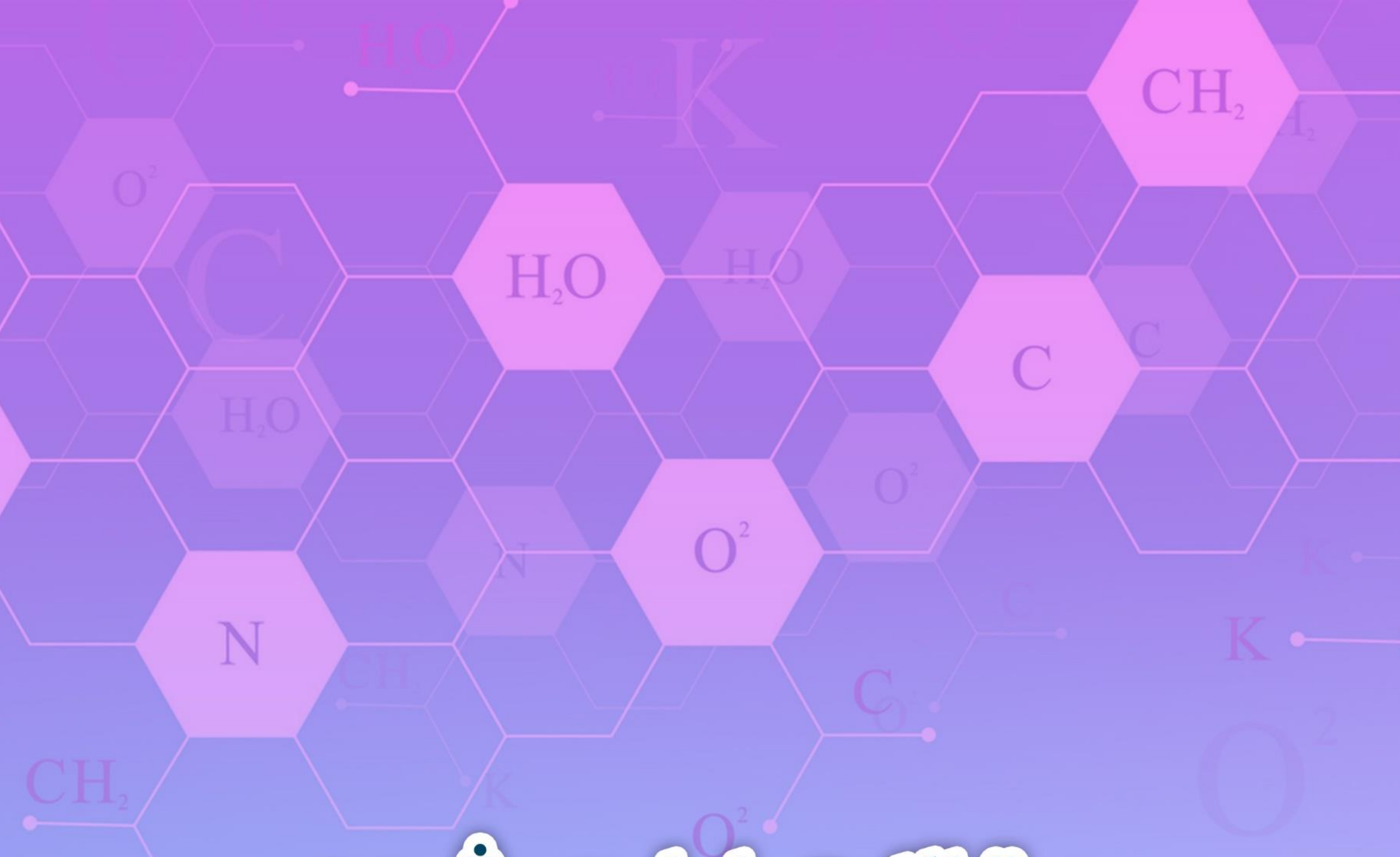

مقالات ارایه شده به صورت سخنرانی

Cellulose and Chitosan Supported Catalysts

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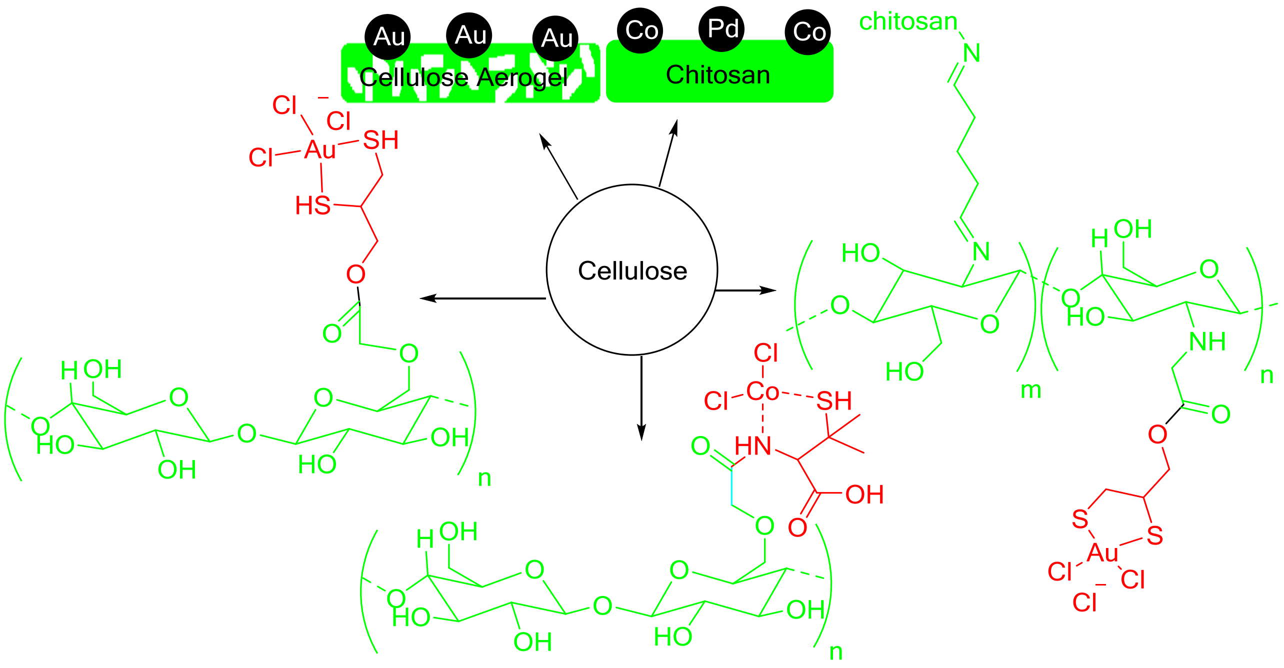
Cellulose has characteristic properties such as hydrophilicity, chirality, biodegradability and high functionality. A great deal of attention has been directed in recent years at cellulose and its derivatives focusing on their biological, chemical as well as mechanical properties. Cellulose and its derivatives can be used as supports since they are renewable, biodegradable and non-toxic.

Chitosan has shown good catalytic activity in organic synthesis without any post-modification. However, chitosan has been modified in most of the research by chemical modifications to serve the desired useful purpose. This biopolymer is interesting for catalytic applications due to low cost, hydrophilicity, chemical or physical modifications susceptibility for obtaining a special property, stability, nontoxic and biodegradable nature and having metal-anchoring functional groups.

With the increasing importance of greener, cleaner and more sustainable chemistry, a growth in applications has been observed for biomaterials such as cellulose and chitosan instead of petrochemical-based feed stocks in recent years [1-5]. Herein, various modifications on cellulose and chitosan was performed to obtain new catalytic systems applicable in the oxidation and reduction reactions.



Scheme 1. Cellulose and chitosan supported catalysts

Keywords: *Cellulose, Chitosan, Catalyst.*

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The Synthesis of C2-symmetric Chiral *S*, *S*-bis (Bidentate Oxazoline Benzamide-Cu (II) Complexes) and Their Applications in Oxidation of Allylic C–H Bonds of Cyclic Olefins

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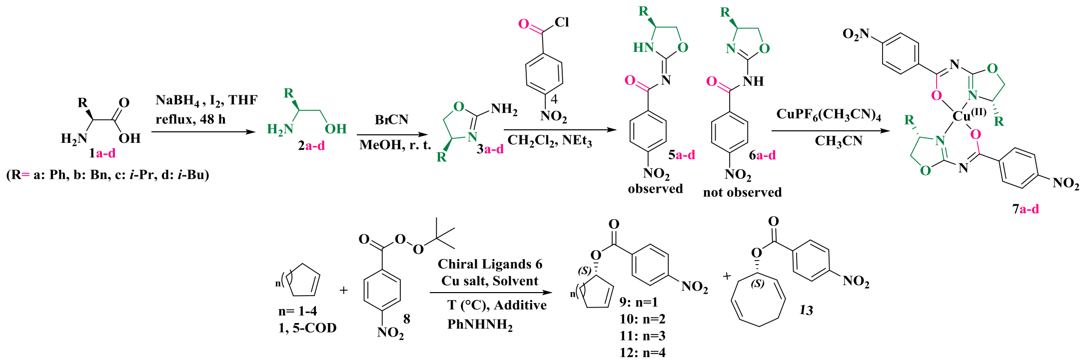
During the last decades, the role of chirality transformation in chiral oxazoline ligands have been confirmed in numerous transition-metal-catalyzed asymmetric transformations. Although chiral bisoxazolines ligands can be extensively used in catalytic asymmetric synthesis, chiral mono oxazoline versions have rarely presented comparable impacts [1-4].

Asymmetric allylic C–H bonds oxidation of olefins to chiral allylic esters and chiral allylic alcohols is considered one of the most important reactions in organic chemistry, in which, unlike hydroxylation and epoxidation, a second functional group is formed while the double bond remains unchanged[5,6].

In this work, a new type of chiral bidentate oxazoline benzamide ligands was conveniently synthesized from inexpensive and commercially available materials in high yields and enantiomeric excesses. The corresponding chiral copper complexes with this class of ligands [C_2 symmetric *S*, *S*-bis(bidentate oxazoline benzamide-Cu(II) complex] were synthesized accordingly. The utilization of these chiral complexes in the enantioselective esterification of allylic C–H bonds of cyclic olefins with *tert*-butyl-4-nitrobenzoperoxoate resulted in the highest activities, yields (up to 95%) and enantioselectivities (up to 94%) in the presence of HZSM-5 zeolite[5,6].



Scheme 1. *Synthesis of C_2 symmetric chiral Cu-oxazoline benzamide complexes 7a–d and their applications in the Enantioselective allylic oxidation of cycloolefins*

Keywords: *Chiral bidentate oxazoline ligands, Enantioselective allylic C–H bonds oxidation, Chiral allylic ester.*

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Synthesis of Efficient TS-1 Zeolite for Selective Oxidation Reactions

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Abstract: Oxygenated organic molecules are important intermediates for synthesis of fine, agrochemical, and pharmaceutical chemicals. Conventional synthesis of oxygenated molecules through stoichiometric approach often lead to low selectivity and generation of large amount of wastes.[1] Oxidation of organic molecules by zeolite catalysts has gained attention because of their stability, selectivity, and tunable physicochemical features.[2] Isomorphous substitution of Si with Ti by Tarammaso et al., from Eni Company in 1983 resulted in microporous TS-1 catalyst with oxidation function with H_2O_2 as oxidant.[3] Despite of enormous research on TS-1 catalyst since its discovery, only a few reactions by this catalyst has been commercialized. This is because of high cost of synthesis, low yield, and generation of wastewater during synthesis of TS-1. In this study, we investigated synthesis of TS-1 by using different silica sources. The obtained TS-1 catalysts showed double yield of that of conventional one. Catalytic tests of hydroxylation of phenol to catechol and hydroquinone resulted in higher conversion than that of conventional one (Figure 1). The method of TS-1 synthesis developed here is a powerful alternative to make low-cost catalysts and promote industrial applications of TS-1 catalysts.

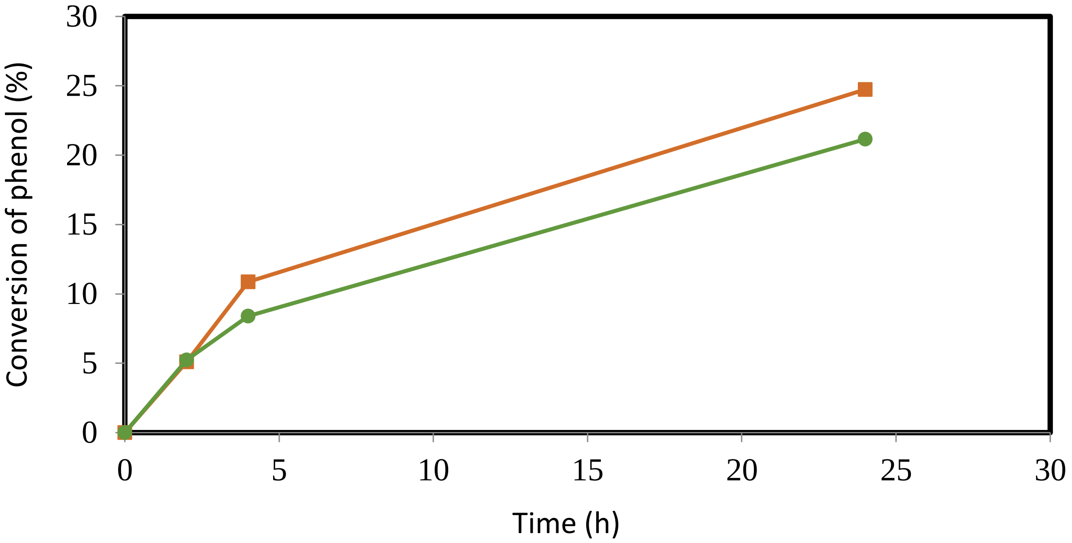

Figure 1. *Conversion of Phenol vs. time for Ts-1 developed in this study (filled square) and conventional (filled circle).*

Keywords: *TS-1 Zeolite, Oxidation, Synthesis.*

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Palladium nanoparticles supported on Fe_3O_4@nitrogen doped carbon cubes as a highly efficient catalyst for the organic reactions

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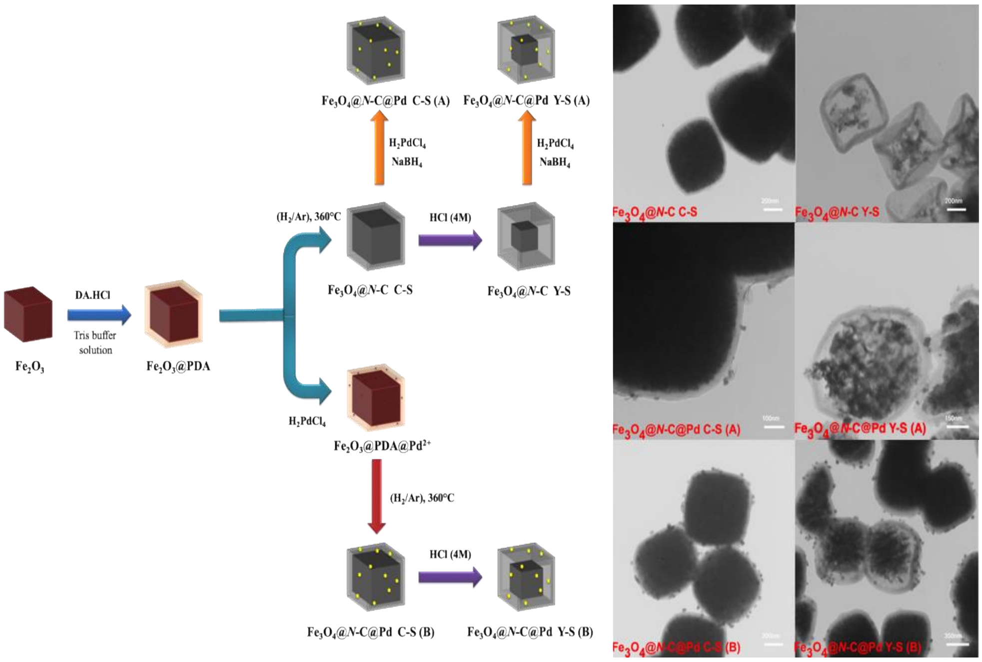
The preparation of palladium nanoparticles (Pd NPs) supported on Fe_3O_4@nitrogen doped carbon (*N*-C) core-shell (C-S) and yolk–shell (Y-S) nanostructures is reported. The Fe_3O_4@*N*-C@Pd C-S nanostructures were synthesized by two different methods. Additionally, the Y-S nanostructures were synthesized by using a HCl solution as an effective etching reagent to the partially etch the Fe_3O_4 [1]. Four types of Pd-based catalysts were tested in the selective reduction of *p*-nitrophenol (*p*-NP) to *p*-aminophenol (*p*-AP). Different catalytic activities were obtained through these catalysts. Furthermore, the reduction of nitroarenes and the oxidation of benzylic alcohols were also studies.



Scheme 1. *Schematic illustration of the formation procedure of Fe_3O_4@N-C@Pd C-S (A), Fe_3O_4@N-C@Pd Y-S (A), Fe_3O_4@N-C@Pd C-S (B), and Fe_3O_4@N-C@Pd Y-S (B) nanostructures*

Keywords: *Carbon, Reduction, Oxidation, Magnetic Separation, Nanocubes, Heterogeneous catalysis*

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Cobalt nano-particles supported on ethylenediamine functionalized magnetic cellulose nanofibers as a novel and efficient catalyst for oxidation of alcoholes

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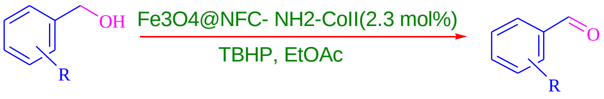
Abstract

Cobalt immobilized on functionalized magnetic cellulose nanofibers (Fe_3O_4@NFCs-NH_2-Co^{II}), as a novel bio-supported catalyst was synthesized. The catalyst system has been well characterized by various techniques like FTIR, TGA, SEM, TEM, EDX, ICP-AES and VSM. The as-prepared nanocatalyst was found to be a highly efficient heterogeneous catalyst for oxidation aromatic alcoholes with Tert- Butyl hydroperoxide (TBHP) in ethyl acetate as a green solvent at 45 °C with a yield over 50−90%. Importantly, the synthesized nanocatalyst can be easily separated by an external magnet and reused for at least five times without any appreciable loss of its catalytic reactivity

Keywords: cellulose nanofibers, Oxidation , Fe_3O_4@NFCs-NH_2-Co^{II}, Tert- Butyl hydroperoxide, metal Complex

Introduction

Oxidation reactions are among the most important transformations in applied synthetic chemistry and provide important methodology for the introduction and modifcation of functional groups. In this context oxidative transformations one major goal is the replacement of stoichiometric procedures, using classical toxic oxidants, with catalytic procedures using environmentally benign oxidant. Oxidants whose use is being contemplated include molecular oxygen, hydrogen peroxide, and tert-butyl hydroperoxide (TBHP) where there is either no by-product, the by-product is environmentally benign, or the by product can be easily recovered and recycled [1] stabilized metallic nanoparticles (NPs) have become as the most important position in developing fields of organic synthesis. In fact, the significance of crystal structure, particle size and nature of ligand to reach metallic NPs with proper catalytic activity has been demonstrated many times [2-4]. Despite of this, its separation technique was energy and time-consuming. On the other hand, up to now magnetic nanocatalysts have been considerable interest for catalytic systems of organic chemists due to their feasible removal and recycling by means of an external permanent magnet which is not time-consuming and prevents losing of catalyst during the separation process. Such a stabilizer is able to control the size of particles, improve the chemical stability, shape the magnetic features of the hybrid materials, avoid the agglomeration and also obtain the catalyst aim [5, 6]. As an important support, cellulose nanofibers (CNFs) is of excellent interest because of its unique specific structure [7, 8] and properties such as hydrophilicity, biodegradability, chirality, broad chemical-modifying capacity, great mechanical strength, fine chemical stability, low toxicity, high purity, high crystallinity and good compatibility [9-11]. In connection with our previous works using functionalized cellulose in organic transformation [12-14], we report a successful synthesis of a novel heterogeneous Co nano-particles bio-supported based magnetic nanomaterials catalyst (Fe_3O_4@ CNPs- NH_2-Co^{II} NPs) and its applications in oxidation of aromatic alcohols using TBHP as an oxidant in ethanol as a green solvent.



Scheme 1. Oxidation of benzyl alcohols catalyzed by Fe_3O_4@ NFC-NH_2- Co^{II}

General

All chemicals were purchased from Merck and Sigma-Aldrich Chemical Companies. CNF gel (3 wt%) was supplied by nano Novin Polymer Co. Iran. The purity determinations of the products and the progress of the reactions were accomplished by TLC on silica gel polygram STL G/UV 254 plates. The FT-IR spectra were recorded on pressed KBr pellets using an AVATAR 370 FT-IR spectrometer. Thermogravimetric analysis (TGA) was carried out using a Shimadzu Thermogravimetric Analyzer. The elemental compositions were determined with an CCERCI Energy-dispersive X-ray analysis (EDX) system .Transmission electron microscopy (TEM) images were obtained with a 906 E instrument (Zeiss, Jena, Germany). The morphology of the products was determined using Scanning Electron Microscopy (SEM) (Hitachi Japan, model S4160). The content of Co in the catalyst was determined by OPTIMA 7300DV ICP analyzer. Room temperature magnetization isotherms were obtained using a vibrating sample magnetometer (VSM, Lake Shore 7400).

Synthesis of the Fe_3O_4 @ cellulose nanofiber

A solution with NaOH–thiourea–urea–H_2O was cooled to -12 °C. cellulose nanofiber (CNF) was added into the above solution under vigorous stirring to form a CNF solution. Then, $FeCl_3.6H2O$ and $FeCl_2.4H_2O$ were dissolved in distilled water with vigorous stirring at room temperature, and then was added dropwise into the CNF solution with vigorous stirring. The resultant Fe_3O_4@CNF composites were separated by an external magnet and washed sequentially with distilled water, ethanol and acetone [15].

Synthesis of the Fe_3O_4 @ cellulose nanofiber-pr-Cl

The Fe_3O_4@CNF was sonicated in dry toluene, (3-Chloropropyl)trimethoxysilane was added dropwise to the resulting suspension. The obtained mixture was refluxed under mechanical stirring. The solid was separated by an external magnet, washed three times with ethanol and dried under vacuum, and thus Fe_3O_4 @Chloro-functionalized cellulose nanofibers (**(**Fe_3O_4 @ CNF-pr-Cl) was obtained**.**

Synthesis of the Fe_3O_4 @ cellulose nanofiber -NH_2

TO a suspension of Fe_3O_4 @ CNF-pr-Cl in absolute ethanol, ethylene1,2-diamine was added and heated under reflux with stirring. The resulting mixture was mechanically stirred. The solid was separated by an external magnet, washed with ethanol and dried in oven under vacuum, and Fe_3O_4 @ CNF-NH_2 was obtained.

Synthesis of the Fe_3O_4 @ cellulose nanofiber- NH_2-Co^{II}

Fe_3O_4 @ CNF-NH_2 was dispersed in ethanol absolute. A solution of $Co(OAc)_2$ in ethanol was added dropwise to the dispersed Mixture and sonicated at room temperature. The reaction mixture was mechanically stirred. Finaly the solid was separated using an external magnet, washed with ethanol sveral times and deried in an oven under vacuum.

General procedure for alcohol oxidation

To a mixture of alcohol, nano catalyst, Fe_3O_4@NFCs-NH_2-Co^{II} in ethyl acetate, TBHP was added and the mixture was stirred at 45°C. After completion of the reaction, the catalyst was separated by an external magnet, washed with ethanol, dried and reused for a consecutive run under the same reaction conditions. Evaporation of the solvent of the filtrate under reduced pressure gave the crude products. The pure products were isolated by chromatography on silica gel eluted with *n*-hexane:EtOAc (10:3).

Results and discussion

The magnetic cellulose nanocomposites were easily synthesized through the co-precipitation method. Fe_3O_4@NFCs was functionalized with ethylenediamine as a ligand with the ability of chemical coordination to Co(II). This nano catalyst was employed for the FT-IR, TGA, TEM, SEM, VSM, EDS and ICP-AES analysis.

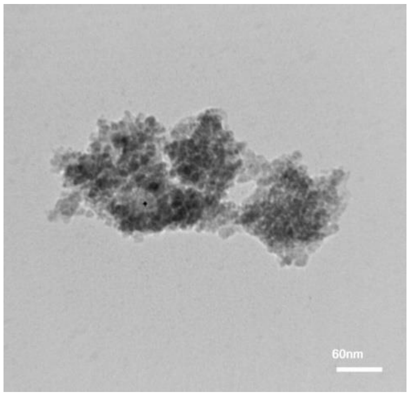


Fig. 1 TEM images of Fe_3O_4@NFC-NH2-Co^{II} NPs

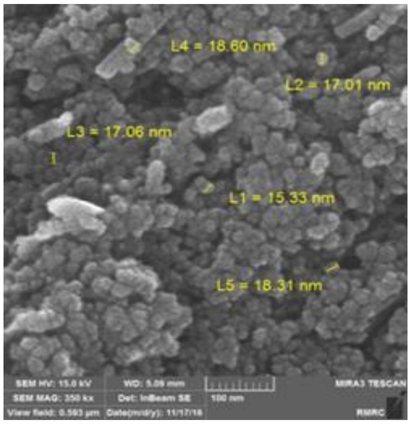
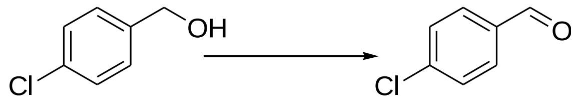


Fig. 2 SEM images of Fe_3O_4@NFC- NH2-Co^{II}

The TEM images of the Fe_3O_4@NFCs-NH_2-Co^{II} NPs (Fig. 1) revealed that a large number of CoNPs with the defind size were formed and uniformly distributed onto the surface of Fe_3O_4@NFCs-NH_2 after deposition. According to the SEM micrograph (Fig. 2)
it was observed that the synthesized Fe_3O_4@NFC- NH_2-Co^{II} NPs has spherical morphology. The EDX analysis confirmed the presence of C, N, O, Si, Fe, and Co elements in the nanocatalyst structure. with FT-IR spectra, TGA and VSM of nano catalyst Fe3O4@ CNPs-Pr -NH2 has been approved Structure of this nano catalyst. In addition, The Co content of Fe_3O_4@NFCs-NH_2-Co^{II} was determined by ICP-OES. The ICP-OES analysis showed that 0.17 gr equal 2.87 mmol of Co was anchored on 1.0 g of the catalyst, which is in agreement with the value determined by EDX.

The catalytic activity of the novel synthesized Fe_3O4@NFCs-NH_2-Co^{II} was evaluated through the oxidation of aromatic alcohols using TBHP as an oxidant in ethyl acetate as a green solvent. Firstly, the oxidation of 4-chlorobenzl alcohol (0.125 mmol) with TBHP (0.25 mmol) was chosen as a model reaction. The obtained data for various temperatures, catalyst loads and solvents are summarized in table 1. It is evident that the best experimental results for oxidation of 4-chlorobenzl alcohol are obtained when the reaction is performed in the presence of 0.001 mg of Fe_3O_4@NFC-NH2-Co^{II} as a nanocatalyst in ethyl acetate as a solvent at 45°C (Table 1. Entry 5). the yield of the oxidation product decreased for the above-mentioned reaction when the nanocatalyst was replaced by Fe3O4@CNFs (40 %) and Co(OAc) (60 %) as well as in the absence of any catalyst under the same conditions.

Table 1. Optimization of various reaction parameters for the oxidation 4-chlorobenzl alcohol[a]



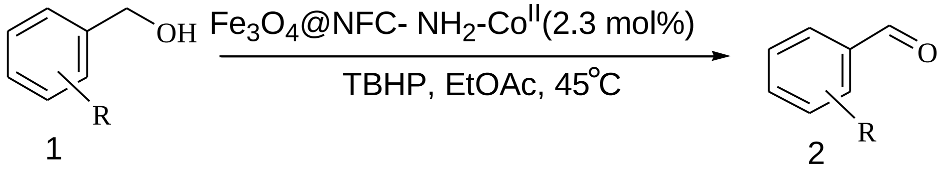
Ent.	Catal. (mg)	Solvent	Tem. °C	Time min	Isolatet[b] Yield%
1[c]	0.001	EtOH	45	120	90
2	0.001	H2O	45	120	50
3	0.001	CH3CN	45	120	90
4	0.001	S.F	45	120	40
5	**0.001**	**EtOAC**	**45**	**30**	**90**
6	0.002	EtOAC	45	60	80
7	0.003	EtOAC	45	60	75
8	0.001	EtOAC	25	60	20
9	0.001	EtOAC	40	30	60
10	0.001	EtOAC	50	60	80
11	0.001	EtOAC	70	30	80
12[d]	2.3%	EtOAC	45	30	60
13[e]	2.3%	EtOAC	45	30	40
14	-	EtOAC	45	120	30

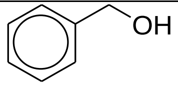
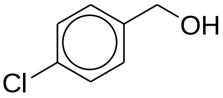
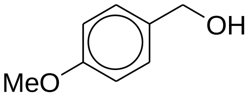
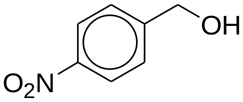
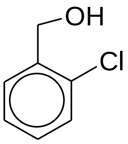
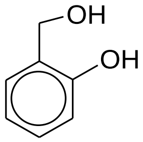
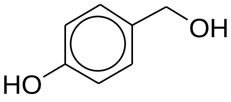
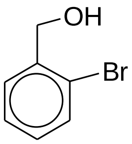
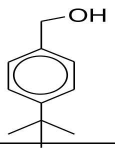
[a] Reaction conditions: 4-chlorobenzyl alcohol (0.125 mmol), TBHP (0.25 mmol)
[b] Isolated yields
[c] 0.001 mg equal 2.3 mol%
[d] The reaction was performed in the presence of $Co(OAc)_2$
[e] The reaction was performed in the presence of Fe_3O_4@CNFs

on the other hand the reaction performed in the presence of various oxidants (O_2, H_2O_2, Oxone) with low efficiency.

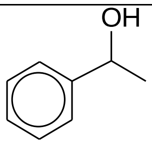
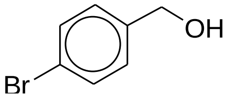
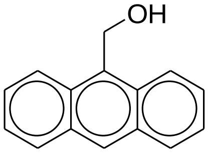
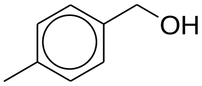
Encouraged by these results, we next examined the generality and efficiency of this approach for the oxidation of a wide variety of aromatic alcohols. The results are summarized in Table 2.

Table 2. Oxidation of various alcohols using TBHP catalyzed by Fe_3O_4@NFCs-NH_2-Co^{II}



Entry	Alcohol	product	Time(h)	Conversion% (Selectivity)
1		2a	1	70 (100)
2		2b	0.5	90 (100)
3		2c	1	75 (100)
4		2d	3	60 (100)
5		2e	3	90 (100)
6		2f	3	30 (70)
7		2g	3	50 (100)
8		2h	1.5	70 (100)
9		2i	1.5	60 (100)

Continuation table 2

Entry	Alcohol	product	Time(h)	Conversion% (Selectivity)
10		2j	2	80 (100)
11		2k	1.5	80 (100)
12		2l	3	40 (100)
13		2m	1	85 (100)

Finally, recycling experiment was conducted to find out the stability and reusability of the catalyst after the reaction. The efficiency of the recovered catalyst was verified with Entry 2, Table 2. The catalyst was easily separated by external magnet, washed with EtOAc, dried and reused for at least five times without any appreciable loss of its catalytic reactivity.

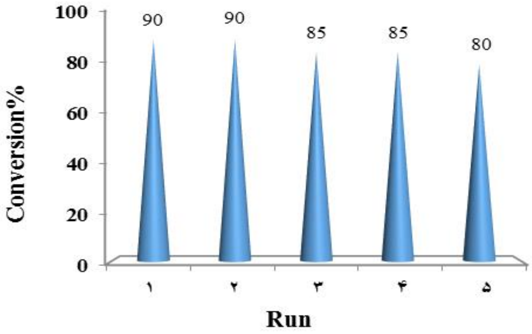


Fig. 3 Reusability of nanocatalyst Fe_3O_4@NFCs-NH_2-Co^{II} In oxidation reaction 2a using TBHP in EtOAc at 45° C

Conclusion

In summary, Fe_3O_4@NFCs-NH2-Co^{II}, a novel, bio-based and efficient heterogeneous magnetic nanocatalyst has been prepared and utilized for the oxidation of aromatic alcohols using TBHP as an oxidant in ethyl acetate as a green solvent at 45° C. Moreover, the broad scope, operational simplicity, practicability, mild reaction conditions, product purity and easy separation of the catalyst with the assistance of an external magnetic field and reusability of the nanocatalyst for up to 5 cycles without significant degradation in activity render it an attractive approach for oxidation of aromatic alcohols.

Acknowledgments

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Graphical Abstract

Cobalt nano-particles supported on ethylenediamine functionalized magnetic cellulose nanofibers as a novel and efficient catalyst for oxidation of alcoholes

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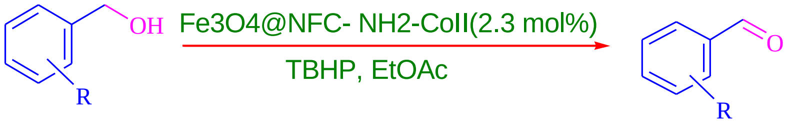

1a-1m

2a-2m

30-90%

تخمین و برآورد اندازه و فواصل ذرات بر اساس مشخصات الکتریکی و مغناطیسی در کاربردهای نانوکاتالیست ها

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چکیده

در این مقاله خواص الکتریکی و مغناطیسی نانو ذرات تحلیل می شود. یکی از مشکلات اصلی در بسیاری از کاربردها کنترل دقیق اندازه، شکل و نحوه توزیع نانو ذرات است. ذرات باردار در ابعاد اتمی و آرایش آنها اندرکنش مواد و الکترومغناطیس را باعث می شوند. نانو ذره به شکل کره در میدان یکنواخت الکتریکی و مغناطیسی، تغییراتی را در میدان بوجود می آورد که مرتبط با خواص الکتریکی و مغناطیسی آنهاست. برای دست یابی به این خواص، معادله لاپلاس با توجه به شکل ذره حل شده و میدانهای ثانویه با استفاده بر هم نهی جوابها بدست می آید اغتشاش در اطراف ذره بر حسب شعاع و زاویه نسبت به حالت اولیه لحاظ می گردد. با پردازش جوابهای مذکور، تاثیر پارامترها و مشخصات الکترومغناطیسی رسانش، دی الکتریک و مغناطیس ذره روشن می گردد. با شناخت خواص الکتریکی و مغناطیسی از این تحلیل می توان راهکارهای مناسبی با توجه به واکنش پذیری، حفاظت و یا ایزوله کردن، پایداری سازی، جداسازی سریع و آسان و استفاده مجدد کاتالیست ها جستجو نمود.

واژگان کلیدی : مشخصات الکترومغناطیسی، نانو ذرات، شکل و اندازه ذرات، میدان و پتانسیل ثانویه

۱- مقدمه

گفته می شود تفاوت اندازه کوچکترین ذرات و بزرگترین اجسام بیش از $۱۰^{۴۰}$ برابر است. اگر فاصله ها را کم کنیم به مولکولها و اتمها و ذرات درون اتمی می رسیم. پرداختن به ابعادکوچک تا حد نانو ما را با دنیای شگفت انگیز همراه با کاربردها و چالشها علمی و فنی مواجه می کند. کاربردهای نانو ذرات نامحدود به نظر می رسد. با وجود کاربردهای بسیار گسترده و زمینه های تحقیق و پژوهش وسیع، هنوز تعریف یکتایی برای نانو ذرات وجود ندارد. معمولا ذراتی که اندازه آنها کوچکتر از ۱۰۰ نانو متر باشد در حوزه نانو قرار می گیرد. در واقع مشخص شده است که ذرات با اندازه های کمتر از ۱۰۰ نانومتر دارای ویژگیهای متفاوتی در مقایسه با مقیاسهای دیگر همین مواد هستند. نانو ذرات ویژگی کامل و یا توسعه یافته ای مبتنی بر اندازه،پراکندگی، شکل، فاز و غیره در مقایسه با اندازه های حجیم همین ذرات از خود نشان می دهند. عمده ویژگی نانوذرات با ویژگی مکانیکی، شیمیایی، حرارتی، نوری، سطحی، الکتریکی و مغناطیسی قابل استخراج است که در اینجا تمرکز بر ویژگی الکتریکی و مغناطیسی می باشد. با گذشت چند دهه طراحی و ساخت در ابعاد نانو به موفقیت های بسیاری دست یافته و مرزهای علوم شیمی، بیولوژی، مواد، فیزیک و مهندسی درهم ریخته است و برای فهم نانو ذرات به همه علوم نیاز می باشد.

در الکترولیز ولتاژ و جریان آند و کاتد تعیین کننده هستند فلزات مختلف برای آند و کاتد، منابع مستقیم و متناوب بکار گرفته می شود. روشهای آزمایشگاهی برای تحلیل بکار می روند. رسانایی آب در حالت عادی و با حضور میدان الکتریکی فعل و انفعالات شیمیایی موجب شده و منجر به نتایج الکتریکی می گردد[1]. استفاده از روشهای شیمیایی برای دانستن مشخصه های الکتریکی کاتالیست ها زمانبر، پیچیده و با هزینه بالاست. پاسخ فرکانسی کاتالیست ها از طریق اندازه گیری ثابت دی الکتریک به روش حفره تشدید موجبری و روش خط انتقال و انعکاس انجام شده است[2] . جداولی از ضریب دی الکتریک برای مایعات در فاصله درجه حرارت ۱۰ تا ۵۰ درجه تا فرکانس 5GHz ارائه شده اند. با استفاده از داده ها، پردازشهای مختلفی برای آب خالص و مایعات دیگر قابل حصول است. در فرکانسهای رادیویی و مایکروویو ضریب دی الکتریک مختلط مایعات قطبی، اتلاف و پلاریزاسیون را توصیف کرده و نیز برای محاسبه نرخ ویژه جذب بکار می روند.[3].

در مورد نانو ذرات مغناطیسی و کاربرد آنها گستره زمانی و کاربردی وسیع تر به نظر می رسد. اول از هر چیزی با کلمه مغناطیس ممکن است که کبالت و آهن و نیکل به ذهن برسد اما امروزه نانو ذرات اکسیدآهن مغناطیسی به دلایل خاصیت مغناطیسی، مساحت سطح گسترده، نسبت سطح به حجم بالا و تاثیر پذیری از میدان مغناطیسی بیشتر مورد توجه قرار گرفته است. برای فهم ارتباط نانو ذرات و خواص مغناطیسی لازم است تا ابتدا علت خواص و پارامترهای که خواص مواد را توصیف می کنند مشخص شود. از تشریح تاریخچه و چگونگی ارتباط الکتریستیه و مغناطیس بخاطر طولانی بودن می گذریم. نانو ذرات مغناطیسی انواع مختلفی دارند و شامل اکسید آهن Fe3O4 ، فلزات خالص co,Fe ، فرومغناطیس های MnFe2o4 , MgFe2O4 , CoFe2O4 و آلیاژها FePt , CoPt می شوند. خواص نانو ذرات مغناطیسی به اختصار عبارتند از : - پایداری شیمیایی در شرایط و محیط های مختلف – اندازه کوچک ذرات – دارای سطح مقطع بزرگ برای جذب و برهمکنش – سرعت کم ته نشینی در مقایسه با فرآیندهای جداسازی – تولید آسان و کم هزینه – پاسخ خوب به میدان مغناطیسی اعمالی – سطح زیست سازگار. همانگونه که اندازه ذرات کاهش می یابد سطح ذرات بیشتر شده و اثر سطح مشترک اهمیت می یابد. وقتی که اندازه نانو ذرات کاهش می یابد به حدی می رسد که به صورت تک حوزه مغناطیس در می آید و دارای سوپر پارامغناطیسی می شود. یک ذره تک حوزه بطور یکنواخت مغناطیده می شود و تمام اسپین ها در یک جهت منظم قرار می گیرد[4,5].

دلیل اصلی و تعیین کننده پیدایش خاصیت کاتالیستی در نانو مواد نسبت سطح به حجم بسیار بالای آنهاست. در اصل دلیل این خواص به تغییر در ساختار الکترونی مواد بر میگردد. چنین موقعیتی با مکانیک کوانتمی قابل تحلیل است. در حالت ذرات خیلی کوچک، چگالی حالات نوار ظرفیت دچار تغییر شده و مجموعه ای از ترازهای گسسته مشاهده می شود. از آنجا که ساختار الکترونی نانو ذرات به اندازه ذره بستگی دارد. قابلیت آنها در واکنش دادن با دیگر نمونه ها نیز به اندازه آنها بستگی دارد. [6] . روشهای بسیار متعددی در منابع جهت تحلیل اندازه و سایر مشخصات ذرات وجود داردکه هر کدام پیچیدگی خاص خود

را دارد. در این مقاله روشی بر اساس الکترومغناطیس کلاسیک برای دست یافتن به اندازه نسبی فواصل ذرات به ابعاد آنها ارائه می گردد. ابتدا به دیدگاه میکروسکوپی خواص الکتریکی و مغناطیسی اشاره می شود. در ادامه روش الکترواستاتیکی متکی بر حل معادله لاپلاس مطرح می شود و در نهایت اثر ذره کروی در اطراف بررسی می گردد.

۲- نگرش میکروسکوپی به الکتریسیته و مغناطیس

هادیهای الکتریکی موادی هستند که دارای الکترونهای آزاد می باشند. توصیف رسانش در آنها، براساس مدل میکروسکوپی ساده امکان پذیر است. تحت تاثیرمیدان الکتریکی به الکترونها نیرو وارد شده و موجب حرکت آنها می شود و در نتیجه جریان الکتریکی ایجاد می گردد. با توجه به ساختار هادیها الکترونهای متحرک به الکترونهای دیگر برخورد می کنند. این برخوردها در اثر نیروی بازدارنده، باعث کاهش سرعت الکترونها می شود با بکارگیری قانون نیوتن و مشخصات ساختاری مواد، حالت پایدار اتفاق می افتد و جریان متناسب با میدان الکتریکی در هادیها جاری می گردد. ضریب تناسب همان ضریب هدایت یا ضریب رسانندگی ویژه مواد گفته می شود. ضریب رسانندگی که طبق قانون اهم رابطه بین جریان و میدان الکتریکی را مشخص می کند یک پارامتر اساسی تمامی مواد است. این ضریب برای هادیهای کامل بینهایت و برای فلزات خوب همانند مس، آلومینیم و طلا عدد بزرگ و برای نیمه هادیها متوسط و در مورد عایق ها کوچک و در نهایت برای عایقهای کامل صفر است. خواص عمده هادیهای کامل که معیار مناسبی برای سنجش رسانش است به اختصار عبارتند از : میدان الکتریکی در داخل آنها صفر است. بارهای الکتریکی در سطح آنها مستقر می شوند و در نه در حجم آنها. مولفه مماسی میدان الکتریکی در سطح آنها صفر است. مولفه عمودی میدان الکتریکی در سطح آنها متناسب با چگالی بار سطحی است. نقاط داخل و سطح هادیها هم پتانسیل هستند.

عایقها الکتریکی موادی هستند که الکترونها براحتی از اتمها جدا نمی شود. مدل مناسب برای توصیف عملکرد آنها، مفهوم دو قطبی است که دو بار غیر همنام با فاصله کوچک را در بر می گیرد. حاصل ضرب بار در فاصله را ممان یا گشتاور دو قطبی گویند. موادی دی الکتریک متشکل از دوقطبیها هستند که در حالت عادی بعلت توزیع تصادفی، اثر همدیگر را خنثی می کنند. با اعمال میدان الکتریکی دو قطبیهای موجود منظم شده و باعث ایجاد پتانسیل و میدان ثانویه می گردند. چنین عملکردی با بردار پلاریزاسیون نشان داده می شود که بصورت زیر تعریف می گردد[7].

$$P = \lim_{\Delta v \to 0} \frac{\sum_{i=1}^{n\Delta v} p_i}{\Delta v} \quad , \qquad D = \epsilon E \ , \qquad P = (\epsilon - \epsilon_0)E \ , \quad \epsilon = \epsilon_0 \epsilon_r$$

که در آن n تعداد دو قطبیها در واحد حجم و Δv عنصر کوچک حجم است. وجود پلاریزاسیون باعث بارهای مقید حجمی و سطحی می گردد. این بارها پتانسیل و میدان ثانویه ایجاد می کنند لحاظ کردن اثر این بارها در قوانین ماکسول تحلیل چنین موادی را امکان پذیر می سازد. روابط بین بردار پلاریزاسیون و میدان الکتریکی و چگالی شار الکتریکی با در نظر گرفتن بارهای

آزاد و مقید منجر به روابط خطی می گردد که ضریب دی الکتریک نقش اساسی آنها دارد ضریب دی الکتریک نسبی ϵ_r یکی از پارامترهای اصلی عایقهاست.

مواد مغناطیسی با حرکت شتاب دار ذرات باردار مرتبط است. بر طبق نظریه های اتمی الکترونها در ساختارهای اتمی دارای دو نوع حرکت، حرکت مداری الکترون حول هسته و حرکت اسپینی الکترون حول قطر خود می باشند. چرخش الکترون با مفهوم جریان الکتریکی توصیف می گردد. حرکت الکترون و جریان بعنوان منبع ایجاد میدان مغناطیسی، با کمیت گشتاور حلقه دو قطبی مغناطیسی مدل می گردد. اندازه بردار گشتاور یک دو قطبی مغناطیسی با حاصل ضرب جریان در مساحت حلقه تعریف می گردد. در حالت عادی مواد مغناطیسی دارای تعدادی زیادی دوقطبی مغناطیسی هستند که بصورت نامنظم توزیع شده اند و اثر همدیگر را خنثی می کنند. وقتی این مواد در میدان مغناطیسی قرار می گیرند. دو قطبیها منظم شده و باعث میدان مغناطیسی ثانویه می گردند. بردار مغناطیس شدگی را می توان بصورت زیر تعریف نمود.

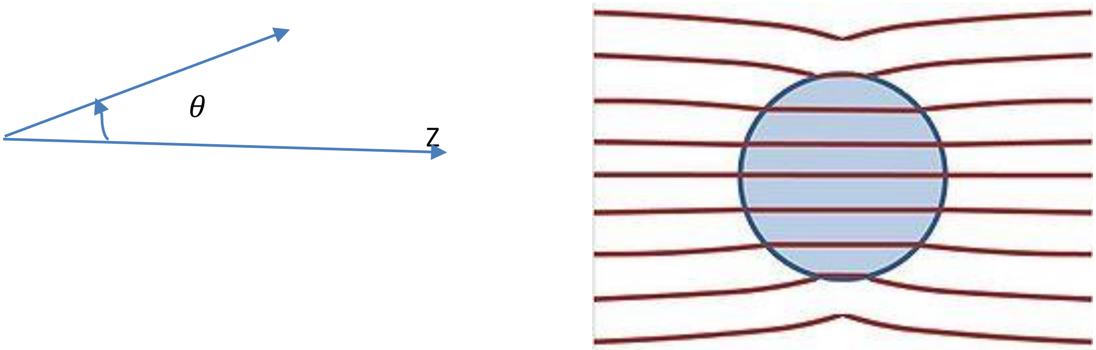
$$M=\lim_{\Delta v\to 0}\frac{\sum_{i=1}^{n\Delta v} m_i}{\Delta v}\ ,B=\mu H\quad ,\quad M=(\mu_r-1)H\ ,\ \ \mu=\mu_r\mu_0$$

مغناطیس شدگی باعث جریانهای مغناطیس شدگی حجمی و سطحی می گردد. تلفیق جریانها در روابط فوق مشاهده می شودضریب μ را ضریب مغناطیسی مواد گویند به اختصار سه پارامتر σ وϵ و μ پارامترهای اساسی الکترومغناطیسی مواد گویند که مشخص بودن آنها خواص الکتریکی و مغناطیسی و اندرکنش مواد و میدانهای الکتریکی و مغناطیسی را امکان پذیر می سازد در ادامه برآورد آنها را مورد بررسی قرار می دهیم.

۳- تحلیل یک ذره کروی در میدان یکنواخت

اندازه مواد در خواص و مشخصات آنها نقشی اساسی دارند. بسیاری از مواد که در ابعاد معمولی خواص الکتریکی و مغناطیسی ندارند با کاهش اندازه تا مقیاس نانو، از خود خواص مذکور را بروز می دهند. شکل ذرات بخصوص نسبت سطح به حجم از معیارهای مهم خواص ذرات به شما می رود. اثر متقابل مواد و ذرات با میدانهای الکتریکی و مغناطیسی نیز به شکل، اندازه و جنس آنها و حتی فواصل ذرات از هم بستگی شدیدی دارند. در اینجا شکل ذرات کروی و میدانهای الکتریکی و مغناطیسی یکنواخت گرفته می شود. اغتشاش و تغییر میدانهای یکنواخت به جنس آنها یعنی ضرایب الکترومغناطیسی وابسته است. در واقعا با استفاده از محاسبه تغییر میدانها می توان به مشخصات آنها پی برد. تحلیل بر اساس حل معادله لاپلاس برای پتانسیل استوار است . در واقع میدانها با محاسبه گرادیان پتانسیل بدست می آیند. بخاطر تقارن کروی جوابهای معادله لاپلاس دو بعدی کارساز است. جواب عمومی معادله لاپلاس متشکل از توابع نمایی برای فاصله و توابع لژاندر برای زاویه در منابع در دست رس

است. با استفاده از اصل جمع آثار و اعمال شرایط مرزی در هر مورد جوابها بدست می آیند. شکل زیر حالت کلی قرار گرفتن جسم کروی و اثر آن در میدان یکنواخت را نشان می دهد.θ



شکل ۱ : جسم کروی در میدان یکنواخت و اثر آن روی میدان در حالت کلی

جواب کلی معادله لاپلاس برای پتانسیل در این حالت بصورت زیر است [8].

$$V(r,\theta) = \sum_{n=0}^{\infty} \left(A_n r^n + B_n r^{-(n+1)}\right) P_n(cos\theta) \quad , \qquad E = -\nabla V$$

با اعمال شرایط مرزی در هر حالت جواب بدست آمده و خواص ذره استنتاج می گردد.

۱-۳ : جسم کروی رسانا در میدان یکنواخت :

قبل از قرار دادن کره در میدان یکنواخت الکتریکی، پتانسیل و میدان بصورت زیر است.

$$E = E_0 a_z \qquad , \qquad E = -\nabla V \quad , \quad V = -E_0 z = -E_0 r cos\theta$$

که در روابط جهت میدان در راستای محور Z گرفته شده است. اگر هدایت ویژه محیط را با σ_0 و هدایت ویژه جسم را با σ نشان دهیم با اعمال شرایط مرزی و محاسبه ثابتها پتانسیل و میدان بعد از قرار گرفتن جسم در میدان یکنواخت، بصورت زیر خواهد بود.

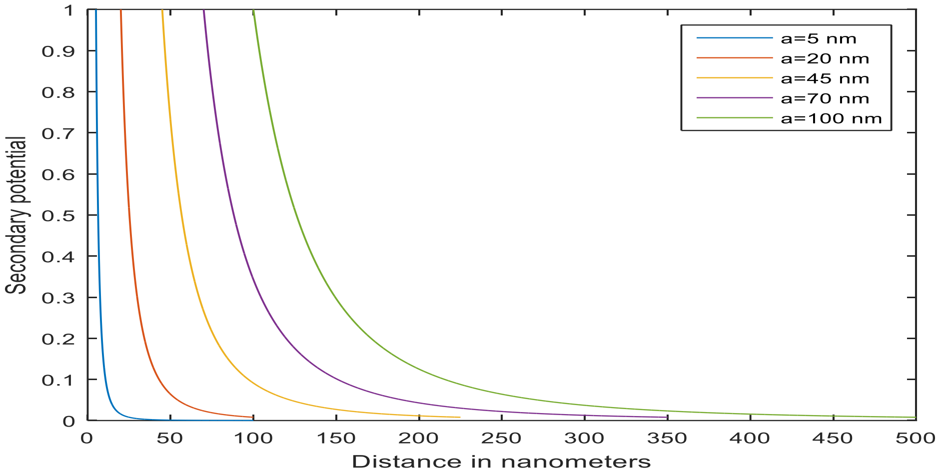
$$V_{in} = -\frac{3\sigma_0}{\sigma + 2\sigma_0} E_0 r cos\theta \qquad , \qquad V_{out} = \left[-1 + \frac{(\sigma - \sigma_0)}{(\sigma + 2\sigma_0)} \frac{a^3}{r3}\right] E_0 r cos\theta$$

در حالت رسانای کامل واقع در محیط بدون هدایت، پتانسیل و میدان در داخل جسم صفر و در بیرون بصورت زیر است.

$$V_{out}(\mathrm{r},\theta) = E_0 \left(-r + \frac{a^3}{r^2}\right) cos\theta$$

چگالی بار سطحی روی کره عبارت از : $\rho_s = 3\epsilon_0 E_0 cos\theta$

پتانسیل ثانویه حاصل از کره رسانای کامل در اطراف آن به ازای شعاعهای مختلف در شکل زیر دیده می شود.



شکل ۲ : پتانسیل ثانویه در اطراف یک ذره کروی فلزی

2-3 : جسم کروی دی الکتریک در میدان یکنواخت :

برای یک کره عایق با ضریب دی الکتریک ϵ_r واقع در میدان الکتریکی یکنواخت، پتانسیل و میدان در داخل کره بصورت زیر بدست می آید

$$V_{in}(r,\theta) = \frac{-3E_0}{(\epsilon_r + 2)} rcos\theta \quad , \qquad V_{out}(r,\theta) = E_0 \frac{a^3}{r^3} \frac{\epsilon_r - 1}{\epsilon_r + 2} rcos\theta - E_0 rcos\theta$$

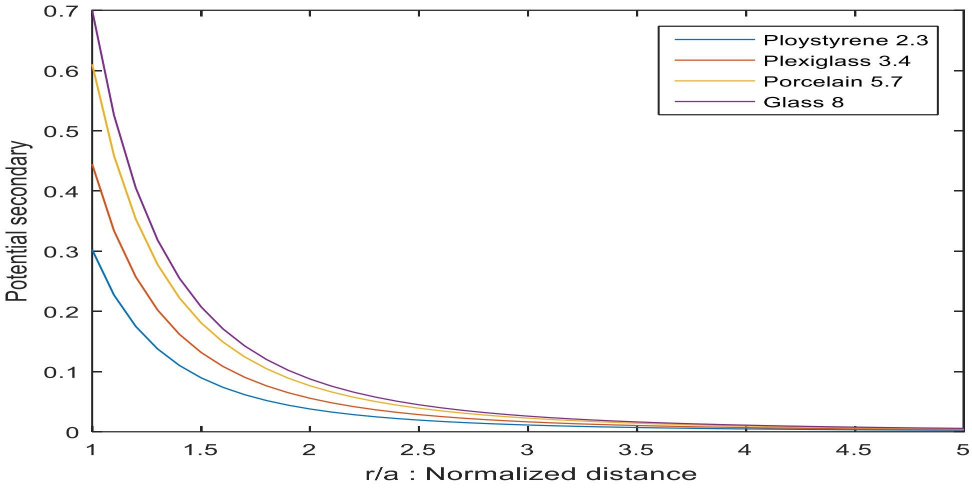
پتانسیل ثانویه حاصل از جسم کروی در میدان یکنواخت برای چند جسم در شکل ۳ دیده می شود

۳-۳ : جسم کروی مغناطیسی در میدان یکنواخت :

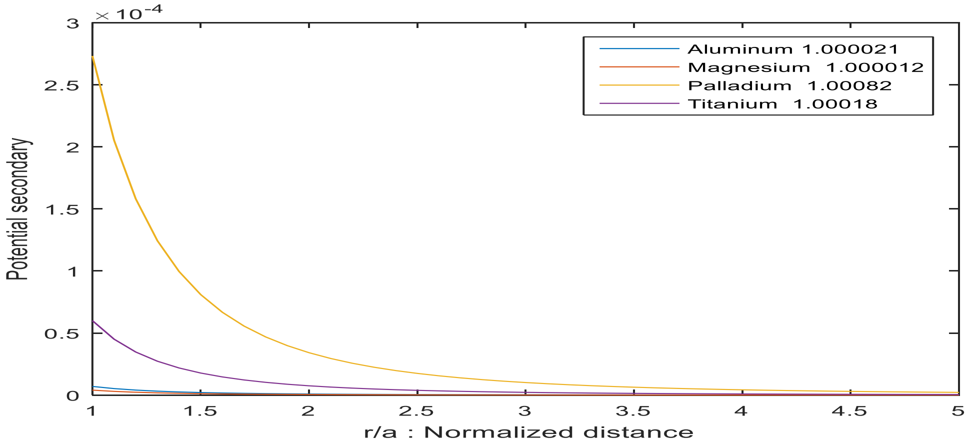
بطور مشابه برای یک جسم کروی با ضریب مغناطیسی μ_r داریم (دو گان حالت الکتریکی)

$$V_{in}^{m}(r,\theta) = \frac{-3H_0}{(\mu_r + 2)} rcos\theta \quad , V_{out}^{m}(r,\theta) = H_0 \frac{a^3}{r^3} \frac{\mu_r - 1}{\mu_r + 2} rcos\theta - H_0 rcos\theta$$

در شکل ۴ پتانسیل ثانویه حاصل از جسم کروی برای چند جسم پارامغناطیسی دیده می شود. علیرغم ماهیت متفاوت میدانها و جسم، اثر آنها در ایجاد پتانسیل و میدان یکنواخت شبیه هم می باشد.



شکل ۳ : پتانسیل ثانویه یک کره دی الکتریک در میدان یکنواخت الکتریکی



شکل ۴ : پتانسیل ثانویه یک جسم مغناطیده برای جسم پارامغناطیس

۳- نتیجه گیری

همانطور که اشاره شد فعالیت کاتالیست یا انتخاب پذیری نانوکاتالیست برای فهم عملکرد نانو کاتالیست دارای اهمیت است. وقتی که مواد به مقیاس نانو برده می شود. خواص الکتریکی، مغناطیسی، نوری و .... دچار تغییر می شوند.سه خصلت حاصل این تغییرات است. اندازه بسیار کوچک. نسبت سطح به حجم بالا. افزایش تعداد اتمها روی سطح . این سه عامل مهم ترین دلایل پیدایش خاصیت کاتالیستی در نانو مواد است. اصولا وقتی ذرات خیلی کوچک می شوند به دلیل انحنای بسیار زیادی که پیدا می کند. دارای اتمهای زیادی روی سطح خود هستند این اتمها پیوند بسیار ضعیفی با اتمهای توده و شبکه دارند. این ذرات انرژی سطحی بسیاری بالایی داشته و به شدت فعال اند و مستعد بسیاری از واکنشهای شیمیایی اند. دلیل اصلی و تعیین کننده پیدایش خاصیت کاتالیستی در نانو مواد افزایش سطح به حجم است. انحنای ذرات تعیین کننده هستند و شکل نانو ذرات باعث

انحناهای مختلف می شوند. هر چه انحنای آنها بیشتر باشد اتمهای آنها فعالترند ذرات غیر کروی همانند مکعب و چند وجهی منظم دارای مکان ها و لبه ها و گوشه های زیاد بوده و بنابراین خاصیت الکتریکی و مغناطیسی و البته نانو کاتالیستی بیشتری از خود نشان می دهند. در اینجا تخمین اولیه از شکل ذرات مورد نظر بود. روشن است که علاوه بر شکل نانو ذرات، هزینه و روش تولید آنها نیز باید مورد توجه قرار گیرد.

نحوه توزیع ذرات و فواصل آنها بر خاصیت کاتالیستی اثر گذار است. از نتایج حاصل دیده می شود که اثر ذرات در ایجاد تغییر در پتانسیل و میدان، مستقل از ماهیت آنهاست. پارامترهای الکترومغناطیسی زمینه و نانو ذره یعنی $\mu_r , \epsilon_r , \sigma$ بصورت مشابه در معادلات نقش دارند. هر چه مقدار آنها بیشتر باشد مقدار عبارت مربوط به این پارامترها به یک نزدیک می شود. همچنین اثر ذره با عکس توان سه فاصله کاهش می یابد. از شکل ۲ دیده می شود که اثر ذره فلزی با فاصله سریعا کاهش می یابد. در فواصل بالاتر از پنج برابر شعاع ذره، اثر ذره به کمتر از یکصدم می رسد. از شکلهای ۳ و ۴ نیز نتیجه مشابه بدست می آید. بدین ترتیب تخمینی از فواصل بدست می آید.

بعنوان نتیجه نهایی می توان گفت که خاصیت کاتالیستی متکی بر خواص الکتریکی و مغناطیسی به اندازه و فواصل ذرات بویژه به نسبت آنها بستگی دارد. کاهش اندازه بصورت مطلق کار ساز نیست. بلکه شکل و اندازه و نسبت پارامترهای الکترومغناطیسی جسم و زمینه بسیار موثرند. عوامل موثر به اختصار عبارتند از : اندازه نانو ذرات، شکل نانو ذرات، نحوه توزیع نانو ذرات، بستر و زمینه نانو ذرات و شرایط انجام واکنش.

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Creating Catalyst Niches, a Breakthrough of Technological development via Uni-Indu collaboration

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In this modern World of embedded technologies, it is a novel discipline to secure and protect research groups that are doing research in a technology focused topic so called as a Technology Niche. Among different technologies, catalyst related technologies and researches got more attention due to importance of this field. it has been reported that over 2/3 of industrial processes need catalyst to handle all or a part of their industrial mission. That seems connecting technology niche discipline to this important field makes a big breakthrough not only in case of improving existed catalytic processes but also can suggest novel and special process to different industries including even non-catalytic industrial processes.

In this work the aim is to suggest a novel tech focused research module entitled catalyst technology niche to prepare a secure and protected environment for research focused on catalyst technologies. Desired result of making such research structure is to create new technologies and process for catalyst industry.[1-2]

Keywords: *Industry collaboration, Technology Niche, embedded technologies.*

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Green synthesis of magnetic $NiFe_2O_4$@CuO nanocomposite using tragacanth gel and its use as an efficient catalyst for the solvent free synthesis of tetrahydrobenzo[b]pyran derivatives

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Multi-component reactions (MCRs) achieve significant role in combinatorial chemistry due to the ability to prepare target compounds with more efficiency and atomic economy by the reaction of three or more compounds together in a single step. Also, MCRs increase simplicity and synthetic efficiency on the conventional organic synthesis [1,2]. The synthesis of tetrahydrobenzo[b]pyran derivatives is important due to their significant anti-coagulant, diuretic, spasmolytic, anticancer, and anti-anaphylactic properties. 2-amino-4H-pyran derivatives can be widely used as photoactive materials. Additionally, substituted 4H-pyrans are observed as units in the structure of some natural products [3,4].

In the present study, for the first time, magnetically $NiFe_2O_4$@CuO nanocomposite was synthesized using tragacanth gel as a green capping agent and biotemplate by the sol-gel method. $NiFe_2O_4$@CuO magnetic nanocomposite was investigated using powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Field emission scanning electron microscopy (FESEM), energy dispersive X-ray analysis (EDX) vibrating sample magnetometer (VSM) and Transmission electron microscopy (TEM). XRD results show that $NiFe_2O_4$@CuO nanocomposite corresponds to the monoclinic of CuO and the spinel cubic structure of $NiFe_2O_4$. Thereupon, a green and efficient method is described for the solvent free synthesis of tetrahydrobenzo[b]pyran derivatives through one-pot three-component condensation of dimedone, an aryl aldehyde, and malononitrile in the presence of $NiFe_2O_4$@CuO nanocomposite as high-performance magnetic catalyst under microwave irradiation (scheme 1). Simple work-up, mild reaction conditions, short reaction times, use of an economically convenient catalyst, and excellent product yields are the advantageous features of this method. The catalyst could easily be recycled and reused five times without noticeable decrease in catalytic activity.

Scheme 1. *Synthesis of tetrahydrobenzo[b]pyran derivatives*

Keywords: *Microwave irradiation; $NiFe_2O_4$@CuO nanocomposite; Tetrahydrobenzo[b]pyran derivatives*

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سینتیک هضم لیپید توسط آنزیم لیپاز تثبیت شده بر سطح نانوکامپوزیت گرافن

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چکیده

آنزیم‌های تثبیت شده، مواد زیست فعال مهمی هستند که کاربردهای گسترده‌ای در صنایع شیمیایی، دارویی و بیوتکنولوژی دارند. با این وجود، مکانیسم عمل آنزیم تثبیت شده در واکنش‌های مربوطه به درستی درک نشده است. به این منظور بسترهای مختلف اعم از ژلاتین، گرافن و نانوکامپوزیت ژلاتین- گرافن با ترکیب درصدهای ۱۰ و ۱۵ درصد وزنی جهت تثبیت آنزیم لیپاز مورد استفاده قرار گرفت. هیدرولیز تری گلیسرید توسط آنزیم لیپاز با تیتراسیون بر حسب زمان مورد مطالعه قرار گرفت. مدل سینتیکی منطبق بر سرعت اولیه واکنش علاوه بر برازش داده‌های تجربی بر معادله مکائیلس-منتون با در نظر گرفتن حجم لیپید و غلظت آنزیم بسط و توسعه یافت. منحنی بررسی زمانی واکنش بر حسب مدل بطور مشخص در توافق با داده های تجربی بود. بررسی نتایج داده‌های تجربی و تئوری نشان می‌دهد که فرآیند هیدرولیز طی دو مرحله انجام می‌گیرد که گاهی اوقات همپوشانی دارند.

واژگان کلیدی : زیست کاتالیست، پارامترهای سینتیکی، لیپاز

۱- مقدمه

هیدرولیز لیپید امولسیون شده توسط لیپازها از نقطه نظر کاربردی از اهمیت بسیار بالایی برخوردار است، زیرا که جایگزین مناسبی برای سنتز اسید های چرب نسبت به روش‌های شیمیایی مرسوم است. علاوه بر این، امولسیون های تری گلیسرید (O/W) محیطی برای بسیاری فرایند مهم و کاربردی کاتالیزوری لیپاز در طبیعت فراهم می‌کنند، مانند تصفیه فاضلاب با مقدار چربی بالا یا در فرایندهای شستشو، که لیپاز به خوبی لکه‌های چربی را در دمای پایین حذف می‌کند[1][2]. علی رغم این واقعیت‌ها، بیشتر مطالعات در مورد سینتیک فعالیت آنزیم روی سیستم‌های همگن انجام شده است. هر چند سیستم‌های ناهمگن با استفاده از آنزیم تثبیت شده دارای مزایایی متعددی ازجمله سهولت بازیابی آنزیم است که پارامتر مهم تعیین کننده کاربرد آنزیم در فرایندهای صنعتی است. با این حال مهمترین نقطه ضعف این روش، کاهش فعالیت آنزیم تثبیت شده در مقایسه با نوع آزاد است. همچنین لازم به ذکر است که اکثر مطالعات سینتیکی هیدورلیز لیپید تا به حال بر سرعت اولیه واکنش متمرکز بوده و اثر بازدارندگی بر فعالیت آنزیم مورد بررسی قرار نگرفته است[3,4]. بنابراین بررسی فعالیت آنزیم

تثبیت شده در طول مدت زمان واکنش جهت ارزیابی عملکرد آنزیم در کاربردهای زیستی علاوه بر حصول دیدگاه کامل بر مکانیسم عملکرد لیپید در فرایندهای تصفیه آب و شستشو بسیار حائز اهمیت است.

هرمانش و همکارانش[5] مدل سینتیکی برای هیدرولیز تری گلیسیرید با آنزیم را با مکانیسم پینگ پونگ بی برای یک واکنش سه مرحله‌ای ارائه دادند. این مدل پیشرفت واکنش در طول زمان را پیش بینی می‌کند، اما منجر به ثابت سرعت و ثابت جذب بالا می‌شود که در قیاس با مطالعات پیشین قابل اعتبار نیست. با وجود پیچیدگی‌های این مدل، پیشرفت جزئی در برازش داده‌ها در مقایسه با مدل میکائیلس-منتون (Michaelis-Menten) مشاهده می‌گردد. تلاش های زیادی به منظور توسعه روش های آنالیز سینتیکی آنزیم برای تفسیر عامل بازدارنده انجام شده است[6,7]. با این حال، هیچ روش عمومی، مستقیم و عملی برای استخراج پارامترهای آنزیمی از منحنی‌های غیر خطی بدست نیآمده است. در تحقیق حاضر مدل سینتیکی برای هیدرولیز لیپید با آنزیم PSSD توسعه یافته است. این مدل جهت بررسی سینتیک هیدولیز لیپید در طی زمان بر پایه‌های مختلف مورد ارزیابی قرار گرفته است. این مدل سینتیکی جهت پیش گویی رفتار آنزیم تثبیت شده در قیاس با انواع آزاد بسیار کاراست. چندین فرضیه درباره جهتگیری فضایی مولکول‌های تری و دی گلیسیرید بر سطح آنزیم بیان شد که نهایتاً با مطالعه نتایج تجربی تایید گردید.

۲- بخش تجربی

۲-۱- مواد

در این تحقیق از ژلاتین نوع B با بلوم[۱] ۸۰-۱۲۰ خریداری شده از شرکت سیگما-آلدریچ[۲] استفاده شد. گرافیت با درصد خلوص ۹۹/۵ و میزان کربن ۹۹/۶ از شرکت Graphit Kropfmühl خریداری شد. محلول‌دی‌متیل‌هیدرازین، اسید سولفوریک، اسید هیدروکلریک، پرمنگنات منیزیم، نیترات سدیم، هیدروکسید سدیم، سولفات پتاسیم، پتاسیم، کلرید منیزیم، کلرید سدیم، تری‌بوتیرین، Triton X-100، کلرید کلسیم، هیدروکسید سدیم و نمک های بافر فسفات همگی از شرکت های سیگما-آلدریچ و مرک تهیه شد. آنزیم PSSD از شرکت آمانو خریداری شد. برای تمامی فرآیندهای این مطالعه از آب مقطر بدون یون استفاده شد.

۲-۲- روش کار

به منظور مطالعه سینتیک آنزیم آزاد و تثبیت شده از روش تیتراسیون بر پایه تنظیم pH استفاده گردید. امولسیون سوبسترا با فراصوت‌دهی توسط دستگاه فراصوت دهنده Dr Kielscher GmbH حاصل گردید. میزان هضم توسط دستگاه تیتراسیون (Titrando, 800 Dosino 2 mL, software tiamo 2.3, Metrohm ۸۴۲) ساخت سوئیس با الکترود پاسخ

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[1] Bloom

[2] Sigma-Aldrich Company

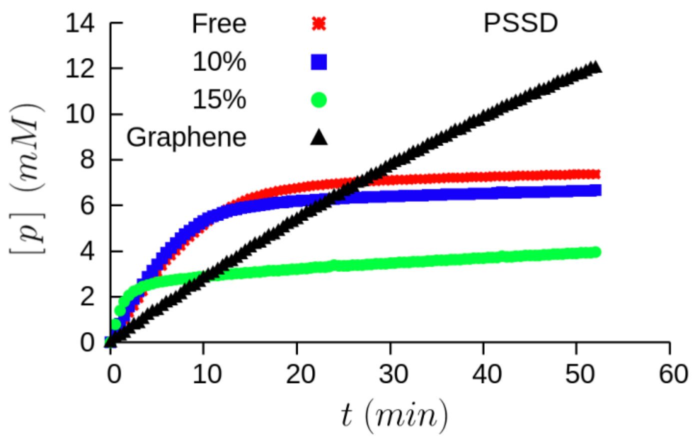
سریع Unitrode Nr. 6.0259.100 انجام شد. میزان اسید رها شده در طی فرایند هضم توسط تیتراسیون خودکار همراه با افزودن هیدروکسید سدیم اندازه گیری شد. دمای مخلوط واکنش با استفاده از حمام دستگاه ثابت نگه داشته شد. آنزیم لیپاز آزاد یا تثبیت شده به امولسیون پیش حرارت داده شده در محفظه تیتراسیون با سرعت هم‌زدن ثابت اضافه می‌شود. سپس داده‌ها با استفاده از معادله سینتیک میکائیلس-منتون برازش گردید.

۳- نتایج و بحث

۳-۱- آنالیز و نتایج مربوطه

در این بخش سینتیک هضم لیپید توسط آنزیم لیپاز PSSD به صورت آزاد و تثبیت شده مورد مطالعه قرار گرفت. در شکل مقادیر تجربی حاصل با روش تیتراسیون گزارش شده است. ابتدا بر اساس رابطه میکائیلس-منتون نتایج مورد ارزیابی قرار گرفت (واکنش ۱). در این رابطه e معرف آنزیم، s پایه و p محصول است.

$$e + s \overset{k_1,\,k_{-1}}{\Longleftrightarrow} e.s \xrightarrow{k_2} e + p$$ واکنش ۱



شکل ۱- هضم لیپید توسط آنزیم PSSD به صورت آزاد و تثبیت شده در طی زمان.

با فرض حالت شبه پایا، می‌توان پارامترهای مؤثر بر این رابطه اعم از $K_m \equiv (k2 + k - 1)/k1$ و $V_{max} \equiv k2\ [e0]$ را بدست آورد که $[e_0]$ غلظت آنزیم استفاده شده در آزمایش می‌باشد[8]. بررسی زمانی سینتیک شامل دو مرحله است که بعد از یک مرحله خطی غلظت محصول[p] به مرحله ترازه می‌رسد. ابتدا باید معادله میکائیلس-منتون را بر اساس حضور بازدارنده (i) در سامانه بازنویسی کرد که فرض شده محصول در این واکنش شرکت نمی‌کند (واکنش ۲).

$$e + s \overset{k_1,\,k_{-1}}{\Longleftrightarrow} e.s \xrightarrow{k_2} e + p + i \xrightarrow{k_3} p + e.i,$$ واکنش ۲

مدل قبلی حالت خاص واکنش عمومی است که کاو و همکاران به آن پرداختند[9]. در این کار آن‌ها نشان دادند که می‌توان بررسی زمانی تولید محصول با تأثیر بازدارندگی را با تقریب خوبی به صورت تابع نمایی ساده توضیح داد.

معادله ۱

$$[P](t) = \frac{v_0}{\eta}(1 - e^{-\eta t})$$

که v_0 و η بستگی به ثابت سرعت‌های متعدد واکنش دارند. در زمان‌های اولیه معادله ۱ به حالت خطی تبدیل می‌گردد، همچنین کاو نشان داد که پارامتر v_0 به این‌صورت بدست می‌آید (معادله ۲).

معادله ۲

$$v_0 = \frac{\tilde{V}_{\max}[S_0]}{\tilde{K}_M + [S_0]}$$

در معادله ۲ $\tilde{K}_M$ و $\tilde{V}_{max}$ ترکیب ثابت سرعت‌های اولیه هستند که در غیاب بازدارنده به پارامترهای استاندارد میکائیلس-منتون تبدیل می‌شوند. در اینجا داده‌های تجربی بر اساس معادله ۱ برازش شده و امکان مقایسه کمی آنزیم تثبیت شده بر پایه‌های مختلف را با توجه به مقدار v_0 می‌دهد. علت انتخاب این پارامترها به این‌صورت است که فرض گرفته شد جذب آنزیم روی پایه بر تشکیل کمپلکس و نه سرعت تشکیل یا جدایش آنزیم از پایه تأثیر می‌گذارد. به بیان دیگر کمپلکس آنزیم و پایه همانند آنزیم آزاد مورد بررسی قرار می‌گیرد. در این صورت در معادله میکائیلس-منتون این فرض به این معنی است که جذب آنزیم روی پایه سرعت تشکیل کمپلکس k_1 و غلظت اولیه آنزیم $[e_0]$ را تحت تأثیر قرارداده و بی‌تأثیر بر سرعت‌های k_{-1} و k_2 است. در معادله ۲ بدون در نظر گرفتن بازدارندگی و در غلظت کم پایه اولیه ($s_0 \ll K_M$) معادله ۳ بدست می‌آید.

معادله ۳

$$v_0 \approx \frac{V_{\max}[S_0]}{K_M} = \frac{k_2}{k_{2+k_{-1}}} k_1[e_0]$$

و در غلظت بیشتر پایه ($s_0 \gg K_M$) معادله ۴ حاصل می‌شود.

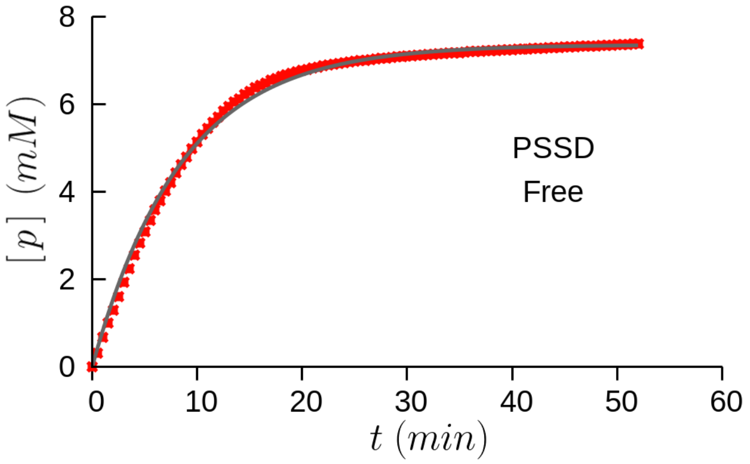
معادله ۴

$$v_0 \approx V_{max} = k_2[e_0]$$

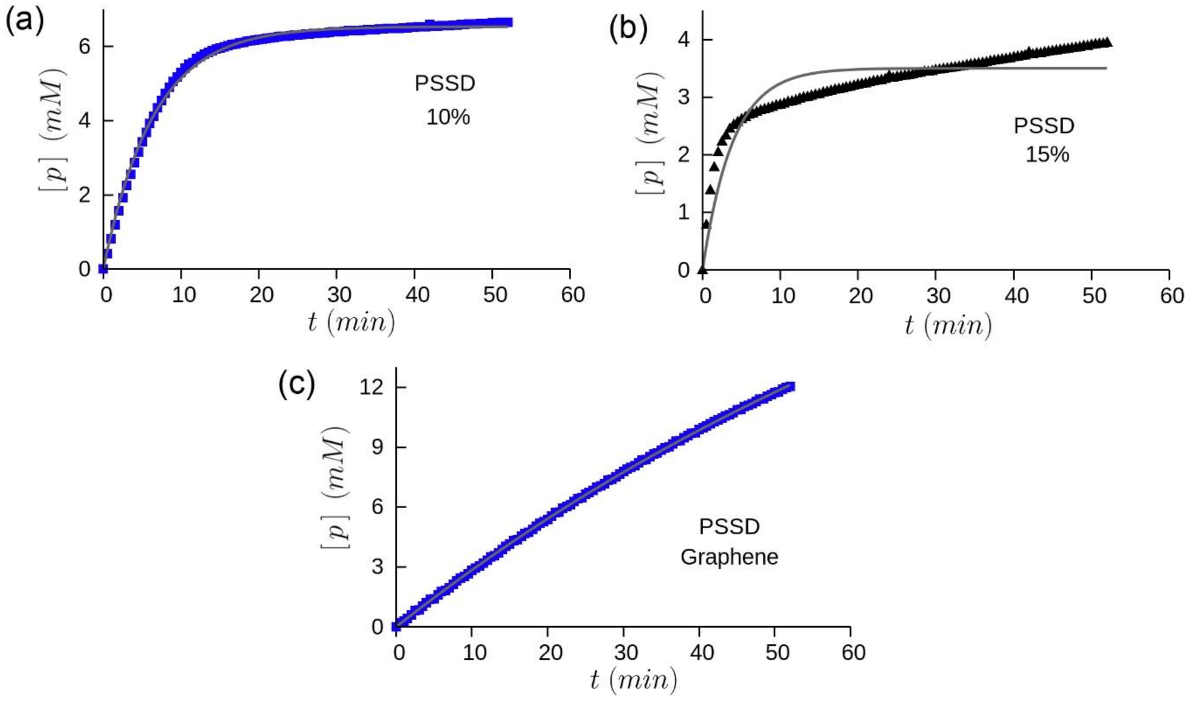
باکمی دستکاری جبری می‌توان آن را به کل محدوده $[s_0]$ تعمیم داد. بنابراین می‌توان با درنظرگرفتن این فرضیه پارامتر را جهت کنترل تغییرات در عملکرد آنزیم آزاد و تثبیت شده به کار گرفت.

همان‌طور که در شکل ۱ و شکل ۲ مشاهده می‌شود، اولین نکته در مورد این آنزیم به صورت آزاد عدم حضور شانه و برازش بسیار خوب داده‌های تجربی با معادله ۱ است. در مورد آنزیم جذب شده، هر دو نانوکامپوزیت ژلاتین-گرافن ۱۰wt% و گرافن خالص برازش خوبی را نشان می‌دهند. در مقایسه، PSSD تثبیت شده بر پایه نانوکامپوزیت ژلاتین-گرافن ۱۵wt% شانه را نشان داده که گواه حضور چندین مقیاس زمانی در سامانه است. با وجود این توضیح رفتار این آنزیم جالب است. برای PSSD

سوبسترا تری‌گلیسیرید است که دوبار به آنزیم متصل می‌شود. بدین‌صورت که به نظر می‌رسد آنزیم ابتدا یکی از شاخه‌های اسید چرب را جدا می‌کند. سپس دی‌گلیسیرید حاصل دوباره برای حذف شاخه دوم به لیپاز وصل می‌شود.



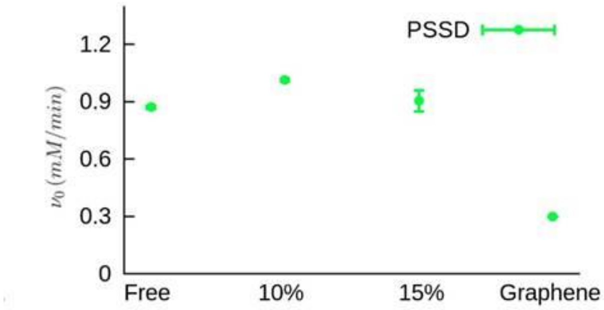
شکل ۱- برازش داده‌های تجربی برای آنزیم PSSD با استفاده از معادله ۱. مقدار نهایی پارامترها حاصله بدین‌صورت است $v0 = (0.0872 \pm 0.007)mM/min$، $\eta = (0.118 \pm 0.001)\ min^{-1}$.



شکل ۲- برازش داده‌های تجربی برای لیپاز PSSD تثبیت شده بر پایه بر اساس معادله ۱. (a) GeG-10 مقادیر پارامتر نهایی عبارت‌اند از $\eta = (0.155 \pm 0.001)\ min^{-1}$، $v0 = (1.013 \pm 0.008)mM/min$. (b) GeG-15 مقادیر پارامتر نهایی عبارت‌اند از $\eta = (0.26 \pm 0.02)\ min^{-1}$، $v0 = (0.90 \pm 0.06)mM/min$. (c) گرافن مقادیر پارامتر عبارت‌اند از $\eta = (0.0100 \pm 0.00009)\ min^{-1}$، $v0 = (0.2990 \pm 0.0005)mM/min$.

به عبارت دیگر محصول واکنش اول غلظت سوبسترا نوع دوم را افزایش داده که با تری‌گلیسیرید وارد رقابت جهت اتصال به آنزیم می‌شوند؛ بنابراین باید رابطه واکنش با در نظر گرفتن عدم حضور بازدارنده تغییر کند که $\bar{s}$ معرف دی‌گلیسیرید است. به

صورت کیفی می‌توان نتایج حاصل برای PSSD تثبیت شده بر نانوکامپوزیت ژلاتین-گرافن ۱۰ % را فرض تمایل یکسان دی‌گلیسیرید و تری‌گلیسیرید به آنزیم بیان داشت، هرچند سرعت تولید محصول کمتری دارد. بدین جهت وقتی مقدار کافی دی‌گلیسیرید تشکیل می‌شود $\bar{s}$ و s شروع به رقابت می‌کنند. لیکن کمپلکس $e.\bar{s}$ زمان بیشتری در مقایسه با e.s برای تولید محصول نیاز دارد. به عبارت دیگر $e.\bar{s}+p$ به‌عنوان گلوگاه در سینتیک عمل می‌کند. در شکل Error! **No text of specified style in document.** پارامترهای برازش حاصل شده در آنالیز گزارش شده است.



شکل **Error! No text of specified style in document.**- پارامترهای برازش شده بر لیپاز PSSD.

نتایج نشان دهنده دینامیک سریع آنزیم PSSD و v_0 بزرگ‌تر برای نمونه‌های حاوی ژلاتین است.

٤- نتیجه گیری

مدل سینتیکی برای هیدرولیز لیپید توسط آنزیم تثبیت شده در طی یک زمان معین توسعه یافت و برای سرعت اولیه هیدولیز علاوه بر بررسی زمانی کل واکنش مورد استفاده قرار گرفت. مدل پیشنهادی موفق در پیشگویی روند واکنش در طی زمان با در نظر گرفتن پیش فرض‌ها و ضرایب بود. نتایج حاکی از پیشرفت واکنش در دو مرحله با مقداری همپوشانی است.

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چکیده مقالات لاتین
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Effect of Support type on the Alpha-olefin oligomerization using $AlCl_3$ catalyst

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Poly(alphaolefin)s (PAOs), due to their range and viscosity, are produced by heavy alphaolefins oligomerization. PAOs have advantages such as more fluidity at low temperatures, low volatility, higher viscosity index, higher pour points, high oxidation/heat stability, low toxicity when compared with conventional mineral oils. Different catalysts such as Lewis acid, metallocene, chromium/silica and ionic liquids are reported so far for the catalytic alphaolefin oligomerization. PAO function can be significantly affected by the catalytic system used in oligomerization process. One of the most suitable methods for the production of PAOs is the use of the $AlCl_3$/donor catalytic system.

The use of Lewis acid catalysts is very practical for achieving desirable properties. In fact, most of the PAO grades are commercially produced by $AlCl_3$/ or BF_3/donor system. However, their highly corrosive and hazardous nature together with the problem of disposal evoked researchers attempt to find new green processes to circumvent such defects. Stabilizing Lewis acid catalysts on different supports is a very promising way to minimize the costs and environmental impacts of these catalysts [1-3]. A valuable research on active species loading, i.e. $AlCl_3$, has been carried out on chlorinated supplements to demonstrate support conditions and fixing conditions [4]. It has been shown that chlorination of support component before catalyst impregnation results catalysts with higher efficiencies.

In this study, to diminish $AlCl_3$ disadvantage, it was fixed on various conventional supports including Al_2O_3 and Silica, Al_2O_3 + $FeCl_3$ and Silica + $FeCl_3$ in the presence of CCl_4 as solvent. After catalysts syntheses, they were characterized by X-Ray, microscopic and spectroscopic methods. Then, oligomerization was conducted in the presence of these catalysts using 1-octene and 1-deccan monomers at 80 °C to produce POct and PDec synthetic oils, respectively. Finally, the properties of the synthesized oils including kinematic viscosity at 40 and 100 °C, viscosity index (VI), molecular weight, and the pour point were fully investigated to unravel the effect of support type on the final PAO characteristic. It was found that support nature has considerable impact on the synthesized PAO molecular weight and its distribution which reflects its effects on the PAO viscosity and grade.

Keywords: *poly(alphaolefin)s,* PAO, *oligomerization , $AlCl_3$ catalyst, cationic.*

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Synthesis and Characterization of Heterogeneous catalyst for Hydrogenation of Benzene in Reformate Gasoline

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A series of nickel catalyst for hydrogenation of benzene in reformate gasoline was synthesized and characterized by various techniques including XRD, FESEM, EDS-map and N_2 adsorption-desorption. The evaluation was carried out in fixed bed reactor at 423-473 K under atmospheric pressure. Different mole ratios H_2/HC and space velocities were investigated by means of optimum condition. The highest conversion of benzene in hydrogenation is achieved at low temperature. In low H_2/HC molar ratio and space velocity, due to higher resident time, benzene molecules find a greater chance of competitive hydrogenation in reformate. Despite the decrease in benzene content, the octane number of the product does not change significantly.

Keywords: *Hydrogenation; Reformate; Benzene reduction; Silica; Green Fuel*

Studding the effects of different additives on the textural properties of RCD catalyst support

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Hydrotreating is called to the reactions that upgrading of hydrocarbon products is the targets, and removing pollutants is done under Hydrogen gas pressure and at present of catalysts, such as hydrodesulfurization (HDS), hydrodenitrogenation (HDN), hydrodematalization (HDM), hydrodehalidation (HDH), or physical properties improving. In this process, gamma alumina catalyst is mostly used as the catalyst support, and nickel and molybdenum as an active metals are homogenously impregnated it. However, catalyst support should have proper surface area and pore distribution for the catalytic hydrotreating process. Concentration and specification of the oil fractions are changing with increasing the boiling point of the oil fractions. Heavy oil fractions have maximum amount and the most resistant of sulfur compounds. Hydrodesulfurization of the atmospheric residual (AR) is the most important process in the preparing low sulfur vacume gas oil (V. G. O). There are various methods to control the pore volume. One of the most effective methods to prepare large pore catalyst support is to use some additives.

Physical properties of the applied residual oil hydrotreating catalysts are conformity with the specific conditions of oil fractions. Pore volume, pore diameter, and pore distribution, are more important factors rather than the surface area. At first, maximum porosity is considered as the most important property of the catalysts, if proper porosity is not achieved, the chemical composition of the active metal is not important, and it is important to maintain the catalyst life time.

In this research, the influence of different additives such as, poly ethylene glycol (low density), ammonia (in different concentrations), ammonium carbonate, poly vinyl alcohol, hexamine, and methanol on the textural properties of the catalyst which is made of boehmite powder of Azarshahr Nephlinsinite mine ores are investigated. In this regard, and in order to prove the different additives influence on the properties of the catalyst within these experiments, different characterization laboratory method and apparatuses have been used, such as X-ray diffraction (XRD), N_2-adsorption/desorption, and radial strength techniques. As a result of all aforementioned experiments and characterization tests, it is shown that, the best additive is ammonia (10%), and catalyst properties which is prepared by ammonia (10%) as an additive is too similar to the commercial sample properties.

Keywords: *additive; Gamma alumina (γ-Al_2O_3); Mesopore support; RCD catalyst.*

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Studding the Effects of the Acidic and Alkaline Treatments on the Properties of Atmospheric Residual Crude Oil Desulfurization (RCD) Catalyst Structure

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Since residual crude oil has a high content of large molecules such as metal containing and asphaltenes (Nickle & Vanadium), the large mesopore structure has been needed for the RCD catalyst. In this research, a specific type of mesopore extrudates gamma alumina which is widely applied as the catalyst support in the atmospheric Residual Crude oil Desulfurization unit (RCD) was prepared. This RCD catalyst support has been prepared by our research team, in which the boehmite powder of Azarshahr Nephlinsinite mine ores for the first time. Then, several RCD catalyst samples have been prepared to perform the ammonia and acetic acid treatments under various operating conditions in order to show the effects of different treatments on the pore volume and diameter in the prepared RCD catalyst during these experiments. Then, nickel and molybdenum as an active metal are impregnated on the catalyst support. In this regard, and in order to compare the acetic acid and ammonia treatments influence on different properties (pore volume and pore diameter) of the prepared RCD catalyst within these experiments, different characterization laboratory method and apparatuses have been used, such as X-ray fluorescence (XRF), N_2-adsorption/desorption, microreactory and radial strength techniques. As a result of all aforementioned experiments and characterization tests, it was shown that, the pore volume and pore diameter of the RCD catalyst support became wider and larger by both treatments. But, the effect of acetic acid treatment was better than ammonia treatment on the properties of RCD catalyst**.** The pore diameter and pore volume of RCD catalyst support which was prepared by acetic acid treatment, were wider and larger than the catalyst which was prepared by ammonia treatment. So, the RCD catalyst which was prepared by acetic acid treatment was applied in demetallization process, and the RCD catalyst which was prepared by ammonia treatment was applied in desulfurization proccess of the RCD unit.

Keywords: *acidic treatment; alkaline treatment, Gamma alumina (γ-Al_2O_3); Mesopore support; RCD catalyst.*

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Development of a Magnetically Recyclable (Ni/Co)MoS_2 catalysts supported on magnetic greigite: high performance and stability in hydrodesulfurization

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Magnetic MoS_2/Fe_3S_4, $CoMoS/Fe_3S_4$, $NiMoS/Fe_3S_4$ composites that consist of greigite as the core and (Co or Ni) molybdenum sulfide catalyst as the top layer were were synthesized and compared to MoS_2/Fe_3O_4 (synthesized and studied in our previous work [1]) for hydrodesulfurization (HDS). The composites prepared in this work containing greigite core were found to have higher hydrogenation (HYD) selectivity in HDS of dibenzothiophene (DBT) compared to the one with a magnetite core and showed higher stability during different cycles of DBT HDS test. When previous techniques [2] failed to utilize promoted sulfide catalysts in slurry reactors, the novel technique used in this study showed the possibility of promoting MoS_2 and increase the activity of the catalyst. The promoting atoms (Ni and Co) were found to be uniformly dispersed over the catalysts and no separate Ni or Co sulfide phase was detected. $NiMoS/Fe_3S_4$ was found to have the highest activity in the hydrodesulfurization (HDS) of dibenzothiophene (DBT) and DMDBT followed by $CoMoS/Fe_3S_4$ and MoS_2/Fe_3S_4. For the promoted catalysts, the direct desulfurization (DDS) pathway was found to be more selectively enhanced than the HYD route in HDS of DBT. HYD pathway was found to be the dominant route in HDS of dimethyldibenzothiophene (DMDBT). MoS_2/Fe_3S_4 was found to be more acidic than the promoted catalysts in the HDS of DBT. This was assigned to the difference in the acidic nature of –SH groups formed through the dissociation of H2S over the coordinatively unsaturated sites (CUS) for the promoted and unpromoted catalysts. In the presence of a weak metal-sulfur bond as in promoted catalysts, the –SH groups were considered to work as nucleophilic centers while over MoS_2/Fe_3S_4 with a strong metal-sulfur bond, they act as Bronsted acid acites. High activity toward the refractory sulfur-containing compounds, high stability, and the magnetic properties associated with these nano-composites as shown in Figure 1, makes them an excellent choice for hydroprocessing of heavy petroleum oils in slurry reactors as they can be easily separated and reused.

Figure 1: *MoS_2/Fe_3S_4 dispersed inside the model oil and b) separated from the model oil after seconds of exposure to an external magnet.*

Keywords: *Heterogenous catalysis, Hydrodesulfurization, Ni(Co)MoS_2/Fe_3S_4.*

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Synthesis magnetic of Cobalt-Ferrite Nanoceramic

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Magnetic spinel ferrites have generated diverse scientific and technological interests, due to their role in developing our understanding of the fundamentals of nanomagnetism and their promising applications in the fields of high-density data storage, ferrofluid technology, heterogeneous catalysis, magnetic resonance imaging, and drug delivery.

Cobalt ferrite magnetic nanoparticles with mean sizes of 40-80 nm were synthesized. Among the various liquid-phase chemical techniques, reported in the literature and employed for the synthesis of cobalt ferrite nanoparticles, the sol–gel process is the most effective and feasible route to develop high purity, homogeneous and crystalline cobalt ferrite nanoparticles [1]. The corresponding oxide obtained was investigated by various methods such as XRD, IR, SEM and magnetic investigation. The strong and sharp reflection peaks in the XRD pattern indicated that products were well-crystallized [2]. Figure 1 shows the hysteresis loops for cobalt ferrite nanoparticles. It can be seen that the saturation magnetization (*Ms*) is about 72 emu/g at calcination temperature 1000 ºC, which is smaller than the bulk value (~80 emu/g). The as-prepared sample displayed homogeneous nanospheres, with the average sizes between 20-30 nm, as can be seen in the scanning electron micrographs.

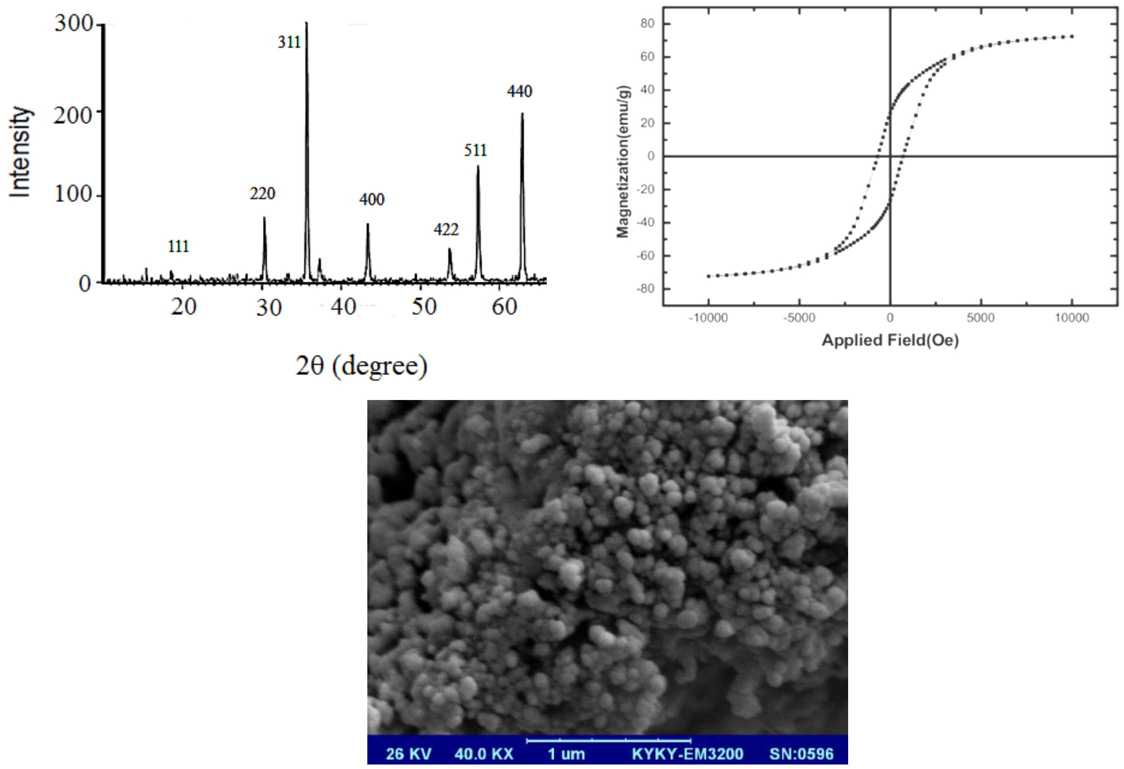

Figure 1. *XRD pattern (left), hysteresis lop (right) and SEM picture of* $CoFe_2O_4$ *nanoceramic.*

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Catalytic Activity of Cobalt-Ferrite Magnetic Nanoparticles for alkenes oxidation

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Cobalt ferrite magnetic nanoparticles used as a clean catalyst for the oxidation of various alkenes with molecular oxygen. The sol–gel technique was followed in the preparation of cobalt ferrite amorphous powder. This study has demonstrated that $CoFe_2O_4$ nanoparticles can act as an efficient catalyst for the conversion of alkenes to the related aldehydes or epoxides in 15-100% conversion at 40 °C. The catalyst can be readily isolated by using an external magnet and no obvious loss of activity was observed when the catalyst was reused in six consecutive runs [1]. The effects of some parameters, such as temperature, types of oxidant and solvents, on the oxidation reactions were also investigated. The results showed that when $CoFe_2O_4$ MNPs is used with O_2 as the oxidant for the oxidation of some alkenes, better results are obtained compared to most of the studied similar ferrites [2].

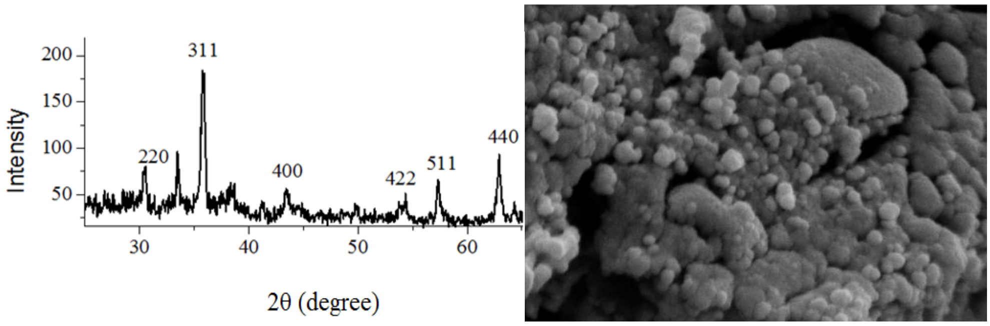
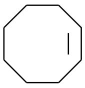
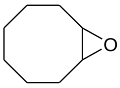
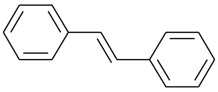
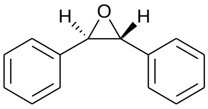
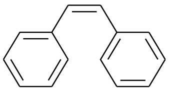
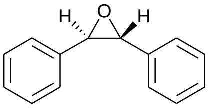


***Figure 1.** XRD pattern (left) and SEM image of recycled $CoFe_2O_4$ nanoparticles.*

***Table 1**. The results of olefin oxidation in presence of $CoFe_2O_4$ nanoparticles.*

No.	Substrate	Products	Selectivity (%)	Conversion (%)
1			98	98
2			100	100
3			85	85

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Efficient synthesis of multiply substituted *7H*-indeno[2,1-*c*]quinolines using LDHs supported 7 ‐ aminonaphthalene ‐ 1,3 ‐ disulfonic acid as catalyst

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The layered double hydroxides@Propyl-7 ‐ aminonaphthalene ‐ 1,3 ‐ disulfonic acid used as a new catalyst for synthesis of *7H*-indeno[2,1-*c*]quinoline derivatives. The catalyst was synthesized according to two-step synthesis. Zn-Cr layered double hydroxides (LDHs) with molar ratio 2:1 by the co-precipitation method.

The main advantages of LDHs are their easy preparation, reusability and giving a visible active catalyst. The synthesized LDH was characterized by FE-SEM, TEM, TGA, XRD, and FT-IR techniques.

LDHs have been known for over than 150 years since the discovery of the layered double hydroxide of general formula $Mg_6Al_2CO_3(OH)_{16}\cdot 4(H_2O)$, which were primarily described by Manasse in 1915. By co-precipitation method, the various forms of anionic species can be directly intercalated or modified with the hydroxide layers, and also, this artificial pathway is often the best method for the preparation of LDHs containing organic bonds which are difficult to attain by other methods.

In the work reported here, in continuation of our research on the synthesis of heterocyclic compounds, a mixture of aryl amine (1.0 mmol) and aromatic aldehyde (1.0 mmol) and LDHs@Propyl–ANDSA (0.06 g) in anhydrous CH_3CN (5 mL) was stirred at 60 °C for 30 min. 1-Indanone (1.0 mmol) was then added, and the resulting mixture was stirred at 60 °C.

Keywords: *layered double hydroxide, co-precipitation, ANDSA, p-anisidine, 1-Indenone*

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Synthesis of 1H-pyrazolo [1,2-b] phthalazine-5, 10 dione derivatives using [SuSA-H]HSO_4 as an efficient catalyst

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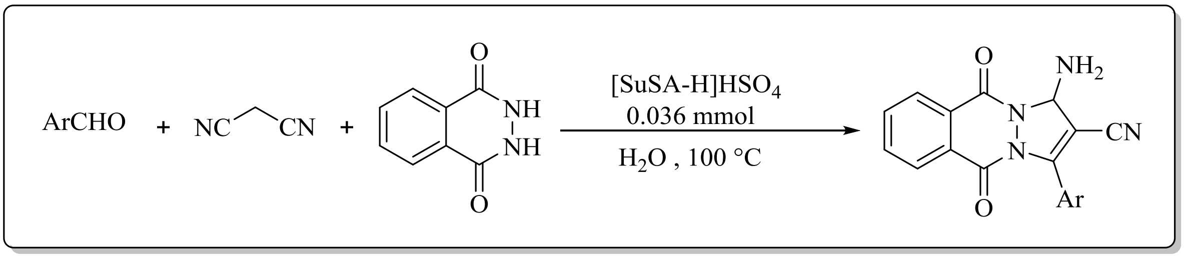
Pyrazoles are important classes of heterocyclic compounds that occur widely in pharmaceutical industry. Synthesis of these compounds is of interest because of their very important pharmacological and biological activities such as antimalarial, antifungal, anti-inflammatory, antimicrobial, fungicide and antitumor [1].

Among these compounds, the synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10 dione derivatives is so attracted the attention of many organic chemists that in the past decade [2-3].

Although these procedures provide an improvement, some of these methods suffer from disadvantages such as long reaction times, harsh reaction conditions, need to excess amounts of the reagent, use of toxic solvents or reagents and non-recoverability of the catalyst.

Therefore, introducing of simple, efficient and mild procedures to overcome these problems is still in demand.

In this work, [SuSA-H]HSO_4, is used as an efficient and reusable catalyst for the promotion of the synthesis of 1H-pyrazolo[1,2-b]phthalazine-5,10 dione derivatives (scheme 1). All reactions were performed under mild conditions and the products were formed over short reaction times in excellent yields.



Scheme 1. *Synthesis of 1H-pyrazolo [1,2-b] phthalazine-5,10-dione derivatives*

Keywords: *Pyrazoles* **,** *[SuSA-H]HSO_4 , Green solvent.*

References

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Introduction of [SuSA-H]HSO$_4$, as an efficient and reusable catalyst for the synthesis of 3,4- dihydropyrimidin- 2(1*H*)- ones/thiones

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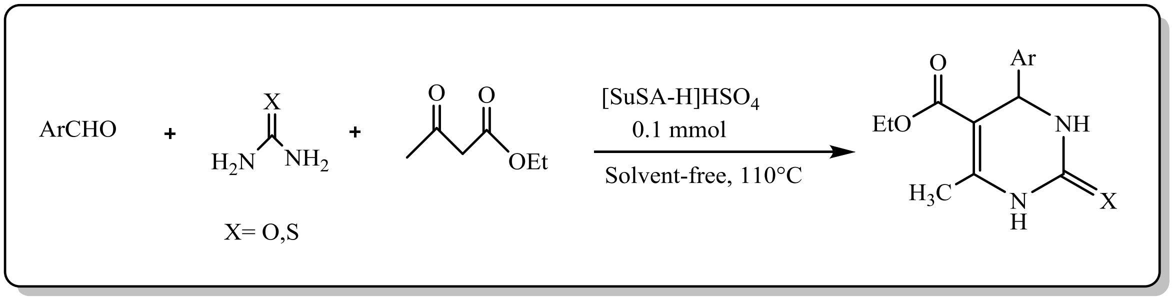
In the past few decades, dihydropyrimidinones (DHPMs), as an important class of heterocyclic compounds, have attracted great attention in medicinal and synthetic organic chemistry owing to their pharmacological and therapeutic properties such as antihypertensive and antibacterial activities. In addition, these compounds exhibit vital medicinal properties as calcium channel blockers, as well as anti-tumor activities. The Bigineli reaction based on a one-pot condensation of *β*-dicarbonyl compounds with aldehydes and urea or thiourea under acidic conditions [1]. However, most of the reported methods suffer from drawbacks such as harsh reaction conditions, use of harmful organic solvents, long reaction times, tedious work-up procedure, expensive and moisture-sensitive reagents, strongly acidic conditions [2-4].

Therefore, it is important to find more efficient conditions and methods for the synthesis of these compounds. Herein, we wish to report the new method for the synthesis of these compounds in the present of [SuSA-H]HSO$_4$, as an efficient catalyst under mild reaction conditions (Scheme 1). Easy preparation of the catalyst, easy work-up procedure, excellent yields of products and short reaction times are some advantages of this work.



Scheme 1. *Synthesis of 3,4 - dihydropyrimidin - 2(1H) - ones/thiones derivatives*

Keywords: *Aromatic aldehydes, dihydropyrimidin, [SuSA-H]HSO$_4$.*

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Catalytic Oxidative Coupling of 2-Naphthols by New Oxidovanadium Complex

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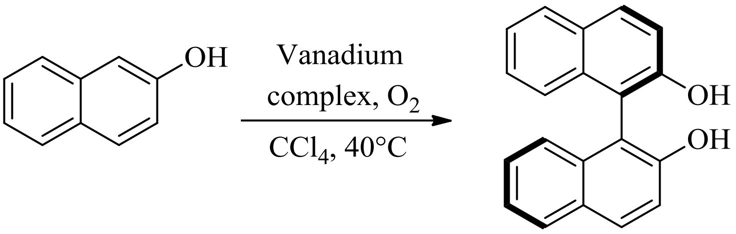
The oxidative coupling of 2-naphthols is a straightforward pathway synthetic transformation as $1,1'$-bi-2-naphthols (BINOLs) are widely used chiral inducers in synthetic organic chemistry [1]. Catalytic coupling of 2-naphthols by using transition metal complexes such as Cu, Fe, Ru, V, etc. is one of the most important methods for preparing BINOLs from the various starting naphthol derivatives [2]. Among the transition metal complexes that catalytically couple 2-naphthol derivatives to BINOLs, vanadium compounds are particularly useful for this process. Vanadium-mediated couplings occur via a favorable one-electron phenolic oxidation in mild reaction conditions with the further advantage that only water is formed as side product. Although several catalytic systems have been reported for preparing BINOLs, development of new catalysts and methods are gaining much attention [3].

By taking the advantage of vanadium complexes toward oxidation reactions, we report here a simple and convenient method for the aerobic oxidative coupling of 2-naphthol to BINOL in excellent yield by using a new vanadium complex as a catalyst. The vanadium complex was synthesized by the reaction of H_3L (H_3L= 2-(5- Bromo-2-hydroxyphenyl)-1,3-bis(2-(5-bromo-2-hydroxybenzylideneamino)ethyl)imidazolidine) and $VO(acac)_2$ in methanol. The vanadium was characterized by elemental analysis and spectroscopic methods (FT-IR and UV-Vis) and was employed as catalyst for oxidative coupling of 2-naphthol. The effects of various parameters, including the temperature, the solvent and the reaction atmosphere were studied. The results of this study indicated that the oxidovanadium complex efficiently coupled 2-naphthol in CCl_4 solvent and the conversion was high when the reaction was carried out at 40 °C and in oxygen rich atmosphere.



***Scheme 1.** Oxidative coupling of 2-naphthol by vanadium complex*

***Keywords:** Oxidative couplings, BINOL, Oxidovanadium complex*

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Multicomponent Click Synthesis of 1,2,3-Triazoles in Water Catalyzed by New Copper(II) Complex

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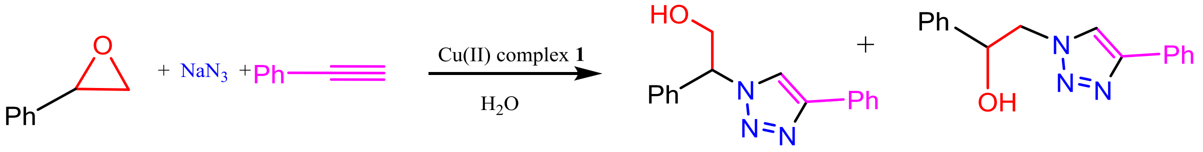
1,2,3-Triazoles are prevalent building blocks of several classes of nitrogen-containing heterocyclic compounds and are commonly employed as a powerful tool in many fields of chemistry such as pharmaceuticals, agrochemicals, dyes and materials. Recently, the catalytic preparation of 1,2,3-triazoles in the presence of transition metal ions, such as Zn, Cu, Ru, Pd, Ce etc., has been developed. Among these, the Cu-catalyzed azide–alkyne cycloaddition (CuAAC) reactions have attracted much attention due to their exclusive regioselectivity, wide substrate scope, mild reaction conditions and high yields [1]. β-Hydroxytriazoles are increasingly useful and important materials in drugs and pharmaceuticals. So, development of a simple and efficient method for their synthesis in a single-step operation is one of the attractive research fields in synthetic organic chemistry. The ability of epoxides to undergo ring opening and hence bringing out the structural diversity in target molecules has made them interesting contenders for in situ azide generation in CuAAC reactions [2]. Nucleophilic addition to epoxides plays a pivotal role in the stereoselective preparation of 1,2-disubstituted products and it has been certainly the most thoroughly studied reaction. It must be highlighted that the multicomponent synthesis of hydroxytriazoles catalyzed by Cu-catalysts is regiospecific with regard to both the azidolysis of the epoxide and the 1,3-dipolar cycloaddition of the in situ generated azidoalcohols with terminal alkynes [3].

In this research we report synthesis, characterization and spectroscopic properties of a new copper(II) complex obtained from the reaction of $Cu(NO_3)_2\cdot 3H_2O$ and 1,3-oxazolidine based ligand in methanol solvent. The obtained Cu(II) complex was used as a catalyst for the green click synthesis of β-hydroxytriazoles in water solvent. Since temperature has considerable effects on the regiospecific opening of the epoxide rings, the effect of temperature was also studied. For this propose, the cycloaddition reaction was studied at 25 (room temperature),40, 50, 60, 70, 80 and 100 °C. The results indicated that increasing the reaction temperature from 25 to 40 and 50 °C increased the catalytic reactivity of copper complex. Further increasing the temperature to 60, 70, 80 and 100 °C also decreased the reaction time but at these temperatures one other product was also obtained. At 100 °C, the ratio of the two products was approximately equal (50 : 50).



Scheme 1. *The structures of two compounds obtained by catalytic reaction at 50 °C < T and T < 50 °C.*

Keywords: *β-Hydroxytriazoles, Copper complex, Click reaction, Regiospecific ring opening*

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Synthesis and Surface Modification of NMOF for its Applications in Biomedicine

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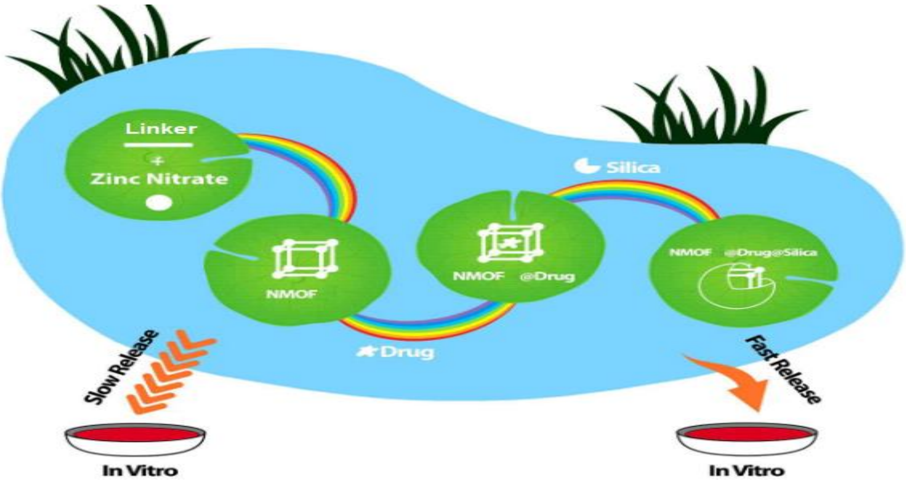
Metal–organic frameworks (MOFs) have fascinated great kindness from chemists due to their fantastic potential applications in catalysis, microelectronics, ion exchange, nonlinear optics, and gas storage [1]. Moreover, MOFs can be considered as good candidates for drug delivery systems due to below reason [2]:

Firstly, the facile synthesis of NMOFs with different compositions, shapes, sizes, and chemical properties allowing that NMOFs are compositionally and structurally various. Secondly, the presence of relatively labile metal ligand bonds triggered that NMOFs are biodegradable. The important issues are stability and surface modification of NMOFs that should be discussed with respect to the biological application of NMOFs. By selecting different metal ions, organic linkers, and crystalline structures can be reached to differences in degradability; thus, a few hours to several weeks could be attuned for their degradation time [3].

We have studied that NMOF coated by silica in order to protect from rapid degradability, then release of drug and cytotoxicity of NMOF explored. Therefore, we developed toxicological studies about coated NMOF by silica. Our results was confirmed by FT-IR, XRD, SEM, and MTT. Observation of releasing of drugs showed that coated NMOF is much better than NMOF alone, due to its slow releasing.



Scheme 1. *Biomedical application of NMOF*

Keywords: *metal-organic framework, drug delivery, silica.*

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Catalytic Oxidation of Cyclooctene by Methoxy Bridged Dinuclear Oxidovanadium(V) Complex

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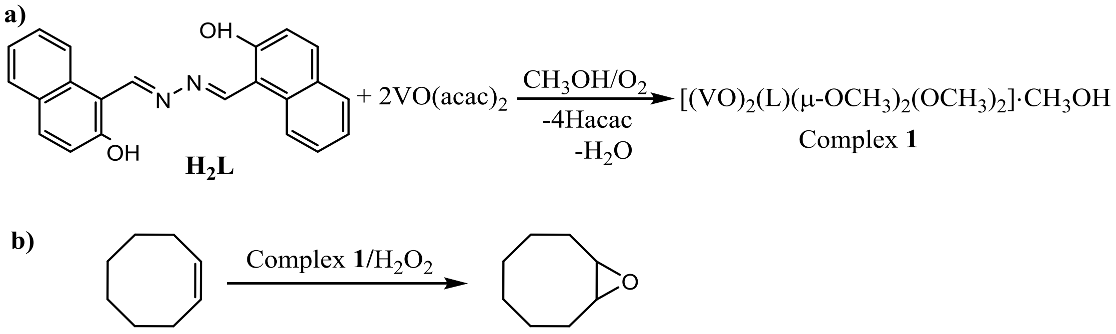
Vanadium plays a vital role in biological systems since the active sites of some enzymes such as haloperoxidases, which are able to catalyze oxidation reactions by hydrogen peroxide, consist of vanadate moieties [1]. The chemistry of vanadium(V) is dominated by the stable oxidovanadium (VO^{3+}) and dioxidovanadium (VO_2^+) cations, which remain intact during many reactions [2]. Vanadium participates in many important catalytic redox processes and its complexes take part in oxo-transfer and oxidation reactions [3]. The synthesis and utility of new vanadium complexes in oxidation reactions is one of the attractive research fields in inorganic and coordination chemistry. In this work we report the synthesis, characterization, crystal structure and catalytic activity of a new neutral dinuclear vanadium complex, $[(VO)_2(L)(\mu\text{-}OCH_3)_2(OCH_3)_2]\cdot CH_3OH$ (**1**). Complex **1** was synthesized by the reaction of $VO(acac)_2$ and tetradentate N_2O_2-donor ligand [H_2L, where H_2L = 1,1'-((1*E*,1'*E*)-hydrazine-1,2-diylidenebis(methanylylidene))bis(naphthalen-2-ol)] in methanol (Scheme 1a). The complex was characterized by spectroscopic methods (FT-IR, UV-Vis, NMR) and single crystal X-ray analysis. The molecular structure of complex **1** was determined by single-crystal X-ray analysis which indicated complex **1** is a neutral methoxy bridged dinuclear oxidovanadium(V) complex. During the formation of complex the V^{4+} is oxidized to V^{5+} by aerial oxygen. The catalytic Complex **1** was employed as catalyst for oxidation of *cis*-cyclooctene in the presence of H_2O_2 as a green oxidant (Scheme 1b). Liquid phase catalytic oxidation of *cis*-cyclooctene was carried out under air (atmospheric pressure) in a 25 mL round bottom flask equipped with a magnetic stirrer. In a typical experiment, aqueous H_2O_2 (1-4 mmol) was added to a flask containing complex **1** (1-3 mg) and cyclooctene (1 mmol) in a solvent (3 mL). The course of the reactions was monitored using a gas chromatograph equipped with a capillary column and a flame ionization detector. In order to obtain the suitable condition of catalytic oxidation, the effect of various parameters including the amount of the catalyst, the ratio of H_2O_2 : cyclooctene, the effect of temperature and also solvent was studied. The results of catalytic reactions indicate that complex **1** is a highly active and selective catalyst in the clean epoxidation reaction of *cis*-cyclooctene using aqueous hydrogen peroxide.



***Scheme 1. a)** Synthesis of dinuclear oxidovanadium(V) complex; b) catalytic oxidation of cyclooctene by complex **1**.*

Keywords: *Catalytic oxidation, Oxidovanadium(V) catalyst, Olefin oxidation.*

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Preparation of pH-sensitive, polymeric prodrug micelles for delivery and controlled release of cisplatin

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Cancer, as a leading cause of death worldwide, has gained much attention in recent decades [1]. Although several anticancer drugs have been introduced as chemotherapeutic agents, the effective treatment of cancer remains a challenge [2]. Cis-diaminedichloroplatinum(II) (cisplatin, CDDP) is one of the oldest chemotherapy drugs available and has been in widespread use to treat a wide range of solid tumors including ovarian, cervical, head and neck, and non-small-cell lung cancer. Treatment is usually limited, however, by side-effects such as nephrotoxicity, emetogenesis, and neurotoxicity. One of the most promising strategies to enhance targeting is to employ polymeric nanocarriers (PNs) to achieve passive targeting via the enhanced permeation retention effect (EPR) and protection of cisplatin from undesirable binding events during drug distribution in the body, while facilitating the transport of the drug across the cell membrane via endocytosis at the site of action [3-4]. Based on what is described, in this work we were designed a novel nontoxic polymeric micelles based on biocompatible polymers such as polyethylene glycol (PEG) and glycidyl azide polymer (GAP) that were modified with pH sensitive amino functional groups. As a result, we were able to provide an active site for conjugation of cisplatin with polymer, and we were able to achieve appropriate loading efficiency of drug into block copolymers and employed this self-assembled block copolymer micelles for efficient intracellular delivery of cisplatin.

Keywords: *pH-sensitive, polymeric prodrug, micelle, cisplatin*

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The effect of polyaniline doping on the TiO_2 and ZnO nanoparticles in the pyrene degradation on the contaminated soils

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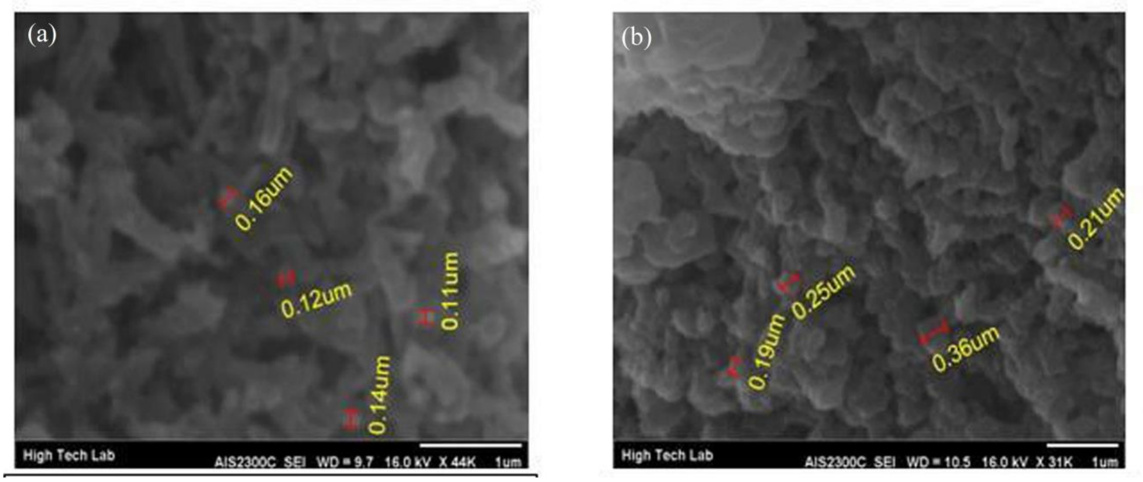
The use of a photocatalyst that is active under sunlight, is one of the cost-effective methods for the removal of pollutants from contaminated soil. In this study, an interfacial polymerization method was used to prepare ZnO- polyaniline (PA) and TiO_2-PA nanocomposites. The SEM images confirmed the particle size distribution ~200 nm in diameter. In both XRD and FTIR data, the peaks relating to PA were identified in the nanocomposites. For the extraction of pyrene of the soil samples, a continuous batch extraction was carried out and evaluated. The data analysis showed the positive effect of PA on pyrene degradation under UV and sunlight radiation, by decreasing the electron hole recombination in modified photocatalysts. The PA coated photocatalysts, improved the extent of pyrene removal, which was more than 95% for both the ZnO and TiO_2 nanocomposites in the bentonite samples under the visible light condition. This value was lower than 80% for the clay soil under UV radiation, which increased to 90% under sunlight. However, only a maximum degradation of 60% was obtained with the unmodified photocatalysts. The increase in the degradation efficiency was due to the increase in adsorption of the organic molecules from the bentonite and clay soils by polyaniline, and also the semiconducting behavior of polymer, that prevented the electron-hole recombination, causing an increase in the photocatalytic activity under both UV and visible radiation. The new ZnO/PA and TiO_2/PA photocatalysts are believed to be promising photocatalytic materials, which can be widely used for the treatment of environmental pollution [1-2].



Scheme 1. *SEM micrographs of (a) TiO_2-PA 4% (b) ZnO-PA 4% NPs.*

Keywords: *Photodegradation, Nanocomposites, Pyrene degradation, Soil contamination, Polyaniline, Titanium, Zinc oxide.*

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Synthesis, Characterization, Crystal Structure and Catalytic Activity of New Dinuclear Cu(II) Complex in Oxidation of Benzyl Alcohol

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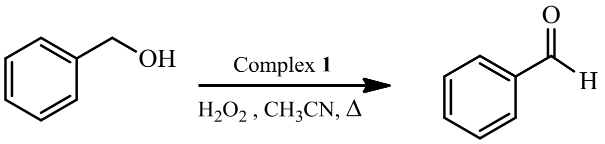
Due to the wide application of carbonyl compounds as intermediates for many chemical compounds, drugs, vitamins and fragrances, the selective oxidation of aromatic alcohols to their corresponding aldehydes is one of the most important transformations in organic chemistry [1]. Therefore, numerous methods have been developed using a variety of reagents for this purpose. Traditional oxidants, such as $KMnO_4$, CrO_3, Br_2, and TBHP (tert-butyl hydroperoxide), used in the oxidation of aromatic alcohols are usually toxic, corrosive or expensive. Thus, offering innovative, “clean” methods that use environmentally friendly oxidants such as hydrogen peroxide and molecular oxygen in non-toxic solvents in particular aqueous media could be a new challenge in this regard [2]. Recently, the catalytic oxidation of alcohols by transition metal complexes in the presence of H_2O_2 has been developed. Various compounds of Cu(II) salts and complexes have been widely used as catalysts in the oxidation of alcohols [3].

In the present work, we report synthesis, crystal structure, spectroscopic properties and catalytic activity of a new dinuclear copper(II) complex, $[Cu(2\text{-}amp)(\mu\text{-}OAc)_2l]_2$ (**1**). Complex **1** was synthesized by the reaction of equimolar amounts of 2-(aminomethyl)pyridine (2-amp) and $Cu(OAc)_2{\cdot}3H_2O$ in methanol. The blue crystals of complex **1** were obtained by thermal gradient method during one week. Single crystal X-ray analysis indicated that these crystals are related to a dinuclear Cu(II) complex which two Cu(II) ions are connected together by two acetate bridging groups. The catalytic potential of complex **1** was tested for the oxidation of benzyl alcohol as representative substrate for primary alcohols using H_2O_2 as a green oxidant. The oxidation products were identified by GC and the progress of the reaction and products were also checked by TLC. In order to obtain the optimum condition for catalytic oxidation of benzyl alcohol, the effects of various parameters, including molar ratio of oxidant to substrate, temperature and solvent were studied. The results of these studies showed that complex **1** catalyzed the oxidation of benzyl alcohol to the benzaldehydes but at higher temperatures a little amount of benzoic acids, produced by over oxidation of benzaldehyde, was also produced in the reaction mixture. The results indicate that the selectivity and the activity of this catalytic system depend on the reaction condition.



Scheme 1.** Oxidation of benzyl alcohol catalyzed by complexe **1

***Keywords:** Oxidation of benzyl alcohol, Copper(II) catalyst, Synthesis.*

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Zeolite-$MnFe_2O_4$: as a novel and highly efficient catalyst for the synthesis of 1,5-benzothiazepine derivatives under solvent free condition

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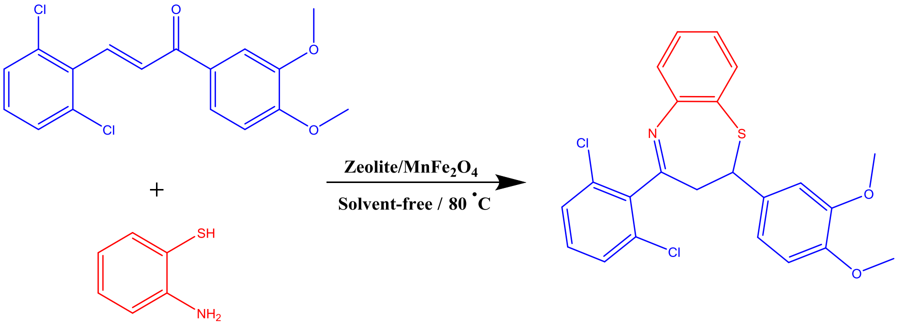
1,5-Benzothiazepines have attracted as an important class of heterocyclic compounds in the field of drug and pharmaceutical research. These compounds are widely used as anticonvulsant, analgesic, sedative, antidepressive, antibacterial, hypnotic agents as well as anti-inflammatory agents.

In the present study, An efficient synthesis of new derivatives of 1,5-benzothiazepine has been developed by the reaction of various chalcones (1,3-diaryl-2-propenones) with 2-amino-thiophenol in the presence of Zeolite-$MnFe_2O_4$ catalyst without solvent.

First, the natural zeolite is activated under appropriate conditions. Then, manganese ferrite were synthesized by reaction of $Fe_2 (SO_4) 3.H_2O$ with $MnCl_2$ and placed on the surface of activated nano zeolite. Under optimized reaction conditions, various 1,5-benzothiazepine derivatives were synthesized and the products were obtained with good to excellent yields and high purities. Ambient reaction temperature, Short reaction times, easy work-up, reusability of the catalyst and no use of harmful organic solvents are among the most important characteristics of the present methodologies. The structures of the synthesized compounds were confirmed by IR, SEM, EDAX and NMR analysis.



Schem1*: Synthesis of 1,5-Benzothiazepines derivatives*

Keywords: *Benzothiazepines, Zeolite, chalcone.*

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An Green and Efficient One-Pot Synthesis of Some Chalcone Derivatives by Zeolite-MnFe$_2$O$_4$ Nanocomposites at Room Temperature

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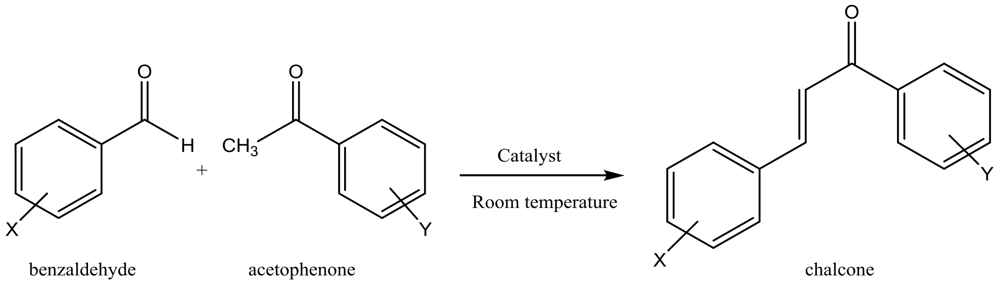
Chalcones (1,3-diaryl-2-propen-1-ones) and their heterocyclic analogues, belong to the flavonoid family, which possess a number of interesting biological properties such as antioxidant, anticancer, antimicrobial, antiprotozoal, antiulcer, antihistaminic and anti-inflammatory activities.

In the present study, a series of chalcone derivatives were synthesized and their structure also confirmed. The compounds were synthesized by various aldehydes and acetophenone derivatives in the ratio of 1: 1 mmol in the presence of a Zeolite/MnFe$_2$O$_4$ based nanocomposites under various solvents and solvent-free conditions. At all experiments, the desired products were synthesized successfully. The described novel synthesis method proposes several advantages of safety, mild condition, short reaction times, high yields, simplicity and easy workup compared to the traditional method of synthesis.

The structures of the synthesized compounds were confirmed by IR, SEM, EDAX and NMR analysis. This method is an easy, rapid, and high yielding reaction for the synthesis of chalcones derivatives.



***Schem1**: Synthesis of chalcone derivatives*

***Keywords:** aldehyde, acetophenone, Zeolite, chalcone.*

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Synthesis of HKUST-1 and studies of its drug release applications

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The metal- organic frameworks (MOFs) are porous crystalline compounds that their structure, connect the metal centers with organic ligands and create a three-dimensional structure. These frameworks are synthesized in a variety of ways under specific temperature and pressure conditions that including hydro (solvo) thermal method, microwave and ultrasonic methods, electrochemical synthesis, diffusion method, solvent evaporation and ionothermal synthesis. In recent years, large numbers of MOFs have shown various potential applications including gas adsorption, sensors, carriers of drugs, Catalyst, separations and etc [1]. In this research, we study the use of drug carrier by MOFs, in which synthesized the metal- organic framework ($Cu_3(BTC)_2$), HKUST-1, with the central metal copper and connector (BTC = 1,3,5-benzenetricarboxylate) and used as a carrier of drugs. This MOF is stable and has a high surface area. HKUST-1 was synthesized by solvothermal method and characterized by (FT- IR) Spectroscopy and X-ray diffraction (XRD), then HKUST-1 was used as drug carrier and the accuracy of drug absorption was evaluated by (FT-IR) spectroscopy and X-ray diffraction (XRD) and thermogravimetry analysis (TGA) spectra.release of drug from HKUST-1 were investigated in PBS (pH = 7) at 37 ^{o}C. To do this, at certain intervals, we take our samples and record UV spectra to obtain the degree of release of the drug in a PBS solution at different time. UV spectra showed ergotamine has a slower release than acetaminophen [2].

Keywords: *Metal organic frameworks, Carriers of drugs, HKUST-1*

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Palladium Supported on Mesoporous Silica/Graphene Nanohybrid as a Highly Efficient and Reusable Heterogeneous Catalyst for C-H Functionalization

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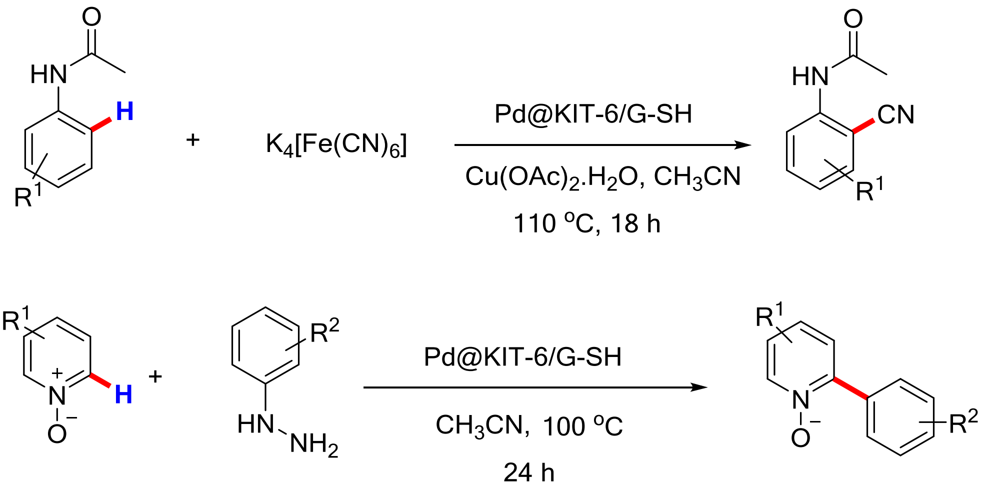
Mesoporous silica/graphene (KIT-6/G) with pendent 3-mercaptopropyl groups has been prepared by condensation of surface silanols and (3-mercaptopropyl)trimethoxysilane (MPTMS). Treatment of the mercaptopropylated with Pd(CH$_3$CN)$_2$Cl$_2$ gave a heterogeneous Pd-catalyst (Pd@KIT-6/G-SH).[1-3] The catalytic activity of the catalyst was investigated in two types of C-H functionalized for the synthesis of 2-cyanoacetanilide and 2- arylpyridine 1-oxide derivatives via C-H activation. Additionally, for the study of the effect of thiol ligand, the Pd@KIT-6/G was prepared from the treatment of Pd(CH3CN)2Cl2 with KIT-6/G. The catalyst has been successfully recovered and reused without loss of activity over seven cycles of reactions[4], scheme 1.



Scheme 1. *Synthesis of 2-CyanoAcetanilide and 2-PhenylPyridine Noxide derivatives*

Keywords: *C-H activation · Graphene · Heterogeneous catalysis · Mesoporous materials · Palladium.*

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Anthraquinone Dyes Degradation Over La-based Nanocatalysts

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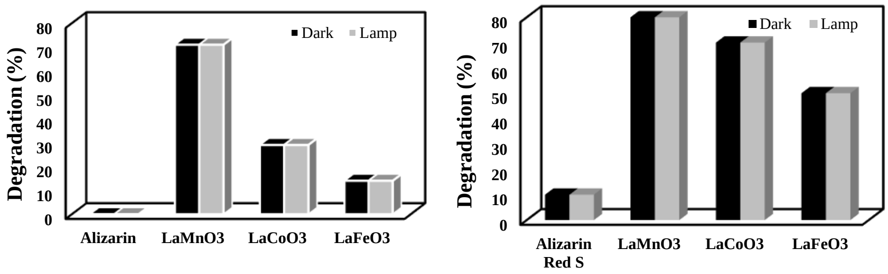
$LaMO_3$ (M = Mn, Fe, Co) nanoperovskites were prepared via citrate method [1]. The synthesized materials were characterized by X-ray diffraction (XRD), FT-IR and UV-Vis spectroscopy. The degradation of anthraquinones dyes [alizarin (A) and alizarin red s (AS)] were investigated in acidic solution in the presence of nanocatalysts under dark and visible-light irradiation. The progress of the reaction was monitored by UV–Vis spectroscopy absorption. The percentage of dye degradation was calculated by the following equation:

$$D\% = \frac{(C_0 - C)}{C_0} \times 100$$

Where C_0 and C are the dye concentration at the initial and after intervals of time, respectively [2]. The controlled experiments revealed that the degradation of A and As were unaltered under dark and visible-light irradiation in the absent of nanocatalyst. Thus, the catalyst was required for an effective degradation of A and AS. Fig. 1 shows the degradation of an aqueous solution of A and AS at pH 2.5 under dark and visible light irradiation. Results show that the A and AS are degraded over $LaMnO_3$ catalyst to ~80% after 180 min under both conditions. Generally, among the three types of nanocatalysts, $LaMnO_3$ is the sample which shows the highest activity and $LaFeO_3$ shows the lowest activity for degradation of A and AS under dark and photo conditions [3]. The greatest activity of the lanthanum manganite is probably due to its high surface area, and also because of its defect structure, which is favorable for development of active sites. Finally, the nanocatalysts reported in this work were effective in anthraquinones dyes degradation when compared to other similar existing catalysts.



(a)

(b)

Scheme 1. *Alizarin 70 ppm (a) and Alizarin Red S 100 ppm (b) degradation*

Keywords: *Nanoperovskites , Degradation , Anthraquinones Dyes.*

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Pd(II)-Supported Complex on Fe_3O_4@SiO_2@SBA-15 for Heck Reaction

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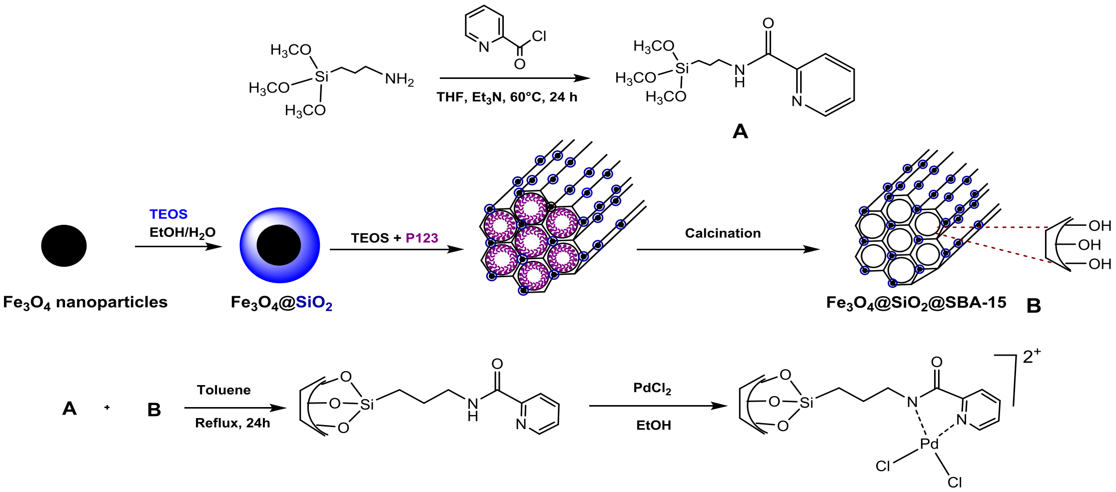
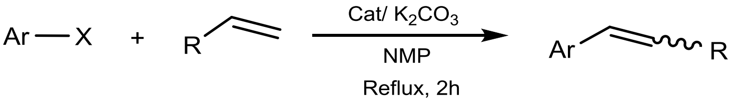
Magnetite nanoparticles were prepared via co-precipitation method and then successively covered by silica and mesoporous silica (SBA-15) layers [1]. N-(3-(Trimethoxysilyl) propyl) picolinamide, obtained from the reaction between 3-aminopropyltrimethoxysilane (APTMS) and picolinoyl chloride [2], was reacted with Fe_3O_4@SBA-15 as supported ligand (Fe_3O_4@SBA-15-PPA) for Pd(II), Scheme 1.



Scheme 1. Synthesis of Fe_3O_4@SBA-15-PPA

Finally, functionalized magnetic mesoporous nanoparticles were reacted with $PdCl_2$ to afford supported Pd(II)-complex that showed excellent efficiency in Heck Reaction of alkenes with aryl halides [3], Scheme 2. The catalyst could be easily separated from the reaction mixture by an external magnet and could be recovered and reused several times.



***Scheme 2**. Heck Reactions of Alkenes with aryl halides in the presence of Fe_3O_4@SBA-15-PPA*

Keywords: Pd(II)-nanoparticles, Heck reaction, , C-C Coupling

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Core cross-linked micelles pH-responsive intracellular drug delivery

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Cancer is one of the most common causes of mortality in the world over the past decades. There are several therapies for treating cancer that chemotherapy is the most commonly used treatment with anticancer drugs [1]. Most anticancer agents are not as effective in cancer chemotherapy as anticipated because of nonspecific toxicity, lack of tumor selectivity, and development of multidrug resistance (MDR) in various tumors. Various carrier systems such as liposomes, polymeric micelles, nano-scaled complexes and microspheres have been investigated to challenge such problems. In particular, polymeric micelles have become attractive because of their small size (10 to 200 nm) for passive accumulation in solid tumors by a process termed 'enhanced permeation and retention' (EPR), improved stability and biodegradability in vivo [2]. In this study, a kind of core cross-linked poly(ethylene glycol)-b-glycidyl azide polymer micelles (PEG-b-GAP) was prepared by a simple chemical cross-linking method for pH-response drug delivery. Curcumin (CU) was then loaded into the micelles in high efficiency [3,4]. The curcumin loaded amphiphilic block copolymer was self-assembled in phosphate buffer (pH 7.4, 0.1 M) into nanosized spherical micelles. In vitro release studies demonstrated that the micelles are relatively stable at normal physiologic conditions but susceptible to tumor relevant reductive and acidic conditions which would trigger the release of chemically loaded drugs. These results suggest that curcumin loaded micelles may offer a promising strategy for CU delivery in the treatment of various tumors, with enhanced efficacy and fewer adverse effects.

Keywords: *Micelles, Nanocarrier, pH-responsive, Curcumin*

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Synthesis of Hierarchical SAPO-34 Using Green Non-Ionic Surfactant Triton X-100 with Improved Catalytic Performance in Methanol to Olefin Reaction

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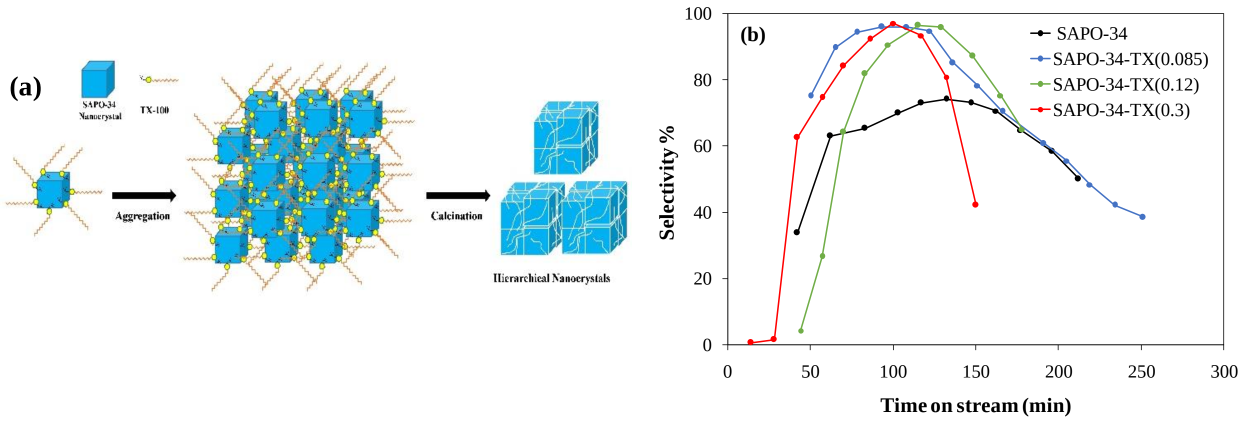
SAPO-34 has excellent performance in the methanol-to-olefin (MTO) reaction because of effective shape selectivity and mild strong acidity [1]. The main problem of SAPO-34 is short life time due to diffusion limitations in its structure. Diffusion limitations cause not only the decrease of catalytic lifetime, but also the low selectivity of light olefins during MTO reactions [2]. Synthesis of SAPO-34 with hierarchically porosity, by decrease diffusion limitations can lead to improve mass transport and catalytic performance in MTO reaction. In this work, the hierarchical SAPO-34 has been successfully synthesized by using tetraethyl ammonium hydroxide as a microporous template and cheap and green non-ionic surfactant triton X-100 (TX-100) as a mesoporous template. The effect of TX-100/Al^{3+} ratio on the structural and textural properties of hierarchical SAPO-34 and its catalytic performance in methanol to olefin (MTO) reaction was investigated. Physical properties of obtained samples were characterized by X-ray diffraction (XRD), NH_3 temperature-programmed desorption, scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FT-IR). The results indicated that with decrease of TX-100/Al^{3+} ratio from 0.3 to 0.085, crystallinity, light olefins selectivity and catalyst life time were enhanced.



Scheme 1. (a) Proposed formation process of hierarchically SAPO-34 using Triton X-100 surfactant as mesoporous template; (b) Light olefins selectivity of prepared SAPO-34 samples at T = 450 ºC and WHSV=4 h^{-1}

Keywords:*SAPO-34, MTO, TX-100, Non-ionic Surfactant.*

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Ruthenium Nanoparticles Immobilized on Nano-silica Functionalized with Triazine Dendrimer (Ru$_{np}$-nSTDP): An Efficient, Selective, and Reusable Catalyst System for the Oxidation of Alcohols

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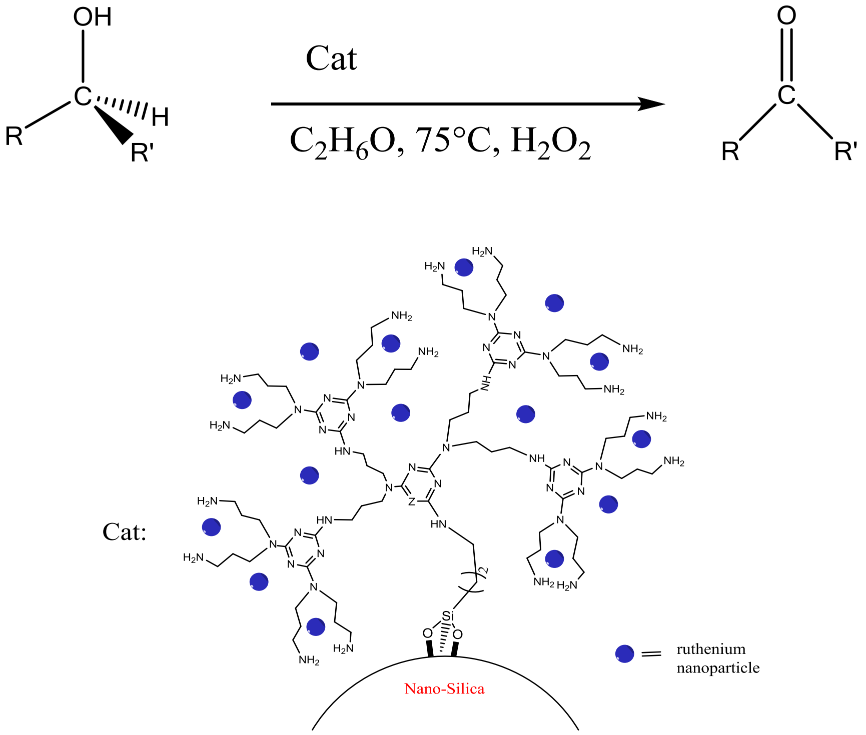
The present study describes the synthesis, characterization, and catalytic activity of ruthenium nanoparticles stabilized with nano-silica triazine dendrimer Ru$_{np}$-nSTDP. To do this, silica nanoparticles were functionalized by triazine dendrimer and finally loaded with ruthenium nanoparticles. Finally, their catalytic activity was investigated in the oxidation reaction of alcohols. However, the preparation of dendrimer containing ruthenium nanoparticles, the ruthenium nanoparticles were produced with reducing of $RuCl_3.H_2O$ by $NaBH_4$.

The prepared catalyst was characterized by FT-IR, TGA, elemental analysis, UV–vis, FE-SEM, SEM-EDX, TGA, TEM, HR-TEM, XPS and ICP-OES techniques. The catalyst was used for the oxidation of various types of alcohols to carbonyl compounds. The present method offers advantages of excellent yields, short reaction times and simple work-up. Also, the catalyst can be easily recycled and reused several times, which makes this method attractive, economic and environmentally benign.



Scheme 1. *Oxidations of Alcohols with Ru$_{np}$-nSTDP Catalyst System*

Keywords: *Ruthenium nanoparticles, Nano-Silica Triazine dendrimer, Oxidation reaction.*

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Effect of Ce addition on catalytic performance of Ni/MCM-41 for hydrogen production via ethanol steam reforming

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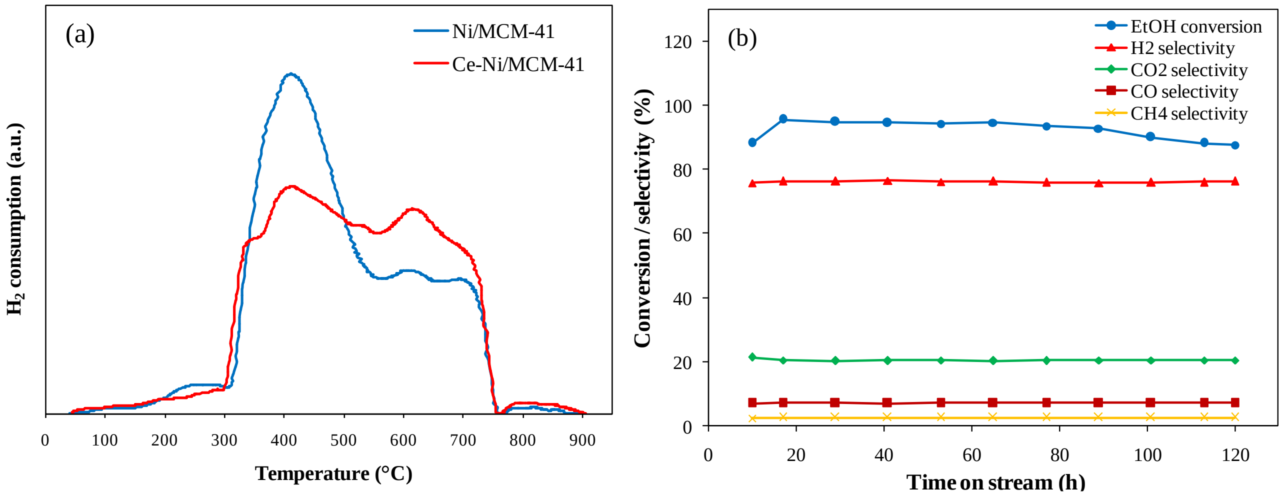
Among different metals that used for ethanol steam reforming, Ni based catalysts has been commonly used since it is highly active and its cost is relatively low [1]. Product distribution and catalyst stability during steam reforming reaction are controlled by the type of utilized support. MCM-41 mesoporous molecular sieves have attracted much interest due to their noticeable surface areas and highly ordered pore structures [2]. In the present study, MCM-41 mesoporous material and highly active and quite stable Ni/MCM-41 catalyst were synthesized through direct hydrothermal and wet impregnation procedure, respectively. The effect of Ce impregnation into Ni/MCM-41 catalyst was evaluated in steam reforming of ethanol. Physical properties of obtained samples characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM) and H_2 temperature program reduction (H_2-TPR). The best catalytic results over ethanol steam reforming reaction, were obtained with Ce-Ni/MCM-41 catalyst, i.e. 94% ethanol conversion and 76.5% hydrogen selectivity. These results remained constant about 90 h time on stream and ethanol conversion decreased to 78% after 120 h.



Scheme1. (a) H_2-TPR of prepared samples; (b) Variations of conversion and selectivities of Ce-Ni/MCM-41 catalyst with reaction time in ethanol steam reforming at 600 ˚C, ethanol/water molar ratio of 1: 6 and WHSV of 1.991 h^{-1}

Keywords: *Ethanol steam reforming, Ni/MCM-41, hydrogen, Fixed bed reactor.*

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New Hydrophobic Cellulose Aerogel Based Titania Catalyst

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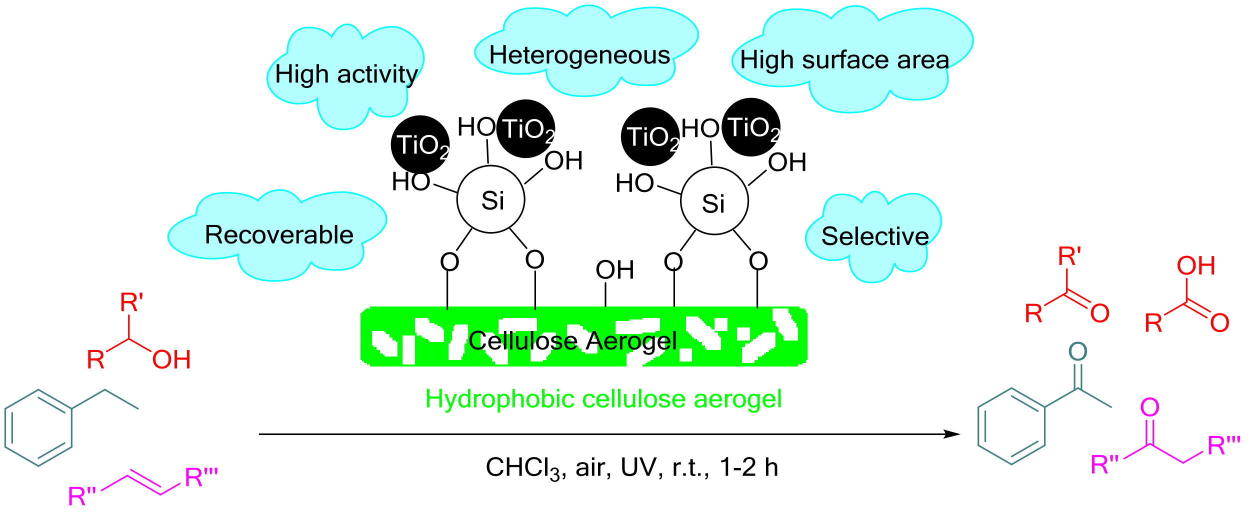
The development of sustainable and efficient catalysts for the oxidation of organic substrates such as alcohols, alkylarenes, and alkenes is an attractive and challenging work respect to the industrial importance of the oxidation reactions [1-5]. Here, novel hydrophobic cellulose aerogel supported TiO_2 nanoparticles with high lipophilicity, superior porosity as well as high catalytic activity was successfully prepared. The nanocomposite aerogel was synthesized in two steps including transformation of cellulose to the cellulose aerogel, and a silanization reaction in the presence of TiO_2 nanoparticles. The aerogel exhibited hydrophobicity with water contact angle of 152.0º. The aerogel exhibited excellent oil/water selective absorption capacity with oil absorption up to 141 g/g. Finally, the nanocomposite was used as a heterogeneous catalyst in the oxidation reaction of alcohols, ethylbenzene, and alkenes. High yields, excellent selectivities, mild reaction conditions, recyclability and biocompatibility of the catalyst are important features of the reactions.



Scheme 1. *Oxidation of organic substrates with hydrophobic cellulose aerogel based titania catalyst*

Keywords: *Cellulose, Aerogel, Hydrophobic, Oxidation.*

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Cellulose Aerogel Supported Graphene Quantum Dots/Pt Catalyst

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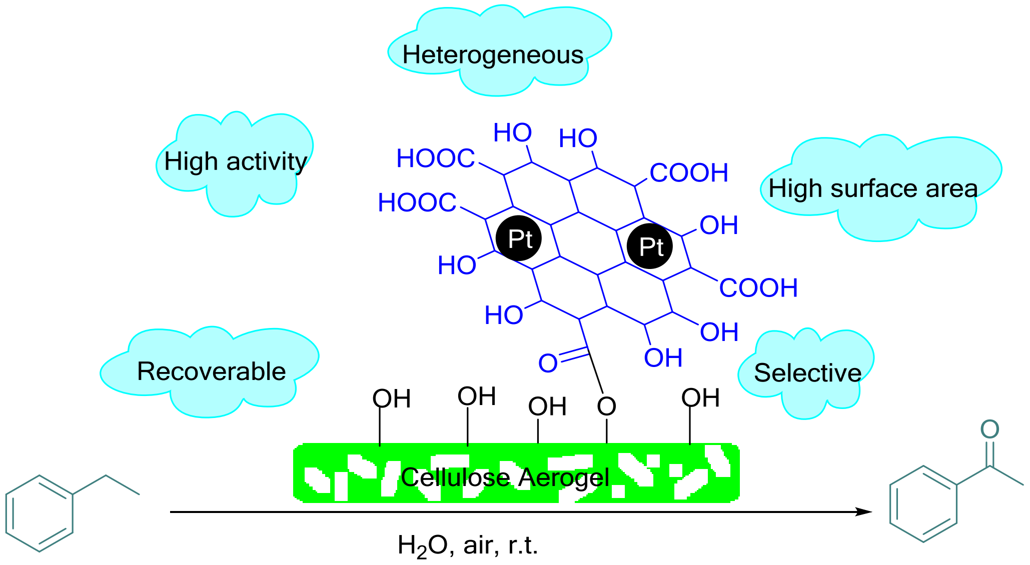
With increasing the importance of green chemistry in human life, heterogeneous catalysts have gained a special place in the catalyst research. Introduction of a large number of heterogeneous catalysts created a competition for selecting a best heterogenized catalytic system for a reaction. High efficiency, non-toxicity, biocompatibility and recyclability are some of the challenging for heterogeneous catalysts. For affording the mentioned conditions various supports such as silica, cellulose, zeolite, alumina, titania and carbon nanotube were applied. Among the supports, cellulose has been attracted great attentions due to some advantages such as hydrophilicity, chirality, biodegradability and high functionality [1-3].

The development of sustainable and efficient catalysts for the oxidation of organic substrates such as alkylarenes is an attractive and challenging work respect to the industrial importance of the oxidation reactions [4,5]. Herein, cellulose aerogel was modified with graphene quantum dots (GQD) and Pt nanoparticles. The catalyst after characterization was used as a heterogeneous catalyst in the oxidation reaction of ethylbenzene at room temperature. High yield and excellent conversion was obtained in green reaction conditions. The catalyst is recyclable for six times without any significant reduction in the yield.



Scheme 1. *Oxidation of ethylbenzene with cellulose aerogel supported GQD/Pt*

Keywords: *Cellulose, Aerogel, Graphene, Quantum dot, Oxidation.*

References

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[3] S. Keshipour and A. Adak, *Appllied Organometallic Chemistry*, **2017**, *31*, e3774.
[4] S. Keshipour, F. Ahmadi and B. Seyyedi, *Cellulose*, **2017**, *24*, 1455.
[5] S. Keshipour and N. Kalam Khalteh, *Appllied Organometallic Chemistry*, **2016**, *30*, 653.

Magnetic Crosslinked Copoly(ionic liquid) Nanohydrogel Supported Palladium Nanoparticles as Efficient Catalysts for the Selective Aerobic Oxidation of Alcohols

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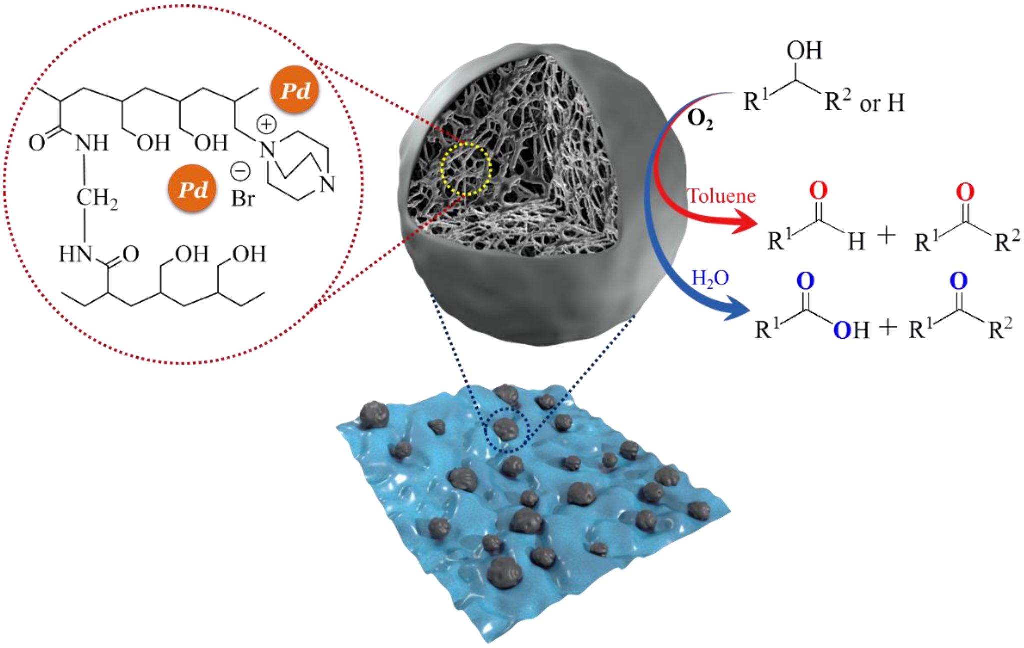
Nowadays it is still a great sustainable processes challenge to produce efficient, selective and easy magnetic recovery and recycling catalysts for oxidation of alcohols using air as the oxidant [1,2]. In this work a new magnetic nanohydrogel comprising [DABCO-allyl][Br] ionic liquid, allyl alcohol and N,N'-methylene-bis (acrylamide) has been used for stabilization of small and highly uniform palladium nanoparticles of 3-4 nm size (MXCPILNHG@Pd). It was characterized by Fourier-transform infrared spectroscopy (FTIR), atomic adsorption spectroscopy (AAS), thermogravimetric analysis (TGA) transmission electron microscopy (TEM), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), SEM-Map, energy-dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectra (XPS), vibrating-sample magnetometer (VSM), and dynamic light scattering (DLS). According to optimization of cross-linking degree and ratio of DABCO-IL, MXCPILNHG-2@Pd found as a highly selective catalyst in oxidations of primary alcohols to the corresponding aldehydes in toluene and to acids in water. Furthermore, secondary alcohols were reacted efficiently to corresponding ketones in both toluene and water. Catalyst was magnetically recovered and recycled for several times in both toluene and water and reused catalysts were characterized by TEM and XPS.



Scheme 1. *Scheme of MXCPILNHG@Pd NPs and selective oxidation of benzyl alcohol.*

Keywords: *Magnetic, Nanohydrogel, Palladium, Oxidation, Alcohols*

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Enhanced photocatalytic degradation of organic pollutant over BiOBr/Ag composite

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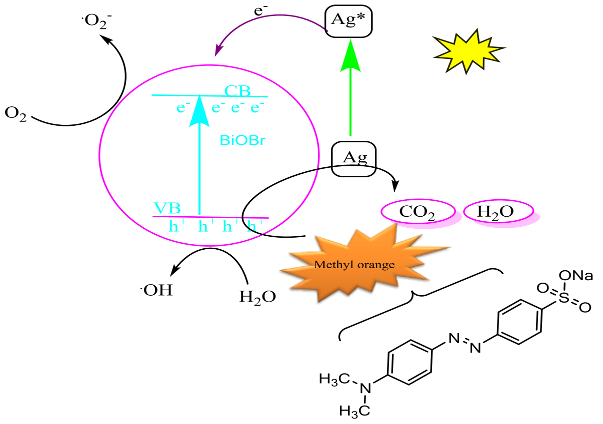
Lately, bismuth oxyhalide BiOX (Cl, Br, I), a new family of promising semiconductor photocatalytic materials, has drawn considerable attention. Within it, BiOBr is the most ideal candidate for its suitable band gap (2.8 eV), nontoxicity, relatively excellent photocatalytic ability and chemical stability in photocatalytic oxidation process. Therefore, many efforts have been devoted to develop the synthesis of BiOBr nanostructures which high surface-to-volume ratio is expected to increase the photocatalytic activity [1].

Silver (Ag) is an attractive material for its specific properties, such as good conductivity, chemical stability, catalytic activity and antimicrobial activity. Ag nanoparticles are used in antimicrobial applications since the antimicrobial effect of Ag ions is well known, it is being used as well as in water and air filtration. Hybrid materials of Ag nanoparticles with amphiphilic hyperbranched macromolecules are synthesized for use in surface coatings because of its antibacterial activity [2]. Newly, the deposition of Ag nanoparticles (NPs) on BiOX (X= Cl, Br, I) has been found can give a singular efficiency in destroy organic pollutants under UV or visible light irradiation. It is generally known that the noble metal/semiconductor oxide composite system could reduce the e^-/h^+ recombination rate due to better charge separation [3].

To prepare this compound, the prepared BiOBr was composed with 2.5 ml of $AgNO_3$ solution. Then, freshly prepared sodium borohydride was added dropwise and then stirred for 5 hours. Eventually, the precipitate was centrifuged, washed with distilled water and dried in oven. The resulting sample was characterized using XRD, SEM, FT-IR and DRS analysis. Furthermore, the photocatalytic activity of the synthesized photocatalyst was investigated using methyl orange (MO) as a model organic pollutant. A maximum degradation efficiency of 61% has been achieved under visible light irradiation over the prepared photocatalyst. The photocatalytic performance of BiOBr/Ag photocatalyst is much higher than that of pure BiOBr.



Keywords: *Bismuth oxyhalide, Photocatalytic degradation, Organic pollutant.*

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Enhanced photocatalytic performance of BiOBr nanoplate with porphyrin complex

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Wastewaters generated from the textile industry contain large amounts of azo-dyes. Azo dyes are synthetic colored organic compounds. They are manufactured and used widely [1]. In order to solve such problems, degradation of aqueous organic pollutants in wastewater through semiconductor photocatalysis has received significant attention over the last decades.

Among the various narrow band gap semiconductors, bismuth oxyhalides, BiOX (X= Cl, Br, I) have been also found to act under visible light irradiation [2], Furthermore, BiOX are nontoxic and the environment compatible photocatalysts with low cost [3]. Therefore, BiOX has attracted increasing attention in practical industrial applications, especially in the degradation of organic pollutants [3] and in the fabrication of photoelectrochemical cells [4]. BiOBr, as one of Bi based semiconductor materials, has attracted the attention of researchers due to its unique lamellar crystal structure, efficient visible light absorption and charge transfer ability [5].

BiOBr nanoplates were synthesized through the co-precipitation method. In a typical experiment to prepare the BiOBr sample, $Bi(NO_3)_3.5H_2O$ powder was firstly dissolved in HNO_3 (solution A). Solution B contained KBr and CH_3COONa in distilled water. Solution A was added rapidly to the solution B under vigorous stirring. Subsequently, the mixtures were vigorously stirred for 12 h. After the reaction was completed, the resulting product was collected by centrifugation, washed several times with distilled water. The resulting nanoplates have a tetragonal phase .To improve the visible light performance of the prepared BiOBr in the photocatalytic reactions, the prepared photocatalyst were functionalized with tin complex of porphyrin photosensitizer (Sn-TCPP). To photosensitize the prepared BiOBr by the Sn-TCPP, BiOBr and the porphyrin complex with weight ratio of 10 to 1 were refluxed in DMF solvent. After washing with DMF, the synthesized product was obtained and named BiOBr/SnTCPP. The prepared photocatalysts were characterized through FT-IR, DRS, XRD and SEM analysis. The photoactivity activity of the synthesized sample was investigated via photodegradation of a colored pollutant of methyl orange (MO) and 2, 4-dicloro phenol. The results showed that BiOBr photosensitized with SnTCPP is able to destroy 78% of MO and 80% of 2, 4-dicloro phenol in 240 min under visible light radiation.

Keywords: *Bismuth oxyhalide, Porphyrin complex, Photodegradation .*

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Synthesis of Tricarboxamides Using Novel Core-shell Nanocatalyst Based on Ionic Liquid

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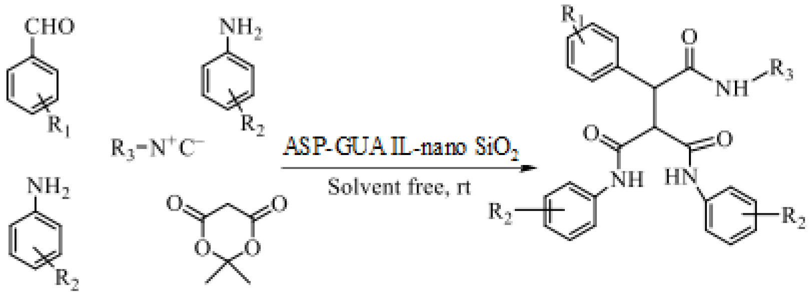
Ionic liquids (ILs) possess green properties such as non-flammability, chemical and thermal stability, extended solvation nature, and negligible vapor pressure. In recent years, many task-specific ionic liquids (TSILs) were designed and utilized for accelerating various organic transformations.

Nano catalysts offer a higher surface-to-volume ratio and lower coordinating sites in comparison to bulk counterparts, which are responsible for the higher catalytic activity as well as selectivity. Furthermore, nano catalysis has the advantage of high atom efficiency, easy product purification, and reusability of the catalyst.

The multi-component reactions (MCRs) are valuable versatile method for affording diverse organic structures with potent applications in medicinal and pharmaceutical chemistry. Because of their benefits such as facile performance, environmentally friendly, and atom economic, MCRs are interested in organic chemistry.

Tricarboxamides are a class of nitrogen heterocycles which have significant biological properties such as neuroprotective, anti-diabetic, anti-bacterial, anti-carcinogenic, and anti-tumor activities. In this research we have prepared a new catalyst based on nano SiO_2 core and a novel ionic liquid containing aspartic acid and guanine. This new nano structure has been characterized by FT-IR, FESEM, EDAX, TGA/ DTG, and BET techniques. Its catalytic efficacy examined in the synthesis of tricarboxamides via a pseudo five-component condensation of isocyanides, aromatic aldehydes, Meldrum's acid, and aromatic amines at room temperature solvent-free conditions. Recovery and recyclability of the nano structure within 3 runs without activity loss, in combination with green reaction media, and high yields of the products, are some highlighted points of the procedure.



Scheme 1. *Synthesis of tricarboxamides*

Keywords: *Tricarboxamides, Ionic Liquid, Heterogenous Nano Catalyst.*

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Impregnated Antimony on $NiFe_2O_4$: An Efficient Magnetically Separable Nanocatalyst for Rapid Acylation of Amines

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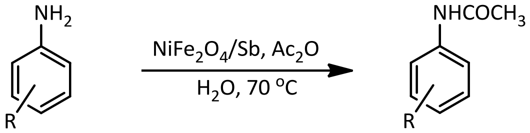
Selective protection of amines is one of the most important methods for multistep synthesis of organic compounds [1-2]. In this context, more attention has been paid to core–shell nano systems with the core of magnetite. They are simply prepared and because of their good magnetic properties are easily removed from the reactions. Functionalized magnetic nanoparticles (MNPs) are robust, air-stable and frequently used for immobilization of various heterogeneous [3-6] and homogenous catalysts. These subjects prompted us to prepare $NiFe_2O_4$/Sb as an efficient and reusable nanocatalyst toward acetylation of arylamines with Ac_2O in H_2O (Scheme 1). Remarkable reusability and easy separation of the nanocatalyst, high yields and mild reaction condition as well as the benefits of using water as a green solvent are the advantages which make this protocol a perfect candidate for the acetylation of amines.



Scheme 1. *Acetylation of amines with $NiFe_2O_4$@Sb/Ac_2O system*

Keywords: *Acetylation, Ac_2O, $NiFe_2O_4$, Sb*

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Synthesis of hydrophilic palladium complex immobilized on nano magnetic support and its catalytic acitivity in coupling reactions

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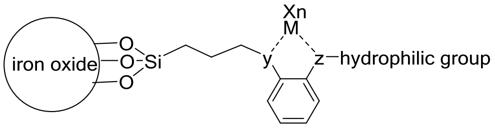
The development of environmentally more benign and efficient synthetic method continues to be a central goal of current research in chemistry. Along this line, it is better that catalysis be associated with both catalyst reusability and green reaction media [1]. Generally, homogeneous catalysis can provide excellent yield, while heterogeneous catalysis offers the advantages of simplified product separation and recycling of the catalyst [2]. These properties make heterogeneous catalysts as suitable candidates for green chemistry catalysis due to their great stability, durability, cost effectiveness, and diminishing heavy metal environmental contamination [3]. To increase the efficiency of heterogeneous catalysts, additives such as phase transfer agents [4], polymers [5], surfactants [6], cyclodextrins [7], organic co-solvents [8] or ionic liquids [9] have been used. A more desirable approach, which avoids using any additives, is designing hydrophilic heterogeneous catalysts. Along this line, in this work, a new heterogeneous palladium complex of supported on nanomagnetic γ-Fe_2O_3 (Scheme 1) was synthesized and characterized by HRTEM, SEM, XRD, XPS, ICP, FT-IR, TGA, VSM and elemental analysis.



Scheme 1.

The synthesized catalyst was used successfully as a new Pd catalyst for Suzuki and Hiyama coupling reactions of aryl iodides, bromides and chlorides with phenylboronic acid and phenylsilanes. The true heterogeneous magnetically-recyclable catalyst can be separated easily using a magnetic bar and reused six times without any drastic loss of its catalytic activity. Using water as a green solvent, facile catalyst recovery and reuse, simple work-up and not requiring any additive or promoter make this method favourable from the environmental and economic point of view for the coupling reactions.

Keywords: nanomagnetic, hydrophilic catalyst, heterogeneous palladium complex, γ-Fe_2O_3

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Synthesis of Copper Nanoparticle on Functionalized Graphen Oxide Support: An Efficient Catalyst for Coupling Reacction

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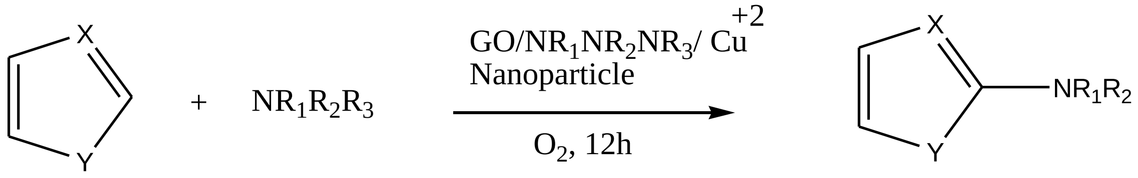
Graphene oxide (GO), a novel and promising two-dimensional (2D) carbon nanomaterial, has attracted extensive attention in catalysis fields, such as photochemistry, electrochemistry, and organic catalysis, for the past few years [1-2]. Graphene-based materials hold unique features, such as large surface, high water dispersibility, intrinsic low mass, easy surface modifications, and ample oxygen-carrying functionalities [3-4], which might be promising candidates as catalysts or supports. Copper is a low-cost transition metal. Efficient catalysts of copper nanoparticles on graphene oxide support are successfully developed for controllably catalyzing the coupling reactions [5].
In this research, we successfully demonstrated GO/amine as a reinforcement for a metal substrate nanocomposite to preparation of homogeneously dispersed GO/amine/Cu nanocomposite powders. Functional groups of GO helped to disperse the GO flakes and form chemical bonds with metal ions. The prepared nanocatalyst were characterized by a variety of techniques, FT-IR, X-ray diffraction, scanning electron microscopy and atomic force microscopy. Prepared nanocatalyst functionalized for coupling reaction at a green condition (Scheme 1).



***Scheme 1.** Amination reaction with nanocatalyst*

***Keywords:** Copper Nanocatalyst, coupling reaction, Amination reaction.*

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Preparation of 2-amino 4H-benzo[h]chromene catalyzed by a Copper complex immobilized on to functionalized $Fe_3O_4@SiO_2$ as a reusable nanocatalyst

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During the past decade, a great deal of attention has been paid to developing greener chemical processes and synthetic methods. Catalysts bound to inorganic solids are widely used for organic transformations due to environmental and economical considerations [1]. Nanoparticles supported on a metal oxide as an inorganic solid, in particular magnetic nanoparticles (MNPs), have been extensively studied in the field of chemical catalysis, environmental protection, sensors, magnetic storage media, and clinical diagnosis treatments. MNPs have great potential in view of their recovery, since the magnetic separation of MNPs from the reaction mixture with an external magnet is simpler and more efficient than conventional separation with filtration or centrifugation. On the other hand, MNPs are accessible from inexpensive materials and can be easily supported organic and inorganic materials. Recently, MNP-supported-copper ions have been used extensively in organic transformations.[2]. In this work, a new magnetically recoverable nanocatalyst was developed by covalent binding of a ligand, 2-amino banzhydrazide and 2-hydroxy naphtaldehyde on the surface of silica coated magnetite nanoparticles (SCMNPs) and followed complexation with $CuCl_2.4H_2O$. Characterization of the prepared nanocatalyst was performed with different physicochemical methods such as FT-IR, TCP-AES, VSM, SEM EDS and TGA analyses. Finally, catalytic activity of the prepared nanocatalyst was examined in the preparation of 2-amino-4*H*-benzo[*h*]chromene derivetives through a one-pot, three component reactions of 1-naphthol, various aldehydes and malononitrile. The synthesized nanocatalyst was efficient. The benefits of this protocol are simple workup procedure, short reaction time and high yields of products. The immobilized complex was reused for several times without meaningful loss in catalytic performance.

Keywords: *Heterogeneous catalysts, Magnetic nanoparticles, Three component reactions*

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Copper Schiff base complex immobilized on surface modified magnetite as a nanocatalyst for the reduction of 4-nitrophenol

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The presence of toxic dyes and nitroarene compounds in waste waters is of great concern as these are biologically and chemically stable; therefore, it is difficult to remove them by natural degradation processes [1]. Recently, magnetic core–shell nano-structures have attracted more attention due to their unique magnetic properties. In contrast to the difficulty observed in recovering and reusing most solid catalysts, core–shell nanostructure magnetic catalysts can be easily retrieved under the influence of a magnetic field and used in subsequent reactions. Due to this property, using magnetic core–shell structure composites as catalysts has been recommended in literature. Schiff base transition metal complexes have been extensively studied because of their potential use as catalysts in a wide range of reactions. These complexes have been extensively used for hydrogenation of organic substrates, epoxidation of olefins, conversion of epoxides into halohydrines, asymmetric ring opening of terminal epoxides and oxidation reactions [2]. In this work, a copper schiff base complex immobilized on surface modified magnetite used as efficient nanocatalyst for reduction reaction. The most important advantages of this work are high conversion, short reaction time, simple work-up procedure, use of non-toxic materials and environmentally benign. Moreover, the nanocatalyst could be separated easily from the reaction mixture using an external magnetic field and reused for several times without significant loss of its catalytic activity.

Keywords: *Schiff base,*
Nanocatalyst, Magnetically, Dye reduction.

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Enantioselective Allylic Oxidation of Cycloolefins Using Chiral Heterogeneous Catalysts Based on Aliphatic Substituted Oxazoline Ligands

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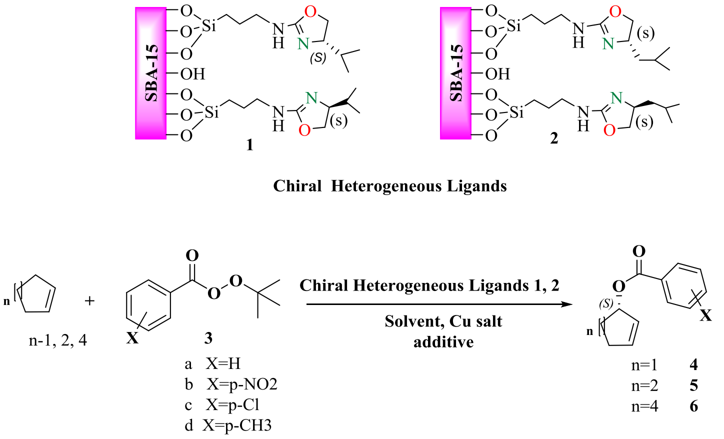
Asymmetric oxidation of allylic C-H bonds of cycloolefins and synthesis of chiral allylic esters, is one of the most important reactions in asymmetric synthesis, that unlike the hydroxylation and epoxidation, the second functional group forms while double bond remains unchanged [1,2]. Despite high selectivity of chiral homogeneous catalysts, because of easy separation of trace amounts of catalyst from the end product, stability under different reaction conditions, reducing metal productions pollution and being consistent with the goals of green chemistry, heterogeneous catalysts have attracted enormous interest. Herein we have focused on the synthesis of recyclable chiral heterogeneous catalysts and their application in copper-catalyzed asymmetric allylic oxidation [3,4]. We first immobilized the chiral amino oxazoline ligands with aliphatic substituent groups ((*S*)-4-isopropyl-4, 5-dihydrooxazol-2-amine or (*S*)-4-isobutyl-4, 5-dihydrooxazol-2-amine) on nanoporous silica SBA-15. To probe the catalytic capability of the chiral heterogeneous catalysts, we used them in copper-catalyzed esterification of allylic sp^3 C–H bonds of cyclic olefins with variously substituted peresters. In continuation, we optimized the conditions for these reactions by changing some parameters such as temperature, solvents and additives. The chiral allylic esters were achieved in good yields and enantioselectivities.



Scheme 1. *Allylic oxidation of cyclic olefins in the presence of chiral heterogeneous ligands*

Keywords: *Allylic oxidation, Heterogeneous catalysts, Cycloolefins, Oxazoline ligands, Nonoporous silica*

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Synthesis of New Chiral Heterogeneous Catalysts by Immobilization of Aromatic Substituted Chiral Amino Oxazoline Ligands on Nonoporous SBA-15 and Their Applications in Asymmetric Allylic C-H Bond Oxidation of Cycloalkenes

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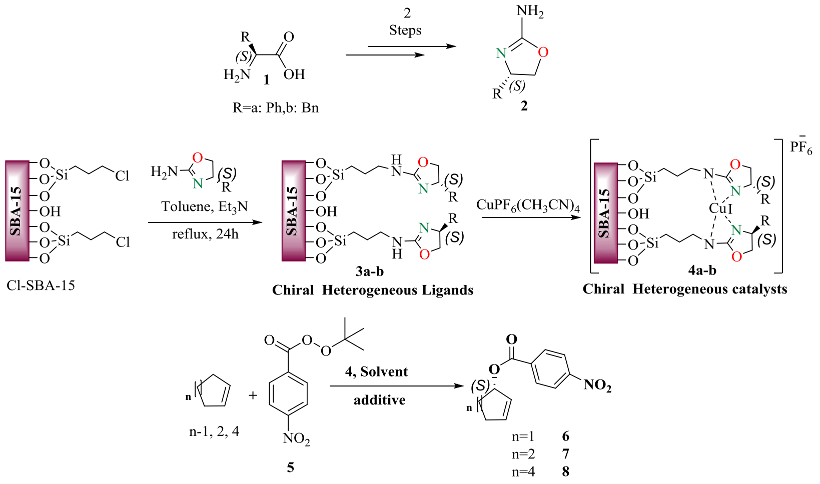
Compounds containing a chiral oxazoline ring are one of the accessible and useful classes of ligands for asymmetric catalysis[1,2]. In the recent decade, using chiral heterogeneous catalysts for the synthesis of asymmetric allylic esters by oxidation of allylic C-H bond has attracted much attention in organic chemistry [3-5]. Herein chiral amino oxazoline ligands with aromatic substituent groups such as (*S*)-4-benzyl-4, 5 -dihydrooxazol-2-amine and (*S*)-4-phenyl-4, 5-dihydrooxazol-2-amine were synthesized from inexpensive and available amino acids. The obtained chiral ligands were grafted on ordered mesoporous silica SBA-15 and Characterized by TGA, DTA, BET, TEM, EDX, SEM and FT-IR. The catalytic and induced asymmetric effects of the copper (I) complexes of these new chiral heterogeneous ligands on the asymmetric allylic oxidation of cycloolefins with tert-butyl p-nitroperbenzoate as oxidant were investigated under different conditions.



Scheme 1. *Allylic C–H bond oxidation of cycloalkenes in the presence of chiral heterogeneous catalysts.*

Keywords: *Allylic oxidation, Heterogeneous catalysts, Amino Oxazoline ligands, Allylic esters, Mesoporous silica*

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Magnetically Nanoparticles of Copper ferrite@antimony: A High Performance Recyclable Catalyst for $NaBH_4$ Reduction of Nitroarenes to Arylamines

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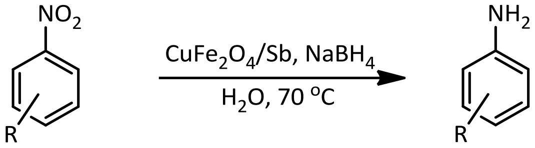
Reduction of nitroarenes to arylamines is one of the most important reactions in organic synthesis due to arylamines are versatile intermediates and precursors in the preparation of dyes, pharmaceuticals, pigments, agrochemicals and polymers [1,2]. In this context, various protocols as well reducing agents are available for the titled transformation [3]. The main limitations of these works were prolonged reaction time, low yields, harsh reaction conditions, use of harmful organic solvents, tedious work-up procedures and the use of expensive catalysts. In this study, we have used magnetically nanoparticles of $CuFe_2O_4$@Sb as a heterogeneous catalyst for reduction of nitroarenes to arylamines in water (Scheme 1). Remarkable reusability and easy separation of the nanocatalyst, high yields and mild reaction conditions as well as the benefits of using water as a green solvent are the advantages which make this protocol a perfect candidate for the reduction of nitroarenes.



Scheme 1. *Reduction of nitroarenes with $NaBH_4$/$CuFe_2O_4$@Sb system*

Keywords: *Amines, Nitro, $CuFe_2O_4$, Reduction, Sb*

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Lipophilic lignocellulose -supported Palladium nanoparticles: A green efficient and recyclable heterogeneous catalyst for the aerobic oxidation of alcohols

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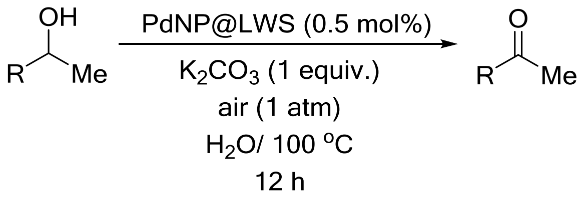
In the recent years, bio-based economy and use of renewable biomass as the raw material have been considered as sustainable options to tackle the problems associated with local and global pollutions [1]. Along this line, lignocellulosic agricultural waste as one of the most abundantly available agricultural wastes has been advocated as a choice for the production of fine chemicals such as nanomaterials [2]. On the other hand, due to cheapness and safety of water, performing organic reactions in this medium is now of great interest.

In this work we have presented a new green, simple and inexpensive method of making palladium nanoparticle (PdNP) catalyst supported on lipophilic walnut shell as an abundantly available lignocellulose-rich agricultural waste. Lipophilization of walnut shell has been performed by Zycosil. Zycosil is low-cost and industrially available organosilicon-based material and the only water soluble product in the world that is used waterproofing of masonry building material, concrete, limestone, marble, stone, stucco, clay tile, plaster, sand, soil, and aggregates. TEM image of Lipophilic walnut shell -supported PdNPs (PdNP@LWS) indicates the formation of 10 nm sized palladium nanoparticles. The catalyst is quite effective for the oxidation of benzylic and aliphatic alcohols under atmospheric pressure of air in aqueous phase.



R	yeild
Ph	96
n-C_6H_{13}	89

Scheme 1. *PdNP@LWS catalyzed aerobic oxidation of alcohols in water*

More importantly, we tested the cytotoxic potential of PdNP@LWS on the erythroleukemia K562 cancer cell lines and peripheral blood mononuclear cells (PBMCs) as normal cells. The K562 cells or PBMCs (1×10^5 cells/100 µL/well) were incubated for 24 h with serial dilution of PdNP@LWS (0, 50,100,200 and 400 µM). After incubation, the survivability of present cells was determined by MTT method. Obtained data showed that PdNP@LWS had cytotoxic effects against K562 cell-line in a dose-dependent manner. Fortunately, the inhibitory concentration (IC50) value of PdNP@LWS against K562 cell line was significantly smaller than an IC50 value of PdNP@LWS against PBMCs (150.54±5.1 µM *vs.* 275 ±9 µM). In conclusion, PdNP@LWS may provide a selective favorable cytotoxicity against K562 cancer cell-line.

Keywords: *Green chemistry, Palladium, Alcohols, Oxidation.* K562, Cytotoxicity.

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Lipophilic perlite-supported Palladium nanoparticles

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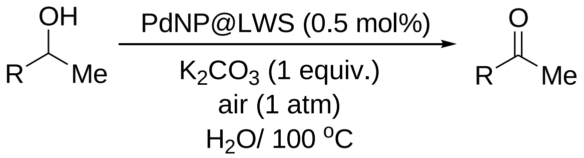
Because of difficulty of recycling/reusing catalyst from the reaction mixture, catalyst separation is a critically important issue in the chemical industry. Thus, the use of support for the preparation of heterogeneous catalysts is often desirable from the perspective of process development due to their easy handling, simple recovery, and recycling [1]. However in the case of nanoparticle-based catalysts supports play role of stabilizer for nanoparticles. Natural aluminium silicate such as perlite can act as an excellent support especially for nanoparticles [2].

In this work we have presented a new green, simple and inexpensive method of making palladium nanoparticle (PdNP) catalyst supported on lipophilic expanded perlite as an abundantly available aluminium silicate. Lipophilization of expanded perlite has been performed by Zycosil. Zycosil is low-cost and industrially available organosilicon-based material and the only water soluble product in the world that is used waterproofing of masonry building material, concrete, limestone, marble, stone, stucco, clay tile, plaster, sand, soil, and aggregates. TEM image of lipophilic expanded perlite-supported PdNPs (PdNP@LEP) indicates the formation of 10-20 nm sized palladium nanoparticles. The catalyst is quite effective for the oxidation of benzylic and aliphatic alcohols under atmospheric pressure of air in aqueous phase.



R	time (h)	yeild (%)
Ph	6	95
n-C_6H_{13}	12	92

***Scheme 1.** PdNP@LEP catalyzed aerobic oxidation of alcohols in water*

Moreover, we tested the cytotoxic potential of the PdNP@LEP on the erythroleukemia K562 cancer cell lines. The K562 cells (1×10^5 cells/100 µL/well) were incubated for 24 h with serial dilution of PdNP@LEP (0, 50,100,200 and 400 µM). After incubation, the survivability of present cells was determined by neutral red uptake assay MTT reduction methods. MTT data showed that the PdNP@LEP had a profound cytotoxic effects against K562 cell-line in a dose-dependent manner (inhibitory concentration (IC50) value: 90.11±4.56 µM). Nevertheless, Based on NR uptake assay, it seems that the PdNP@LEP only at a high dose (400 µM) can interfere with cell membrane functions. In conclusion, PdNP@LEP may provide a favorable cytotoxicity against K562 cancer cell-line by damaging the electron transfer function by mitochondria.

***Keywords:** Green chemistry, Palladium, Alcohols, Oxidation, Cytotoxicity. K562.*

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Energy Decomposition Analysis of the P…N interaction energy between different halo-dienophiles and trivalent phosphorus-based catalyst at the transition state of a cycloaddition reaction

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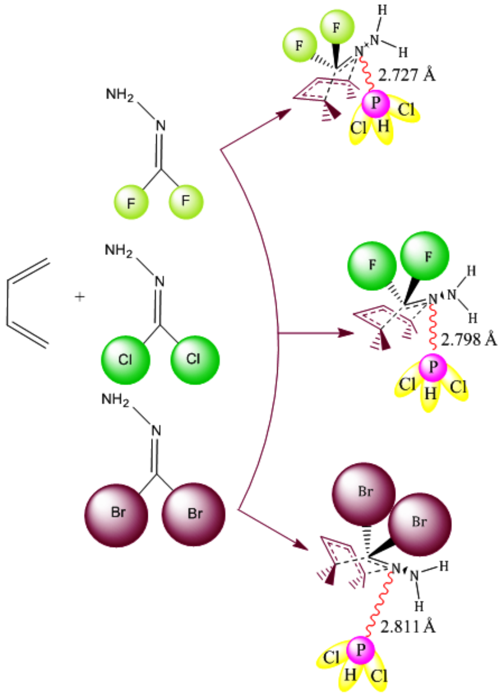
The energy decomposition analysis [1] of the noncovalent intermolecular P…N interaction energy (E_{int}) between different the dienophiles of $X_2C{=}NNH_2$, where X = F, Cl, and Br and trivalent phosphorus-based catalyst ($PHCl_2$) was performed using with the Amsterdam Density Functional program package, ADF2009.01 [2] at the M06-2X/TZ2P-(ZORA)//M06-2X /def2-TZVPP level of theory. The size effect of the X substitutions of dienophile molecule on the interaction energy (E_{int}) and its decomposed components [electrostatic (E_{ele}), Pauli (E_{Pauli}), and interactions between the occupied andunoccupied molecular orbitals energy (E_{orb})] were studied. The aim was to investigate the relation and nature of the P...N bonding at the transition state (TS) of aza-diels-alder [4π+2π] cycloaddition reaction [3] with the size effect of the X substitutions of dienophile molecule at the TS. The calculations showed that the E_{int} between the dienophile molecules and $PHCl_2$ catalyst shows considerable changes with the size of the X substitutions of dienophile molecule. Also, it was found that the value of the E_{elec} is nearly insensitive to the size of the X substitutions of dienophile molecules, especially for the $F_2C{=}NNH_2$ and $Cl_2C{=}NNH_2$ molecules, while for the $Br_2C{=}NNH_2$ observed a small dependency. Similarly, the E_{Pauli} showed a nearly size independent value for the $F_2C{=}NNH_2$ and $Cl_2C{=}NNH_2$ molecules while it was some size-dependent for $Br_2C{=}NNH_2$ molecules.



Scheme 1. *Illustration of the size effect of the halogen substitutions of dienophile molecule on the P..N interaction energy*

Keywords: *Energy decomposition analysis, catalytic effects, pnicogen-bond.*

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The potential of Trivalent Phosphorus-based catalysts for pnicogen-bond activating

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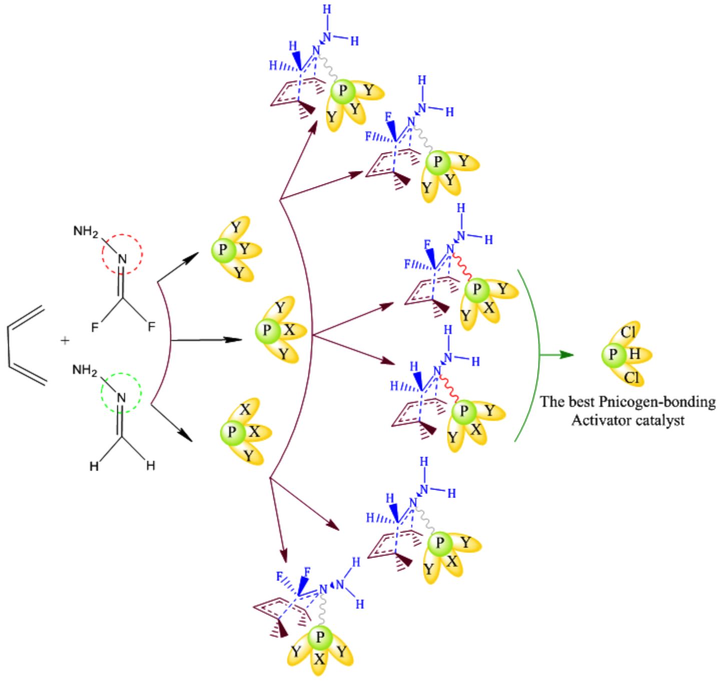
The catalytic power of trivalent phosphorus compounds (TPC) in order to activate the noncovalent interactions -particularly pnicogen-bonding [1]- was investigated. The Aza–Diels–Alder reaction [2] between a diene of 1, 3–butadiene and the dienophiles of $H_2C{=}NNH_2$ and $F_2C{=}NNH_2$ were chosen to study. The catalytic effect of three different kinds of TPCs including PY_nX_m, where Y and X are H and Cl, respectively, n, m = 0, 1, 2, on the transition state (TS) of these reactions was studied. Geometry optimization of all the minima and TSs studied was carried out at the M062X-D3 level of theory with the TZVPP basis set [3,4]. Investigations showed that the $PHCl_2$ catalyst is more capable of the pnicogen-bonding activating comparing to $PHCl_2$ and PCl_3 catalyst. In other words, the investigation of the catalytic effects of PH_2Cl, $PHCl_2$, and PCl_3 on the TSs of the Aza–Diels–Alder reaction shows that the $PHCl_2$ catalyst is of the most effects for lowering of the TS. Therefore, according to the obtained results, the orders of the catalytic effects of PH_2Cl, $PHCl_2$, and PCl_3 on the TS studied in the present work are $PHCl_2 > PCl_3 > PH_2Cl$, respectively. Corresponding TS energy values in the presence of the used catalysts for the dienophiles of $H_2C{=}NNH_2$ and $F_2C{=}NNH_2$ are 16.04, 16.74 for $PHCl_2$, 17.16, 17.12 for PCl_3 and 18.67, 18.06 for PH_2Cl, respectively. Therefore, it could be concluded that the $PHCl_2$ as the trivalent phosphorus-based catalyst is capable of the activation potential of pnicogen bonding in the Aza–Diels–Alder cycloaddition reactions with respect two other catalysts studied here.



Scheme 1. *Illustrations of the catalytic effects on activating pnicogen bonding in the Aza−Diels−Alder reaction between cis-1,3-butadiene and $H_2C{=}NNH_2$ and $F_2C{=}NNH_2$ at the transition state (TS) of reaction.*

Keywords: *Phosphorus compounds, catalytic effects, pnicogen-bond.*

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Effect of calcination temperature and percentage of Mn_3O_4 catalysts derived from used battery powder on Al_2O_3 for removal of VOC in a plasma system

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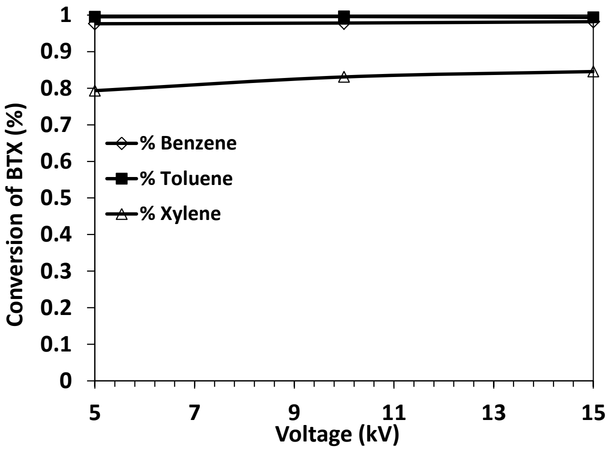
Mn_3O_4 catalysts that derived from used alkaline battery powder were synthesized using hydrometallurgical method[1]. After using H_2SO_4 as leaching acid catalysts were calcined in four different temperatures; 400°C, 500°C, 600°C, 700°C. Tests showed 600°C was the best temperature for calcination of catalysts, and then different percentage of Mn_3O_4 was used as active phase on Al_2O_3. Plasma tests were conducted on Mn_3O_4(5, 10, 15%)/Al_2O_3 catalysts for degrading of Benzene, Toluene and Xylene[2]. Different voltages of plasma was tested for understanding the effect of voltage on VOC removal efficiency. Results showed that Mn_3O_4 (10%)/Al_2O_3 had better performance in abatement of xylene, also the conversion of benzene and toluene were 99% and 98% respectively. Using these catalysts for degrading the volatile organic compounds has a great potential according to their economical advantages and their great performance.



Scheme 1. *Conversion of BTX using Mn_3O_4 (10%)/Al_2O_3 in different voltages of plasma*

Keywords: Mn_3O_4, Catalyst, Volatile Organic compounds, Plasma

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Pd@-Functionalized Haloysite: A new Catalyst for Hydrogenation of Poly α-olefins

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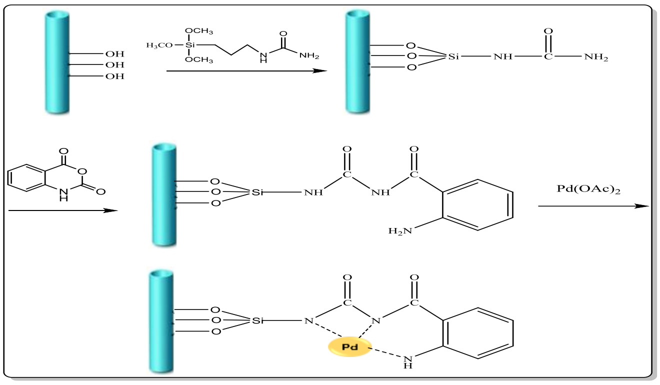
Poly α-olefins (PAOs) are saturated oligomers obtained from polymerizing of linear alpha-olefins. They are widely used as oils in the industry and considered as alternative source for the production of various types of engine oils, hydraulic, compressors, airplane fuel, etc. In fact, poly α- olefins are mostly synthesized by cationic method. In this method, the presence of unsaturated hydrocarbons with different types of double bond in oligomer decreases the stability of the produced oils. To solve this problem, hydrogenation is performed on the unsaturated oils to obtain a stable white oil with higher performance. Catalytic systems play a very important role in hydrogenating of polyα-olefins and production of white oils. Most hydrogenation catalysts partially hydrogenate PAO chains [1, 2]. Hence, development of efficient heterogeneous catalysts that could fully hydrogenate polyα-olefins is of the great importance.

Halloysite nanoclays (HNTs, $Al_2(OH)_4Si_2O_5.2H_2O$), possess high surface area, tubular morphology and high mechanical strength. They belong to the class of kaolinite group hydrated layered aluminosilicates. Recently, functionalization of the HNTs surface has been considered as a potent method for modification of the features of HNTs and expanding their applications [3].

In this regard, a novel heterogeneous catalyst was designed and synthesized through a multi-step process, including, functionalization of HNT with organosilane followed by the reaction with isotonic anhydride and immobilization of Pd(0) nanoparticles (Scheme 1). Then, the activity of the catalyst was examined for hydrogenation of polyα-olefins.



Scheme 1. *The schematic representation of the catalyst. synthesis steps*

Keywords: *Poly α-olefins, Hydrogenation, Haloysite, palladium, catalyst.*

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RAFT Synthesized Polymer Supported Pd Nanoparticles as an Effective Heterogeneous Catalyst for Alcohol Aerobic Oxidation Reactions

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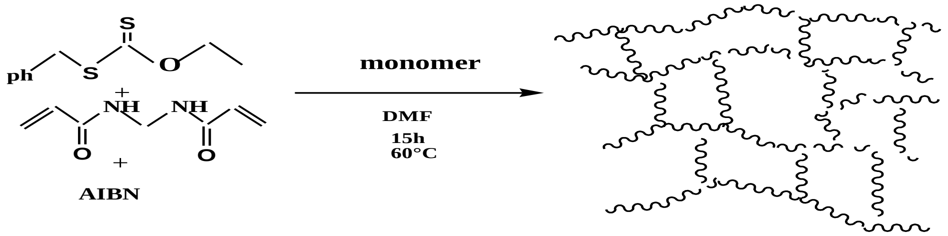
During the last decades much interest have been focused on the applications of functionalized polymers as a support for heterogeneous catalysts because they provide great ease in separation of the catalyst and isolation of the products[1,2]. However, the higher cost, the lake of physical and chemical stability and lower activity are disadvantages of traditional insoluble polymer supported catalysts [3]. Today, new methods for the preparation of controlled polymeric polymers are used which the most important of these methods are the living radical polymerization techniques and among these methods, the Reversible Addition Fragmentation chain Transfer (RAFT) polymerization is more diverse and efficient [4].

The catalytic behavior of palladium nanoparticles has already been proven in various types of reactions and has been investigated even in the stabilized form on the different polymers. In this study diallyldimethyl ammonium chloride and acrylamide were used as monomers in the RAFT polymerization process in the presence of a suitable crosslinking agent and these polymers was utilized for stabilization of Pd nanoparticles. The fabricated supported catalyst was used in the oxidation reaction of alcohols. The results indicated that these supported catalyst had a suitable selectivity and efficiency. Some analysis such as FESEM, TEM and XRD were used for characterization of catalyst structure and also the effect of crosslinking and polymerization method on the catalytic efficiency was investigated.



***Scheme 1.** RAFT polymerization*

Keywords:RAFT polymerization, crosslinking,aerobic oxidation.*

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Investigation of Photocatalytic Activity of the Mixed Matrix Membrane Containing TiO_2-POM Hybrid Mineral Fibers

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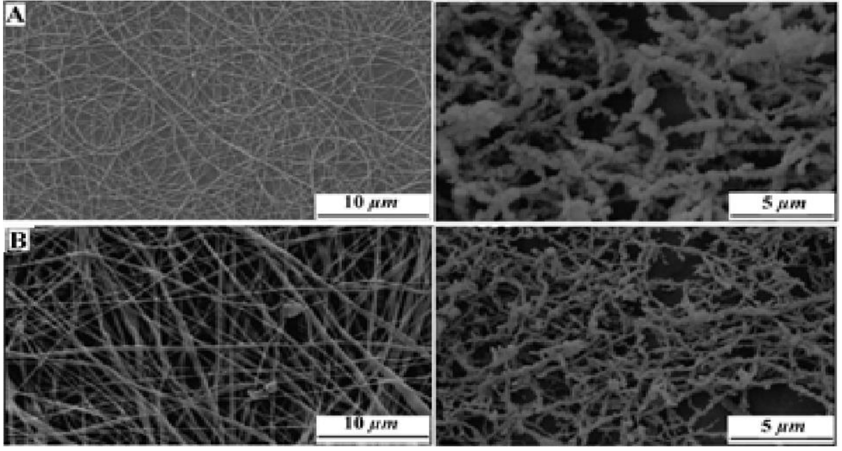
A photocatalytic membrane can be defined as a combination between a photocatalyst and a membrane [1]. The presence of a photocatalyst gives rise to an enhancement of the rate of a chemical reaction or its initiation under ultraviolet, infrared, or visible light illumination and the role of light is to photoexcite the solid that works as the photocatalyst [2]. The membrane has the task to immobilize the photocatalyst and to act as a molecular separation barrier for the reagents and/or reaction products[3,4]. In this study, the photocatalytic activity for the polyethersulfone membranes was achieved by incorporation of a special additive into the polymeric matrix.in order to prepare the photocatalyst, $H_3PMo_{12}O_{40}$ as a poluoxometalate was blended with TiO_2 and SiO_2 particles by electrospinning method and then the fabricated fibers were calcinated. Consequently, the mineral hybrid fibers were mixed with the polymer solution and used for preparation of membranes by phase inversion method. FT-IR and XRD analysis were used for characterization of synthesized compounds. The FE-SEM manifest that the average diameter of the hybrid composite fibers is about 1 µm. Membrane morphology was investigated by FE-SEM. The performance of system was examined by several analysis such as pure water flux, contact angle, salts and heavy metal rejection. Photocatalytic experiments confirm that membranes display highly efficient and durable activity for the photo degradation of methylene blue (MB) and humic acid (HA). Experiments show that the prepared membranes have a good stability under UV irradiation and can be used potentially for separation of different components from water.



Scheme 1. *Prepared fibers before (left) and after (right) calcination, A: POM, B: POM/TiO_2*

Keywords: *Photocatalytic Activity, POM, Mixed Matrix Membrane*

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Synthesis of Chiral Nano Heterogeneous Catalysts by Immobilization of Chiral (*S*)-2-amino-2-phenylethanol and (*S*)-2-amino-3-phenylpropanol Ligands on Nanoporous Silica MCM-41 and Their Applications in Enantioselective Kharasch-Sosnovsky Reaction

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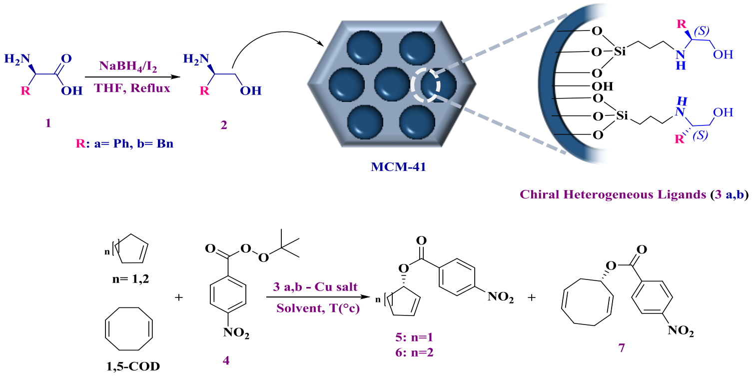
Heterogeneous catalysts have attracted a lot of attention in comparison to other catalysts due to their ability to reuse them through recovering and easy separation [1].
A method for preparation of a practical heterogeneous catalyst is to immobilize the chiral amino alcohol ligands on nanoporous silica MCM-41 [1,2].
Enantioselective Kharasch-Sosnovsky reaction can be used as one of the most considerable synthetic methods for the preparation of highly functionalized olefins such as allylic esters and allylic alcohols that are important intermediates in the synthesis of compounds that are used in the preparation of pesticides and pharmaceutical compounds [3,4].
For this purpose, MCM-41 was prepared and modified by (3-chloropropyl) trimethoxy silane. Afterward, the chiral amino alcohols (*S*)-2-amino-2-phenylethanol and (*S*)-2-amino-3-phenylpropanol which are synthesis by reducing their corresponding amino acids, immobilized on MCM-41 mesoporous silicas. Then copper complexes of these chiral ligands for the first time were examined in the asymmetric allylic C-H bond oxidation of cycloolefins. The chiral allylic esters were achieved in good yields and enantioselectivities (Scheme 1).
The catalyst could be easily recovered and reused fifth times without remarkable loss of the reactivity, yield, and enantioselectivity.



***Scheme 1.** Enantioselective Kharasch-Sosnovsky reaction of cycloolefins in the presence of chiral heterogeneous catalysts*

Keywords: *Chiral Heterogeneous catalysts, Kharasch-Sosnovsky reaction, Chiral allylic ester.*

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Bimetal Ni-Pd Immobilizing into the Hierarchical Beta Zeolite synthesized by using Steam Assisted Conversion Method and Mesoporous Silica KIT-6 and its catalytic application in a Tandem Organic Reaction

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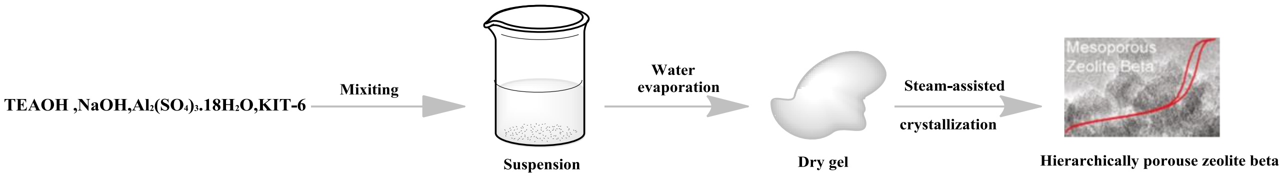
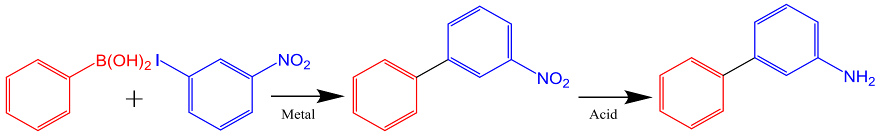
Zeolite Beta exhibits remarkable catalytic performance in reactions involving relatively bulky compounds as those involved in Fine Chemistry reactions. Nevertheless, when the molecular size of the latter approaches or is even larger than the micropores of Beta zeolite, important diffusional and/or steric hindrances may appear. A high interest has emerged in past years for the development of hierarchical zeolites, featuring mesoporosity and therefore enhanced accessibility. When used as catalysts, hierarchical zeolites present usually lower steric and diffusional limitations [1]. A hierarchical mesoporous network of Beta zeolite with very high micropore as well as mesopore volume has been synthesized by using Steam-Assisted Conversion (SAC) to induce a burst of nucleation in presence of the organic template (tetraethylammonium hydroxide, TEAOH). Moreover, the mesoporous silica KIT-6 has been applied as a silica source. Physicochemical properties of the resulting samples have been investigated by XRD, SEM, BET, TG, FT-IR, DLS, NH_3-TPD and DRS-UV. These characterizations show that using the SAC method incorporation with mesoporous silica KIT-6 led to hierarchical crystalline Beta zeolite with a small crystal size. Here, water plays a pivotal role in the crystallization mechanism, providing for a pool of concentrated nutrients affording fast nucleation, as well as for the recrystallization into ordered, more extended crystallite networks. A complete transformation of silica precursors into zeolite beta materials is thus only possible if the amount of water present in the reactor exceeds the requirements for simple saturation because water condensation in the gel is necessary. Thus, the amount of water needs to be adjusted not only for a specific temperature and reactor volume, but also for the sample loading [2]. This zeolite possesses large surface area (630 m_2/g) and mesoporous volume (0.59 cm_3/g) resulted from the formation of intercrystalline mesopores and the small crystal size. This hierarchical zeolite was used as acid-metal bi-functional heterogeneous catalysts in a tandem Suzuki-reduction reaction. The catalyst showed a superior activity in the water/ethanol solvent with high reusability.



Scheme 1. *Synthesis of hierarchical zeolite Beta*



Scheme 2*. Suzuki-reduction reaction*

Keywords: *Hierarchical Beta zeolite, Dry gel conversion method, Acid-metal catalyst.*

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Heterogenization of Chiral Amino Alcohol Ligands by Grafting onto Mesoporous Silica SBA-15 and Their Applications in Asymmetric Allylic C-H Bond Oxidation of Cycloolefins

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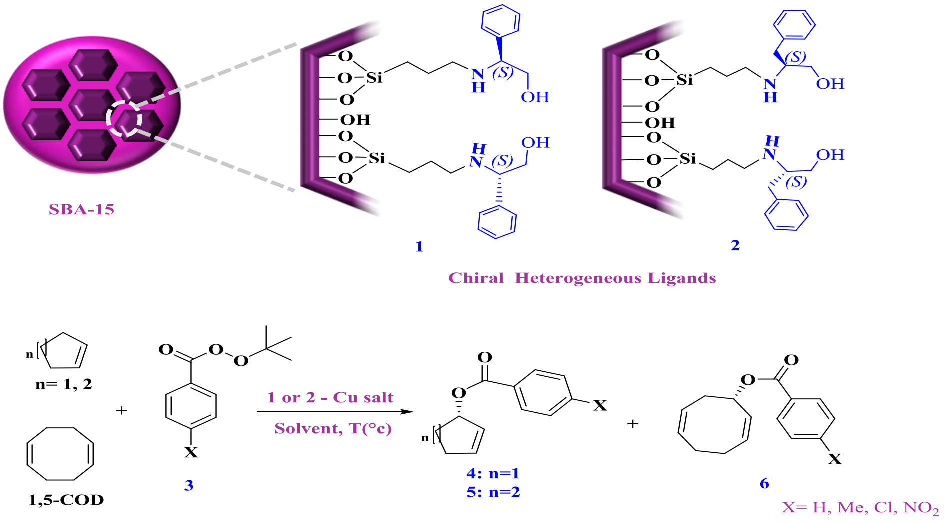
Enantioselective allylic oxidation of alkenes using organic peresters and copper chiral complexes has been a subject of great interest during the last decade. This reaction provides an access to chiral allylic alcohols which are key intermediates in the synthesis of natural products [1].

Limited natural resources and an increasing demand for enantiomerically pure compounds render catalysis and especially chiral heterogeneous catalysis a key technology and many researchers have taken great interest in these catalysts which is mainly due to the simple filtration and reuse of expensive chiral catalysts and ease of separation [2,3].

In this project, we use (*S*)-2-amino-2-phenylethanol and (*S*)-2-amino-3-phenylpropanol which are synthesis by reducing of their corresponding amino acids, as ligands and immobilizing on the modified silica nanoporous SBA-15 [4]. Obtained new heterogeneous ligands characterized by TGA, DTA, XRD, EDX, SEM, and FT-IR. The catalytic potential of these new heterogeneous ligands was applied for the copper catalyzed allylic C-H bond oxidation of cycloolefins. The allylic esters were prepared in good yields and moderate to good enantioselectivities (Scheme1).



***Scheme 1.** Allylic oxidation of cycloolefins in the presence of chiral heterogeneous catalysts*

***Keywords:** Enantioselective allylic oxidation, Silica nanoporous SBA-15, Cycloolefins.*

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Copper-catalyzed C-N Bond formation/ C-H Activation of Heteroarenes

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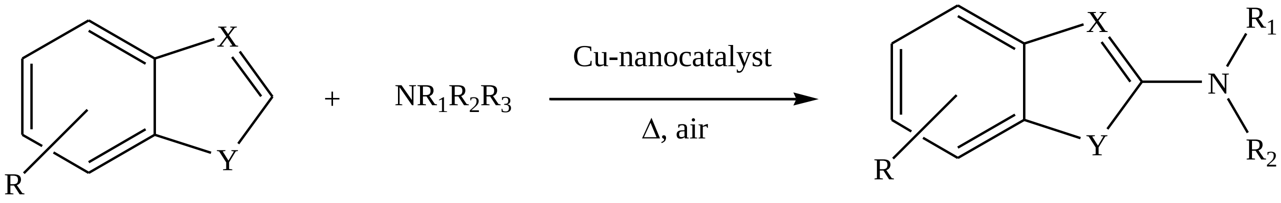
The transition-metal-catalyzed selective C-N bond formation reaction of heteroarenes is a highly important transformation in synthetic chemistry since five-membered heterocycles with amine group are widely employed in biological, pharmaceutical, and material sciences [1]. Methods to synthesize this skeleton include cyclocondensation reactions from two functionalized precursors, copper catalyzed Ullmann and Goldberg couplings [2-4]. There is description of successful copper catalyst systems with O_2 as oxidant, which can construct the C-N bond of heteroarenes efficiently either by decarboxylative coupling with formamides or by a direct C-H amination protocol with secondary amines under mild reaction conditions [5].

This research involved an efficient, clean and facile synthetic route for C-H amination of substituted heteroarenes with all types of amines using Cu-nanocomposite as eco-friendly nanocatalyst under solvent-free conditions at ambient temperature and affording excellent yields.

(Scheme 1).



Scheme 1. *Amination reaction with Nano-catalyst*

Keywords: *Copper Nano-catalyst, C-H activation, C-N Bond formation*

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Catalytic reduction of aromatic nitro compounds by copper-schiff base complex immobilized covalently on magnetic nanoparticles as a new, efficient and recyclable catalyst

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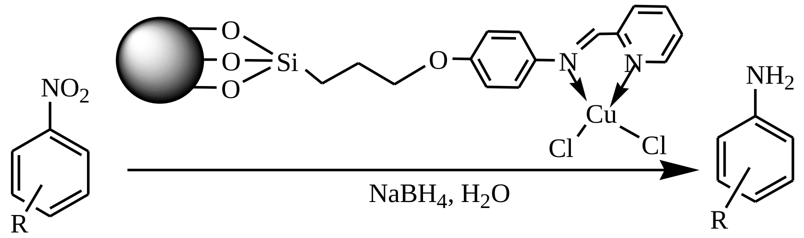
Compounds containing a nitro group are valuable substrates in organic synthesis. In particular, nitroarenes are one of the most readily available starting materials in organic synthesis since they can be produced from a range of aromatic starting materials [1]. One of the major pathways for the transformation of nitroarenes is their hydrogenation into anilines. Moreover nitro compounds are highly toxic and do not undergo biodegradation easily. Thus the elimination of nitro groups can be achieved by the reduction of amines with low toxicity and easily biodegradable [2]. A number of techniques for the reduction of nitroarenes have been developed. Although the reported methods are acknowledging, most of them suffer from one or more of the following drawbacks: high temperature, low yields of the products, prolonged reaction times, tedious work-up procedures, use of expensive or non-recyclable catalysts, hazardous solvents and generating large amounts of waste [3].

In this work, magnetically recyclable Cu-iminopy-MNPs has been synthesized and characterized by different methods. The catalytic activity of this newly synthesized catalyst for the reduction of nitro compounds in water has been studied (Scheme 1). The results showed high catalytic activity of this catalytic system for the hydrogenation reaction of various nitroarenes using $NaBH_4$ as hydrogen donor. Good to high yields (60-98%) of the products, using water as green reaction media and ease of separation and reusability of the catalyst are the advantage of this method.



Scheme 1: *Cu-iminopy-MNPs* catalyzed reduction of nitroarenes in the presence of sodium borohydride in aqueous media.

Keywords: *magnetically recyclable catalyst, nitroarene, reduction*

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Green Synthesis of Magnetically Separable and Recyclable Fe_3O_4-Ag Nanocomposites with Photocatalytic degradation for azo dyes

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We report the successful synthesis of Fe_3O_4-Ag nanocomposites as magnetically recyclable nanocatalyst via reflux process at 80 °C for 3h followed by reduction of Ag^+ using green tea leaves extract as the natural source of reducing and stabilizing agent without any surfactant. The process starts with $FeSO_4 \cdot 7H_2O$, $Fe_2(SO4)_3$, $AgNO_3$. The structure, morphology, thermal behaviour and magnetic properties of the product were characterized by XRD, FT-IR, FE-SEM, EDX, TG, VSM respectively. The photocatalytic degration of product for azo dyes such as methylen blue (MB), methyl orange (MO) were studied. We designed a new self-made labrotory photocatalytic reactor and then photocatalytic properties of Fe_3O_4-Ag nanocomposites are studied by mercury lamp and photodegration of MB and MO as a water pollutant evaluated until the photocatalytic process optimized with the process parameters. The parameters that were examined include: initial dye concentration, the mass of Fe_3O_4-Ag nanocomposites, pH value, and Fe_3O_4-Ag nano-sized composites. Absorbance spectra were measured using a spectrophotometer and the concentration of the test solution was calculated by using the Beer-Lambert Law. Our test results showed that the photocatalytic Hg lamp/ Fe_3O_4-Ag is a promising method for treating wastewater. The photocatalyst activity increases with increasing surface area. The work is very interesting in recent years due to the development of new nano-materials.

Keywords: *Green chemistry, azo dyes, photocatalytic degration*.

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Preparation and characterization of Pd/Beta zeolite with a hierarchical pore structure by using KIT-6 and trimethoxy silyl propanthiol: an efficient acid-metal bi-functional catalyst for the one-pot C-N bond reaction

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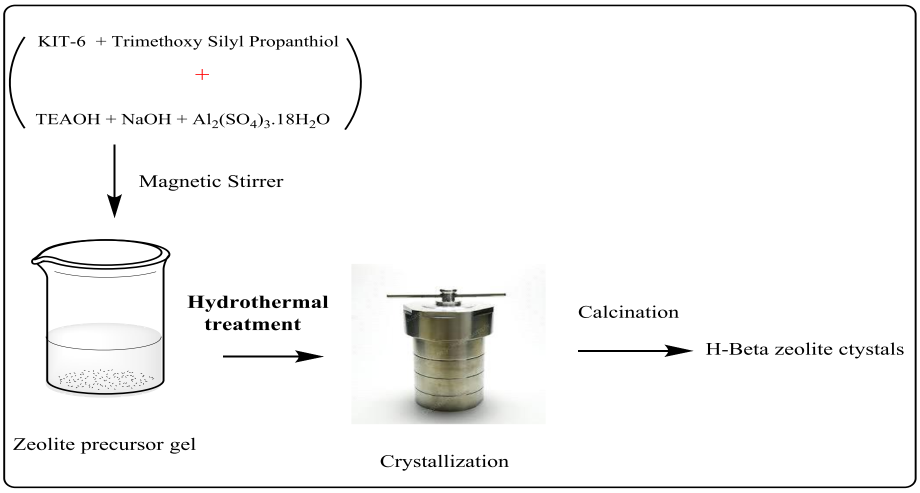
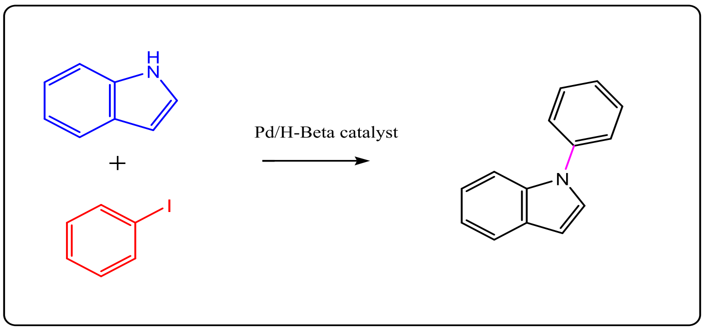
Palladium nanoparticles supported on hierarchical Beta zeolite (Pd/H-Beta) was evaluated as a novel acid-metal bi-functional heterogeneous catalyst. Hierarchical Beta zeolite was synthesized by an indirect method from KIT-6 as a silica source and trimethoxy silyl propanthiol as a crystal size controlling. Moreover, trimethoxy silyl propanthiol was used as an agent in the regularization of the mesopores. It also increases the surface area of the Beta zeolite. The structural and morphological characterization of the prepared catalysts was investigated using XRD, BET, ICP, FT-IR, SEM, and DRS UV techniques. . This zeolite possesses large surface area (742.19 m^2/g) and mesoporous volume (0.55 cm^3/g) resulted from the formation of intercrystalline mesopores and the small crystal size. The catalyst has been applied to the one-pot C-N bond formation reaction and demonstrated high catalytic activity even after several times.



Scheme 1. *Synthesis of H-Beta zeolite*



Scheme 2. *Synthesis of 1-phenylindole*

Keywords: *Hierarchical zeolite, Palladium nanoparticles, Beta zeolite, acid-metal catalyst*

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Preparation and characterization of Vanadium complexes supported on phyllosilicate and investigation of its catalytic properties

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Epoxides are intermediates to produce valuable chemicals Such as polymers, pharmaceuticals, food additives, dyestuffs and fragrance compounds which are commonly used in commercial scales [1]. Reduction, rearrangement or ring opening reactions of, epoxides with various nucleophiles convert, epoxides to diols, amino alcohols, allylic alcohols, ketones and polyether's [2]. They are regularly manufactured by mild oxidation of alkenes which required the presence of metal based catalysts to coordinate and activate the oxidant for selective production of them [1, 3].

An amine-functionalized layered magnesium-phyllosilicate (AMP) was prepared using a direct alkaline co-polymerization method between magnesium chloride and 3-aminopropyltriethoxysilane. The surface of AMP was further reacted with aldehydes (salicylaldehyde) in order to form Schiff base chelating ligands with N-donor groups incorporated in the layer surface. After than the product was reacte with VO (acac)$_2$ and used them as Heterogeneous catalysts in epoxidation of some alkenes.

The optimal conditions for a yield of 95% include 20mg of catalyst, 2ml $C_2H_4Cl_2$ as solvent and 0.4ml THBH as oxidant at 80 °c after 90 min.

The final products were thoroughly characterized by Fourier Transform Infrared spectroscopy (FT-IR), X-ray powder diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM) along with Energy Dispersive X-ray (EDX) Spectroscopy, thermo gravimetric and differential thermal analysis (TG/DTA) and X-ray photoelectron spectroscopy (XPS).

Keywords: *Organoclay, Schiff base chelates, Epoxidation, Pyllosilicate*

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Synthesis and modification of phyllosilicate by Schiff base Molybdenum complexes: characterization and catalytic application in epoxidation of alkenes

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An aminopropyl-functionalized magnesium phyllosilicate (AMP clay) contains a trioctahedral smectite with an organic propyl amine group. Therefore, the interest in the use of organically modified clays has increased with time. In fact, they possess the swelling ability, high cation exchange capacity, high layer aspect ratio, high specific surface area, film formation and adsorptive properties [1]. In particular, smectites appear to be good candidates in industry, agriculture, environmental remediation, catalysis, coatings, ceramics, and polymer materials due to their submicron size [2].

Epoxidation reactions represent a high added value for transformation of olefins. As a result, the technology of olefin epoxide production is an area with great development potential [3]. Molybdenum (II) complexes have been used to synthesize effective catalysts for the epoxidation of olefins using *tert*-butyl hydroperoxide (TBHP) as oxidant, a process which starts with the oxidation of the precursor complex to an active species of molybdenum (VI) [4].

An aminopropyl-functionalized magnesium phyllosilicate clay was synthesized. The surface of AMP was further reacted with aldehydes (salicylaldehyde) in order to form Schiff base chelating ligands with N-donor groups incorporated in the layer surface. After that the product was reacted with $MO_2(acac)_2$ and was used them as heterogeneous catalysts in epoxidation of some alkenes. It was found that the optimized conditions with over 95% yield for epoxidation of allkenes was 20 mg of catalyst, 2 ml $C_2H_4Cl_2$ as solvent and 0.4 ml THBH as oxidant at 80 °C after 90 min.

The final products were thoroughly characterized by fourier transform infrared spectroscopy (FT-IR), X-ray powder diffraction (XRD), field emission scanning electron microscopy (FE-SEM) along with energy dispersive X-ray (EDX) Spectroscopy, thermogravimetric and differential thermal analysis (TG/DTA) and X-ray photoelectron spectroscopy (XPS).

Keywords: *Pyllosilicate, Schiff base chelates, Epoxidation, alkene*

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Pd embedded on halloysite-cyclodextrin nanosponges hybrid: an efficient catalyst for promoting ligand and copper-free Sonogashira reaction

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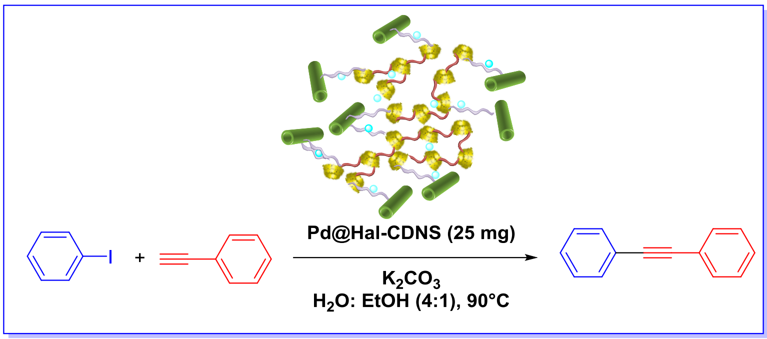
A novel hybrid was developed through covalent conjugation of halloysite nanoclay and cyclodextrin nanosponge and used for embedding Pd salt to afford Pd@Hal-CDNS with utility for promoting ligand and copper-free Sonogashira coupling reaction in aqueous media (Scheme 1). The reason behind this design was the fact that CDNS is composed of cyclodextrins with capability to encapsulate various guest molecules. On the other hand, Hal is an efficient support for immobilizing the catalysts. The formation of Pd@Hal-CDNS was confirmed by applying ICP-AES, TEM, SEM, TGA, XRD and FTIR analysis (Figure 1). CDNS could encapsulate the hydrophobic reagents and bring them near the catalytic active sites and allowed the reaction proceed in aqueous media. Notably, the catalyst was reusable up to five runs and could be recycled with negligible loss of catalytic activity and Pd leaching.



Scheme 1. *Sonogashira coupling reaction catalyzed by Pd@Hal-CDNS as a heterogeneous nano-catalyst*

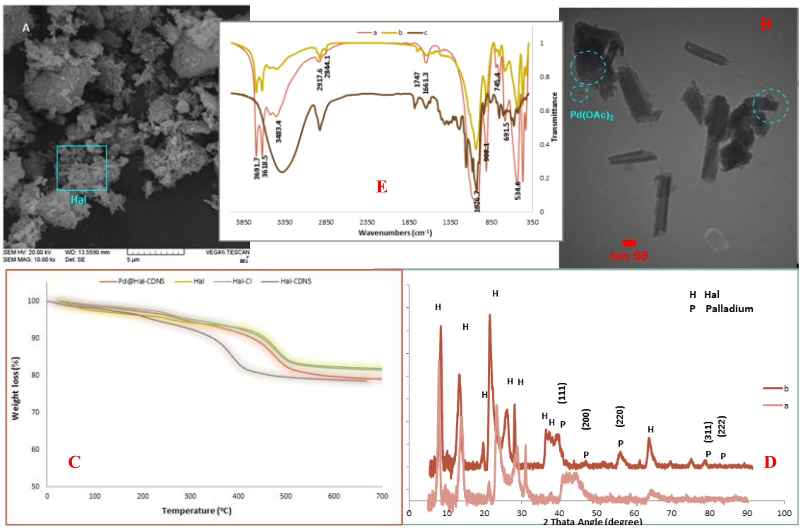


Figure 1. *(A) The SEM image of Pd@Hal-CDNS, (B) The TEM image of Pd@Hal-CDNS, (C) The TGA analyses of Hal, Hal-Cl, Pd@Hal-CDNS and Hal-CDNS, (D) The XRD patterns of the Hal (a) and Pd@Hal-CDNS (b), (E) The FTIR spectra of Hal (a), Pd@Hal-CDNS (b) and CDNS-N (c)*

Keywords: *Halloysite Nanoclay, Heterogeneous Catalyst, Sonogashira Coupling Reaction.*

NaY Zeolite Modified with Monoethanol Amine (MEA-NaY) as a Green and Reusable Catalyst for the One pot Three-Component Synthesis of Spirooxindole in Water

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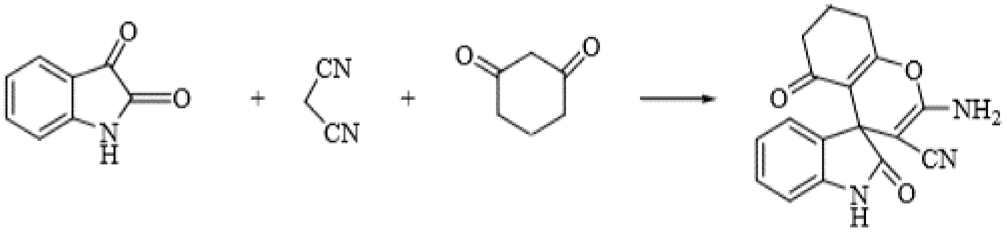
Abstracts: Modified zeolite (MEA_NAY) has been applied as an effective heterogeneous catalyst for one-pot synthesis of spirooxindole via reaction of various isatins with malonitrile and 1,3-cyclohexandione in water at 90^{0}C [1, 2]. The corresponding products were obtained in high yields. The catalyst was easily recycled and reused without loss of its catalytic activity (scheme 1, table 1).



Scheme 1. *Synthesis of Spirooxidoles derivatives*

Reaction between isatin, malonitrile and 1,3-cyclohexandione				
	Solvent	Temperature (°C)	Catalyst	Yeild%
1	H_2O	90	-	30
2	H_2O	90	MEA-NaY	90

Table 1. *Conditions and reaction efficiency*

Keywords: *Spirooxindole,isatin, malonitrile ,1,3-cyclohexandione.*

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Oxo-vanadium Schiff base supported on Fe_3O_4 nanoparticles as a magnetically separable nanocatalyst for epoxidation of olefines

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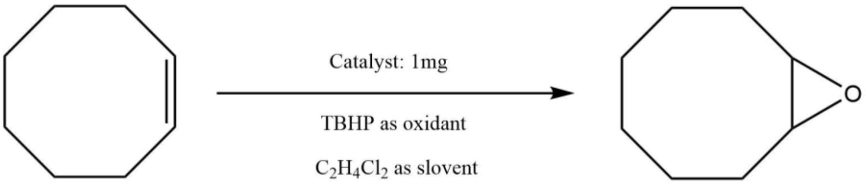
Oxidative catalysis is an important part of research for the preparation of chemical products in industry and chemistry. Oxidation in the presence of metal that has the ability to activate the oxidant for oxidation reaction is one of the most important chemical reactions [1]. In the last decade, due to the rapid development of nanoscience, nanocatalysts developed for different reactions such as C-C coupling and oxidation reactions. The separation of nanocatalysts using magnetic nanoparticles enables us to easily recover nanocatalysts after reaction. Also, due to the size of nanoparticles, magnetic nanocatalysts exhibit high activity [2].

A new magnetically recoverable nanocatalyst has been developed via covalent grafting of the vanadyl acetylacetonate complex onto silica-coated magnetic nanoparticles (MNPs) was functionalized with 3-APTS. The nanocatalyst was characterized by elemental analysis (CHN), FT-IR, X-ray powder diffraction (XRD), field emission scanning electron microscopy (FE-SEM), inductively coupled plasma optical emission spectrometry (ICP-OES) and thermogravimetric analysis (TGA). The resulting nanoparticles were used as a recyclable catalyst for the epoxidation of olefines (Scheme 1). To find suitable condition for epoxidation reactions, different parameter such as solvent, temperature, reaction time, amount of the nanocatalyst and oxidant/substrate molar ratio has been investigated. Eventually, conversion of various substrates is measured by gas chromatography (GC). To examine the stability and reusability of the nanocatalyst, at the end of each reaction, the nanocatalyst was magnetically separated from the reaction mixture, washed with $C_2H_4Cl_2$ and dried to prepare for the next reaction.



***Scheme 1.** Epoxidation of cis-cyclooctene*

***Keywords:** Magnetically nanocatalyst, Epoxidation, Olefine.*

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Preparation of Ag-doped Nano Magnetic γ-$Fe_2O_3@SiO_2$ Core–Shell Hollow Spheres: Investigation of the Catalytic activity for ligand-free *N*-arylation Coupling Reaction

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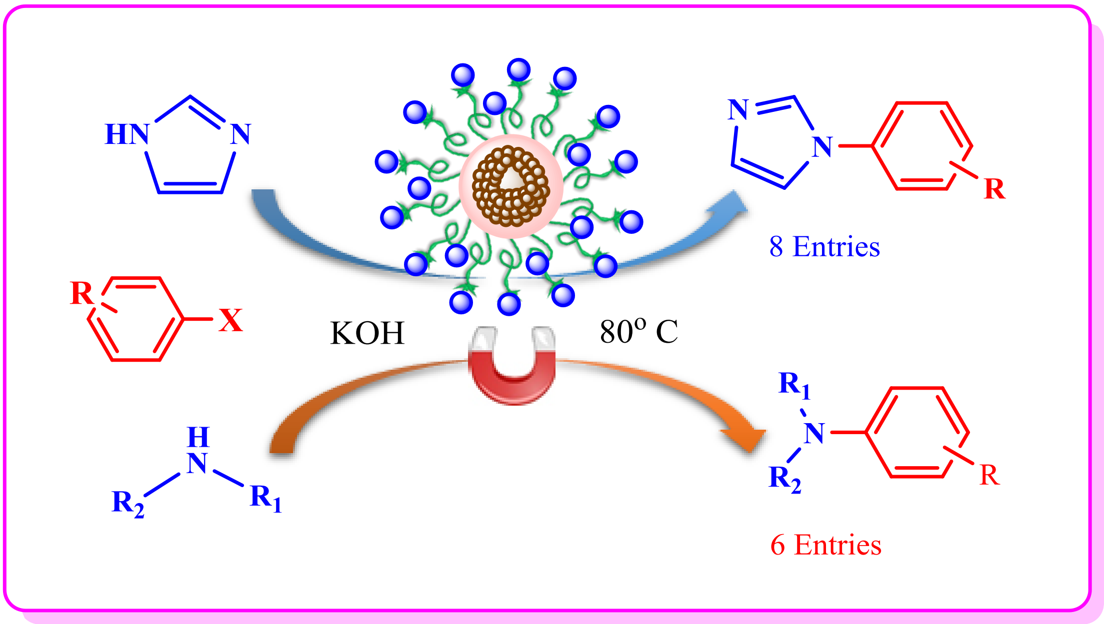
A novel heterogeneous nano-catalyst, (h-$Fe_2O_3@SiO_2$/Ag), was fabricated *via* biosynthesis approach. The design of the catalyst was based on the synthesis of core-shell h-$Fe_2O_3@SiO_2$ followed by amine functionalization and subsequent Ag(0) doping using *Achillea millefolium flower* as reducing and stabilizing agent. The novel catalyst was fully characterized by using SEM, TGA, ICP-AES, FTIR, VSM and XRD techniques. The hybrid catalyst was successfully applied for promoting *N*-arylation of azoles and aliphatic amines with aryl halide (Scheme 1). The hybrid catalyst is found to be applicable to a variety of nitrogen-containing heterocycles, such as imidazole and indole as well as aliphatic amines in high yields and practical simplicity under cost-effective "ligand-free" condition. However, the catalyst was still super-magnetic and could be simply separated from the reaction mixture by using an external magnet. The heterogeneous nature of the catalysis was also confirmed by studying the reusability and stability of the catalyst and silver leaching. Upon reusing for the seven run, however, slight leaching of Ag(0) and consequently loss of catalytic activity was observed.



Scheme 1. *N-arylation reaction catalyzed by nano magnetic h-$Fe_2O_3@SiO_2$/Ag catalyst*

Keywords: *Heterogeneous catalyst, Bio-synthesis, N-arylation reaction.*

Prepration of Cu/Fe_3O_4 nanoparticles using tea leaves extract as a catalyst for reduction of para-nitrophenol

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In this paper, we report the green synthesis of the Cu/Fe_3O_4 nanoparticles using tea leaves extract and their application as magnetically separable nanocatalyst for the reduction of 4-nitrophenol. 50 g of dried leaves powdered of green tea was added to 100 mL double distillated water and 100 mL ethanol in 500 mL flask and well mixed. The preparation of extract was done by using magnetic heating stirrer at 60°C for 1 h. The colorless extract obtained was centrifuged in 7000 rpm then filtered and filtrate was kept at refrigerator to use further. For green synthesis of Cu supported on magnetite nanocatalyst, 0.55 g $FeSO_4 \cdot 7H_2O$, 1.6 g $Fe_2(SO4)_3$ and 10 g $CuSO_4.5H_2O$ were dissolved in 25 mL colorless extract of the leaves of green tea at 60 °C under vigorous stirring. Then, a solution of 0.5 M Na_2CO_3 was added dropwise to the mixture to obtain alkaline pH which caused to change the color of the mixture to dark and monitoring the product formation using UV–vis at times raining 5–40 min. After being stirred again for 5 min at the same temperature, a suspension was formed which gave precipitate of the Cu/Fe_3O_4 nanoparticles on centrifugation at 7000 rpm and the obtained nanoparticles were washed with water and ethanol, respectively, and then dried. The nanocomposite was characterized by X-ray diffraction (XRD), Fourier transformed infrared (FT-IR) spectroscopy, field emission scanning electron microscopy (FE-SEM), energy dispersive X-ray spectroscopy (EDS), Vibrating sample magnetometer (VSM) and transmission electron microscopy (TEM). The catalytic activity for the reduction of 4-NP to 4-AP in water was also evaluated. The conversion of 4-NP to 4-AP in aqueous medium was monitored by using UV-visible measurements at room temperature. There was a shift of the peak of 4-NP from 317 to 400 nm, observed immediately after the addition of $NaBH_4$. This was due to the formation of 4-nitrophenolate ions under alkaline conditions caused by the addition of $NaBH_4$. After the Cu/Fe_3O_4 magnetic nanocomposite was added into the reaction system, the reduction process was monitored by measuring the time-dependent adsorption spectra of the reaction mixture solution. The magnetic nanocomposite can be easily separated from the reaction media by means of an external magnet and recycled several times without marked loss of activity.

Keywords: *Green chemistry, NaBH4, 4-nitrophenol, catalyst*

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Combination of Graphene Oxide, Chitosan, Cyclodextrin Nanosponge and Ionic Liquid as a Magnetic Heterogeneous Nano Catalyst for Pd-Catalyzed Reactions

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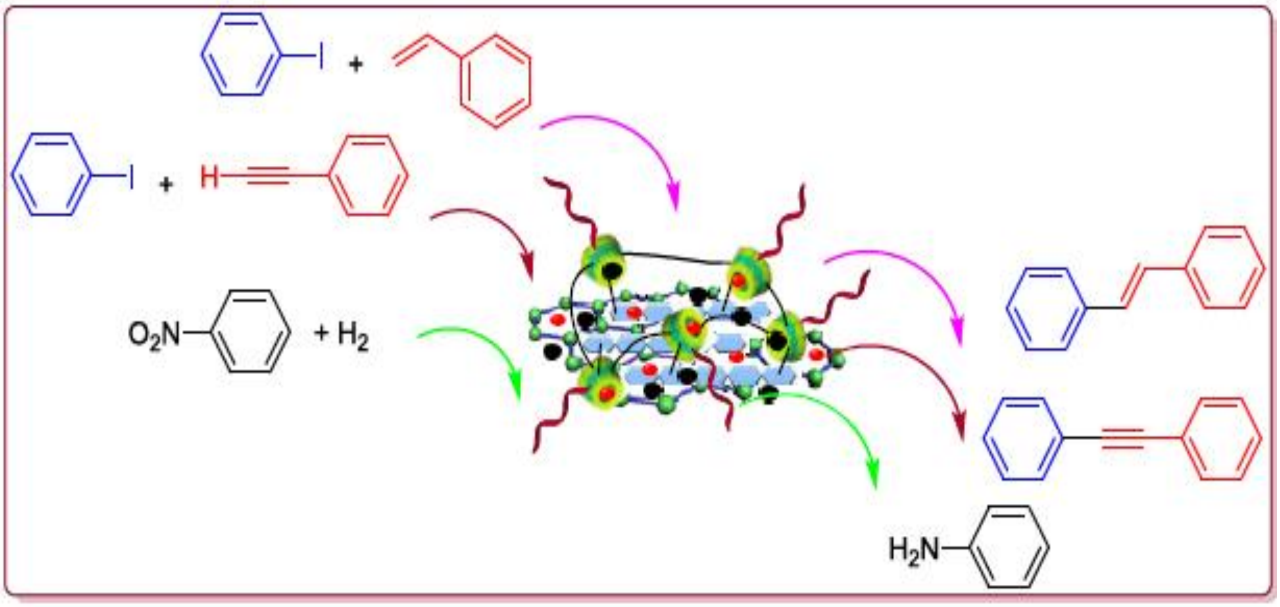
In continuation of our effort to demonstrate the use of cyclodextrin nanosponge (CDNS) as a support for embedding catalytic species [1], a hybrid of graphene oxide (GO), chitosan (CS), CDNS and ionic liquid (IL) was used as a support to embed Fe_3O_4/Pd nanoparticles. Also, the unique properties of graphene for the catalytic active species has been proved [2]. The obtained catalyst, Fe_3O_4/Pd@Hybrid could promote hydrogenation and ligand and copper free Heck and Sonogashira coupling reactions under mild reaction condition. All hydrogenation, Sonogashira and Heck coupling reactions proved high to excellent yields of the products in short reaction time. The result of this study confirmed that the catalytic activity of Fe_3O_4/Pd@Hybrid was superior to that of Pd@CDNS-IL, Pd@GO, Pd@CS and Pd@Go-CS due to the synergetic effect between the components of the hybrid system. Moreover, Fe_3O_4/Pd@Hybrid exhibited negligible Pd leaching after several reaction runs.



Scheme 1. *Model reaction of Mizoroki–Heck and Sonogashira coupling and hydrogenation catalized by Fe_3O_4/Pd@Hybrid*

Keywords: *Graphene Oxide 1, Cyclodextrin Nanosponges 2, Chitosan 3, Ionic Liquid 4*.

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A novel bifunctional heterogeneous catalyst for one-pot reduction-acetylation reaction in water

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Nature has developed enzymetic catalysts for the multistep synthesis of complex chemical building blocks needed for the cells' metabolism from nutrients in a perfect chemical factory which is called living cells [1]. The multistep synthesis of metabolites occurs *via* a series of sequential reactions in which the product of one reaction serves as a substrate for the subsequent reaction. The efficient catalytic ability of enzymes in these multistep reactions is due to cooperative interactions between accurately positioned functional groups such as metal centers, acids, bases, hydrogen bond donors and hydrogen bond acceptors in the active sites. These groups perform many important roles including activation and stabilization of transition states and substrate recognition through hydrogen bonding, electrostatic or covalent interactions [2]. Mimicking of the bio-system in artificial heterogeneous catalysis would be a great interest for chemists not only in industry but also in academia [3]. In this regard, most chemists have focused their attention on the development of heterogeneous multifunctional catalysts for performing multistep organic synthesis of a desired compound *via* one-pot tandem reactions. Using multifunctional catalysts in tandem reactions, that combine two or more catalytic transformations in the one-pot process, eliminates the time and yield losses associated with the isolation and purification of intermediates in multistep sequences [4]. These processes become green, sustainable and attractive with low-cost, step-saving, a reduced energy consumption and waste production as well as decreasing the quantities of reagents and solvents used.

To benefit the valuable applications of multifunctional catalysts in one-pot tandem reactions, and as a continuation of our recent works on the development of new heterogeneous catalysts [5], herein, we report the synthesis of immobilized palladium catalyst containing an acidic functional group on the surface of iron oxide (Scheme 1). After characterization of this newly synthesized catalyst by different methods such as ICP, CHN, SEM, TEM, XRD, TGA and FT-IR, we have successfully used it as a bifunctional heterogeneous catalyst for the synthesis of acetamides in water *via* reduction of nitro compounds followed by acetylation reaction. The catalyst could be easily recycled and reused repetitively. Its structure remained intact after five recoveries according to the FT-IR spectrum.

Scheme 1. *Heterogeneous acidic palladium catalyst*

Keywords: *Bifunctional catalyst, palladium, heterogeneous catalyst*

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The effect of rare earth element (neodymium) on coke deposition in Pt/γ-Al_2O_3-Cl catalyst for reforming reaction

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Catalytic reforming is a major conversion process in petroleum refinery and petrochemical industries. In this process, naphthenic compounds and straight-chain (normal) paraffins are transformed into the branched-chain (isomers) paraffins and aromatic compounds. With this process, the octane number of naphtha increases by increasing the concentration of branched-chain paraffins and mainly of aromatics. There has been an enormous amount of work over the years involved with understanding the role of the second metal on activity, selectivity and coke deposition, but these findings have rarely been reported about Pt-Nd/γ-Al_2O_3 catalyst. Rare earth elements play an important role in the modification of some catalysts. There are only a few studies about rare earth influence on some materials like silica, alumina and Beta zeolite. So the influence of neodymium on the catalytic preference of n-heptane over Pt/γ-Al_2O_3-Cl was studied in this work. We also report activity, selectivity and the deposition rate and amount of coke in the n-heptane reforming process with bimetallic Pt-Nd that compared with Pt-Pb supported on γ-Al_2O_3 catalysts. The Pt-Nd/γ-Al_2O_3-Cl catalysts were prepared with different amounts including x:y=0:0.6, 0.06:0.54, 0.2:0.4, 0.3:0.3, 0.4:0.2, 0.54:0.06, 0.6:0 which x is weight percent of Pt and y is weight percent of Nd. The effects of temperature (450-500 °C) and pressure (15-30 atm) also have been compared and discussed. The results indicate that the coke formation on Pt-Nd/γ-Al_2O_3-Cl catalysts is less than Pt/γ-Al_2O_3-Cl. The higher amount of activity was observed in Pt-Nd/γ-Al_2O_3-Cl which is 99.8% at 15 atm and 500 °C [1-3].

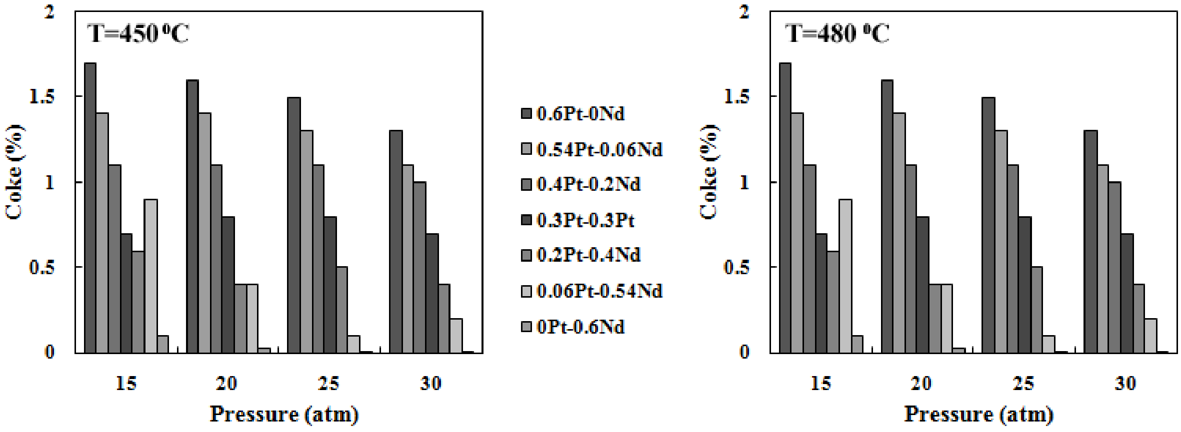

Figure 1. *The amounts of coke laid down over various prepared catalysts in different pressures (15-30 atm).*

Keywords: *Reforming, Coke, Neodymium, Catalyst.*

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Catalytic activities of various types-supported nickel nanoparticles for benzene hydrogenation

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Benzene is naturally present in gasoline, but since this compound is severely carcinogenic, and environmental laws limit the amount of this compound in less than 1%, several methods have been developed to remove this compound. Hydrogenation of unsaturated compounds as benzene for producing the eco-friendly intermediate materials such as cyclohexane is one of the most low-cost and useful methods in industry [1]. It has been found that the activity of the nickel catalysts for this reaction depends on various parameters. One of them is the nature of the supports as it may affect the properties of the active phase (metallic function). Other parameters include of the dispersion and the reducibility of the metallic phase, the preparation method, the pre-treatment conditions as drying and calcination, and reduction of catalyst [1, 2]. In this research, we prepared a series of different Ni-supported catalysts as HZSM-5, SBA-15, activated carbon (AC) and MIL-101. These powder catalysts were characterized by FT-IR, UV-vis DRS, XRD and N_2 adsorption-desorption techniques. The impregnated catalysts were loaded in the fixed-bed microreactor and tested in the range of 403-463 K and at atmospheric pressure. The reactor results indicate that the best benzene conversion and selectivity to cyclohexane is achieved for Ni-SBA-15 (>88%) at 423 K and Ni-AC (>61%) at 443 K. Also, by calculating the benzene yield, it can be concluded that the acceptable performance was obtain for Ni-AC catalyst at 443 K.

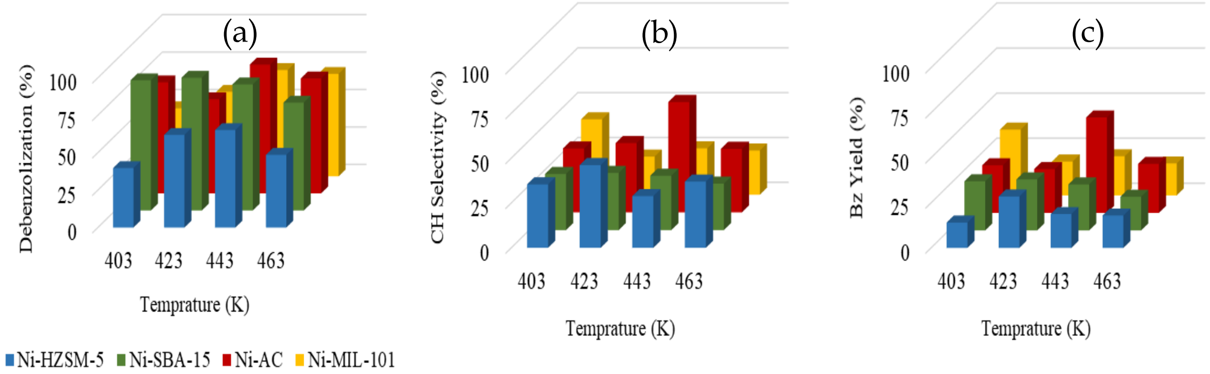

Figure 1. *Temperature effect on a) activity, b) CH selectivity and c) benzene yield of Ni catalysts.*

Keywords: *Benzene hydrogenation, Unsaturated compounds, Fixed-bed reactor.*

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Activity study of the MOFs-supported Ni catalysts in the benzene elimination

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The selective hydrogenation of C-C multiple bonds is an effective method to reduce the benzene in gasoline in accordance to the environmental regulations and aromatics important role in the octane number of fuels. One of the most important points in reducing benzene from gasoline is that the used method has the least effect on other aromatic compounds in order to prevent the loss of fuel octane number. Accordingly, it is important to provide a catalyst that can selectively remove and reduce the target compound (benzene) from the reaction mixture [1-3].

Nickel nanoparticles supported on MOFs (MOF-5 and MIL-101) were prepared by wet impregnation method. The results of the characterization techniques such as powder X-ray diffraction, Fourier transform infrared and Uv-visible diffuse reflectance were used to establish a relationship between the obtained structural properties and the catalytic activity in the selective hydrogenation of benzene at 130–190 ^{o}C and ambient pressure.

A mixture containing the aromatic hydrocarbons (6 vol% of benzene and 8 vol% of toluene dissolved in an excess of liquid n-heptane) was used as feed model and the tests were conducted in the fixed-bed microreactor. Catalytic data’s and evaluating the performance of these nano catalysts present that the best activity (> 98%) and good selectivity (> 52%) were obtained for Ni/MOF-5 catalyst at 130 °C.

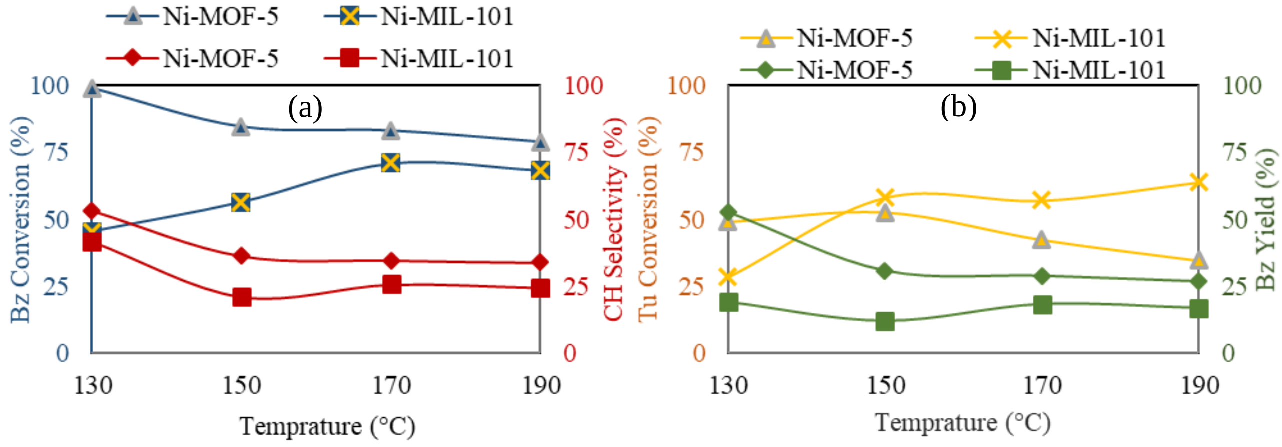

Figure 1. *Temperature effect on (a) Bz Conversion/Selectivity and (b) Tu Conversion/Bz Yield of catalysts.*

Keywords: *Selective hydrogenation, Environmental regulations, Nickel nanoparticles.*

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Catalytic reforming of n-heptane over bi and trimetallic supported catalysts

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Catalytic naphtha reforming is a major petroleum refining process for the production of high octane hydrocarbons in gasoline and aromatic hydrocarbons used in the petrochemical industry. The used catalysts in this process are formed from two functions: the metallic function (noble metals especially Pt) and a porous support that plays as an acidic function. The major reactions that occur are the isomerization, dehydrogenation, and dehydrocyclization [1, 2]. In the present work, a series of HMS-HZSM-5 composites impregnated by 0.6 wt% Pt catalysts promoted by different amounts of Sn, Re or Sn-Re were prepared and characterized as reforming catalysts by N_2 physisorption, XRD, TGA-DSC and FT-IR. The solid catalytic activities were evaluated through reforming of n-heptane employing fixed-bed microreactor directly connected to a gas chromatograph analyzer.

The catalytic evaluations show that Pt-(Re-Sn)/HMS-HZSM5 catalysts had a high activity for reforming of n-heptane. Pt-(Re-Sn)/HMS-HZSM5 have more ability compared to HMS and HZSM-5 catalysts because they have both properties of mesoporous HMS and microporous HZSM-5. The results show that bimetallic and trimetallic catalysts revealed better performance than monometallic catalysts for n-heptane reforming. The analyze of carbon deposited after the stability test shows that the coke deposition on trimetallic catalysts is lower than mono and bimetallic catalysts. The catalytic activity results indicate that the trimetallic (0.3Pt–0.3(Re, Sn))/HMS-HZSM5 catalysts are the most active towards n-heptane reforming while (0.3Pt–0.3Sn)/HMS-HZSM5 catalyst can be recognized as the worst catalyst due to its rapid deactivation.

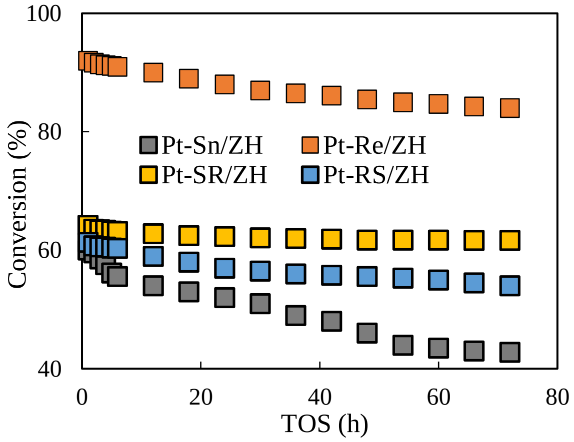

Figure 1. *n-C_7 conversion versus time on stream at 300 °C for different catalysts.*

Keywords: *Reforming, Refining process, Bimetallic catalyst, Trimetallic catalysts.*

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Montmorillonite-Fe_3O_4 a valuable heterogeneous nanocatalyst for the one-pot synthesis of indeno[1,2-b]indolone derivatives in aqueous media

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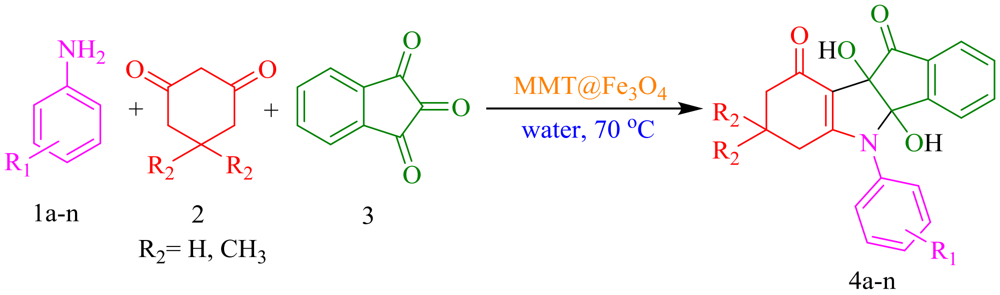
Fe_3O_4 magnetic nanoparticles has attracted a lot of attention because of their fundamental application properties in various field such as sensors, clinical use, and high density magnetic recording media [1]. Arc discharge, mechanical grinding, laser ablation, microemulsion, and high temperature decomposition of organic precursors can produce magnetic nanoparticles [2].
Clay minerals such as montmorillonite has large surface area, stable chemical properties, low-cost, well defined layered structure, therefore it has been widely applied in catalyst [3]. Montmorillonite K10 (MMT-K10) is a nanolayered alumina silicate clay can be act as a nanoreactor for the chemical reactions and a drug nanocarrier for pharmaceutical targets.
Indeno[1,2-*b*]indoles are a significant class of heterocyclic compounds because of their potential biological applications [4] and pharmacological studies [5].

A highly efficient one-pot synthesis of Indeno[1,2-*b*]indoles derivatives **4** has been developed *via* three component reaction of anilines **1**, dimedone **2** and ninhydrin **3** in the presence of recyclable and magnetic organocatalyst MMT@Fe_3O_4 in aqueous media at 70 °C (Scheme 1).



Scheme 1. *Synthesis of dihydroxy indeno[1,2-b]indolone*

Keywords: *Fe3O4-MMT nanoparticles, indeno[1,2-b]indolones, multicomponent reactions.*

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Immobilization of A Diamine onto Fe_3O_4@SiO_2@SBA-15 via Click Reaction: A New Pd(II) Supported Nanocatalyst for Hiyama Cross-Coupling Reaction

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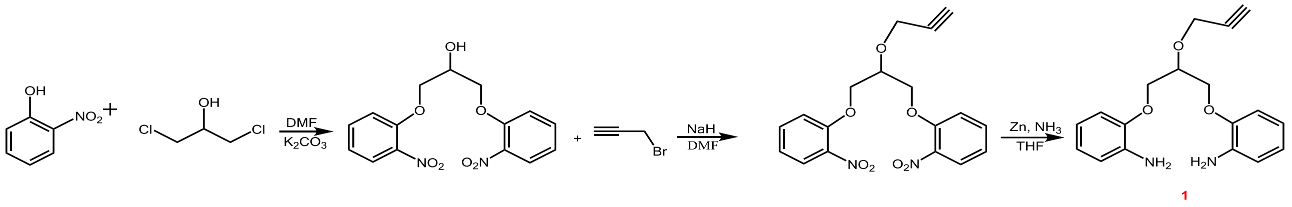
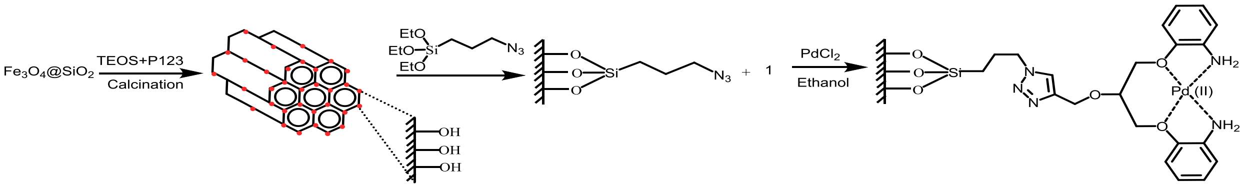
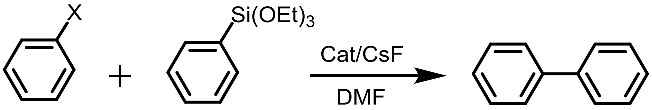
In this study, a new ligand, i.e. 2-(3-(2-aminophenoxy)-2-(prop-2-ynyloxy)propoxy)benzenamine (APPB), has been prepared in three steps starting from *o*-nitrophenole, according to Scheme 1 [1-3]. Magnetite nanoparticles (MNPs), obtained via co-precipitation method and covered by silica and mesoporous silica (SBA-15) layers, were silylated with 3-azidopropyltriethoxysilane (Fe_3O_4@SiO_2@SBA-15-N_3) [4]. The synthesized ligand (APPB) was then anchored on Fe_3O_4@SiO_2@SBA-15 via click reaction. The core shells of the supported ligand were stirred in EtOH solution of Pd(II) to afford the supported Fe_3O_4@SiO_2@SBA-15-APPB-Pd(II) complex, Scheme 2. The obtained nanoparticles were used in Hiyama coupling reaction of aryl halides with triethoxyphenylsilane, Scheme 3 [5]. The nanoparticles of the supported catalyst could be magnetically separated from the reaction mixture by simple magnetic decantation and reused.



Scheme 1. *Synthesis of ligand*



Scheme 2. *Synthesis of MNP-supported diamine-Pd complex*



Scheme 3. *Hiyama reaction*

Keywords: *Magnetic Nanoparticle, Click chemistry, Hiyama coupling reaction.*

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Lead adsorption using Magnetic multiwalled carbon nanotubes

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The pollution of water resources due to the disposal of heavy metals has been causing worldwide concern. Therefore, the removal of heavy metal ions from water has become an important subject today. Many techniques and methods to remove heavy metal ions from water have been developed, such as ion-exchange, evaporation and concentration, chemical precipitation, reverse osmosis, adsorption, and electrolysis [1]. Numerous materials can be used as adsorbents to remove heavy metal ions from water. Because CNTs possess a high chemical and thermal stability and a large specific surface area, they have been applied to remove heavy metal ions from aqueous solution [2-5].

In this study, magnetic multiwalled carbon nanotubes (MMWCNTs) were successfully synthesized. These MWCNTs were used to lead ions adsorption from aqueous solution. The pristine and MMWCNTs were characterized by Fourier transform infrared, scanning electron microscopy and X-ray diffraction. The optimal conditions of experimental such as pH, amount of adsorbent and contact time were investigated. The adsorption capacity was evaluated using both the Langmuir and Freundlich adsorption isotherm models. The results showed that MMWCNTs have a good potential for adsorption of lead from aqueous solution.

Keywords: *Lead adsorption, magnetic MWCNTs, Adsorption isotherm*

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Lead adsorption using TEOS-Functionalized multiwalled carbon nanotubes

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Heavy metal ions in water have been a worldwide concern for many years because of their toxicity toward aquatic-life, plants, animals, human beings and the environment. Water contaminated by heavy metal ions had become much more serious with a rapid development of industries and competitive use of fresh water in many parts of words. Therefore, heavy metal ions removal from water has become an important subject today[1]. Many technologies and methods for heavy metal ions removal from wastewaters have been developed, such as ion-exchange, evaporation and concentration, chemical precipitation, reverse osmosis, adsorption, and electrodialysis. Considering from economy and efficiency point of view, adsorption is regarded as one of the most promising and widely used methods. In current years, carbon nanotubes have shown a high potential for absorbing lead [2-4].

In this study, multiwalled carbon nanotubes (MWCNTs) were modified by strong oxidizing agents and were functionalized with tetra-ethoxy-silane (TEOS). These MWCNTs were used to remove lead ions from aqueous solution. The pristine and functionalized MWCNTs were characterized by Fourier transform infrared, scanning electron microscopy and X-ray diffraction. The optimal conditions of experimental such as pH, amount of adsorbent and contact time were investigated. The adsorption capacity was evaluated using both the Langmuir and Freundlich adsorption isotherm models. The results suggest that functionalized MWCNTs can be good Pb(II) adsorbers and have great potential applications in environmental protection.

Keywords: *Lead adsorption, Functionalized MWCNTs, TEOS.*

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Functionalization of multiwalled carbon nanotubes using Isocyanate groups for Lead adsorption

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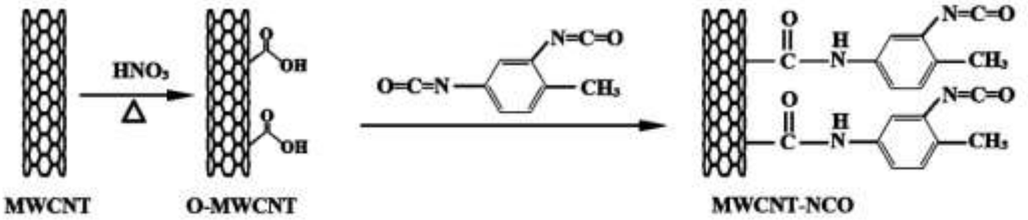
Heavy metal ions are highly toxic even at low concentrations and can accumulate in living organisms, causing several disorders and diseases. Unlike organic pollutants, heavy metals are nondegradable. Once in the food chain, they are able to accumulate in living organisms and cause extremely high toxicity. There are many conventional methods that are being used to remove the metal ions including oxidation, reduction, precipitation, membrane filtration, ion exchange and adsorption. Among the above methods, the promising process for the removal of metal ions from water and wastewater is adsorption, because the employed adsorbent can be regenerated by suitable desorption process and it is highly effective and economical. Several adsorbents which have been studied for adsorption of metal ions [1,2]. In current years, carbon nanotubes have been applied as a novel adsorbent to remove the heavy metal ions and various contaminants from an aqueous solution [3,4].

In this study, multiwalled carbon nanotubes (MWCNTs) were modified by strong oxidizing agents and were functionalized with Isocyanate groups. These MWCNTs were used for adsorption of lead ions from aqueous solution. The pristine and functionalized MWCNTs were characterized by Fourier transform infrared, transmission electron microscopy, scanning electron microscopy and X-ray diffraction. In other to study lead adsorption behaviors, the optimal conditions of experimental such as pH, amount of adsorbent and contact time were investigated. The adsorption capacity was evaluated using both the Langmuir and Freundlich adsorption isotherm models. The results showed that functionalized MWCNTs have a greater potential for adsorption of lead from aqueous solution.



Scheme 1. *Modification and functionalization of MWCNTs with COOH and isocyanate groups*

Keywords: *Lead adsorption, Functionalized MWCNTs, Isocyanate groups.*

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Functionalization of multiwalled carbon nanotubes with thiol groups for Lead adsorption

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Water contaminated by heavy metal ions had become much more serious with a rapid development of industries and competitive use of fresh water in many parts of the world. Heavy metal ions are highly toxic even at low concentrations and can accumulate in living organisms, causing several disorders and diseases. The heavy metals hazardous to human health include Pb, Hg, Cd, As, Cu, Zn, and Cr. As and Cd cause cancer, Hg can cause mutations and genetic damage, while Cu, Pb, and Hg can cause brain and bone damage [1]. There are many conventional methods that are being used to remove the metal ions. Among the different physicochemical processes, adsorption offers the best prospects for overall treatment, especially for effluents that contains moderate and low concentrations of metals [2]. Due to a large surface area, small, hollow, and layered structures, carbon nanotubes have already been investigated as promising adsorbents for various organic pollutants and metal ions and can be easily modified by chemical treatment to increase their adsorption capacity. [3,4].

In this study, multi-walled carbon nanotubes (MWCNTs) were modified by strong oxidizing agents and were functionalized with thiol groups. These MWCNTs were used for adsorption of lead ions from aqueous solution. The pristine and functionalized MWCNTs were characterized by Fourier transform infrared, scanning electron microscopy and X-ray diffraction. In batch tests, the influences of solution pH, contact time, and amount of adsorbent were studied. The Langmuir and Freundlich isotherms were used to describe the adsorption behavior of heavy metal ions by CNTs. The results showed that functionalized MWCNTs have good potential application in environmental protection.

Keywords: *Lead adsorption, Functionalized MWCNTs, thiol groups.*

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Reduction of 4-nitrophenol by GO/Fe_3O_4 supported Cu(Ⅱ) complex composite as an efficient a recyclable nanocatalyst

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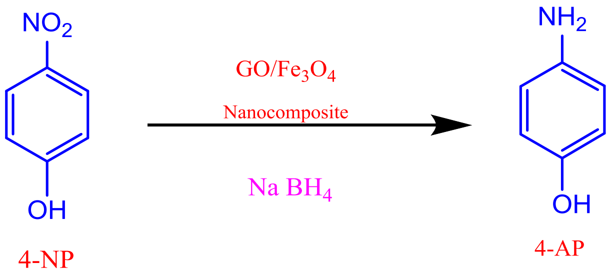
Most of the dyes are toxic to aquatic organisms. Thus, there is a drastic need to develop ecofriendly treatment methods for the elimination of these pollutants from the environment, because of their toxicity and carcinogenic properties. Thus, the need for 'greener' methods or chemical products that reduce or eliminate the use and generation of hazardous compounds is essential. Graphene Oxide has been a lot of attention because of its unexampled properties, such as large surface area and high conductive and electromagnetic parameters and so on. Fe_3O_4 nanoparticles are superparamagnetic and have been studied in many aspects such as structural, morphological, optical, magnetic and catalytic properties and superconductivity. GO/Fe_3O_4 nanocomposite were synthesized to incorporate the properties of both Fe_3O_4 and graphene. In this work, a Cu(Ⅱ) Schiff base complex supported on magnetic GO and used as efficient nanocatalyst for reduction reaction. Also, the synthesized nanocatalyst could be separated easily from the reaction mixture using an external magnet and reused for several consecutive times for dye reduction.



***Scheme 1** The reduction for the conversion 4-NP to 4-AP*

Keywords: *Graphene oxide, Schiff base complex, Dye reduction.*

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Regioselective methanolysis of epoxides by urea-functionalized metal-organic frameworks as heterogeneous organocatalysts

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Abstract

Hydrogen-bonding organocatalysis has emerged as a promising biomimetic alternative to Lewis acid catalysis. Urea moieties represent the most common hydrogen-bond donors used for the preparation of these catalysts. However, their significant tendency to undergo self-quenching often decreases their solubility and reactivity. Recently, scientists have found a promising way around this problem by immobilizing the hydrogen-bonding organocatalysts on Metal–organic frameworks (MOFs). [1,2] Compared to other porous materials, MOFs have given chemists the opportunity to tune the topology, pore size and functionality by rational selection of organic linkers and inorganic metal centers.

Ring opening of epoxides is one of the most important reactions producing vital intermediates in organic synthesis. There are some reports for this reaction catalyzed by MOFs containing Lewis acid sites, especially with Cu, Fe and Hf metal nodes.[3] In this regard, there is no report of urea-containing MOFs as hydrogen-bond catalysts in this reaction.

In this paper, we report an extension of these studies aimed at investigating the organocatalytic role of urea-containing MOFs in the activation of epoxides. A novel Zn-MOF was synthesized by combining the ditopic urea strut, 4,4′-oxybisbenzoic acid and $Zn(NO_3)_2.6H_2O$ using the solvothermal method at 90°C for 120 h to give suitable X-ray quality crystals, Fig.1.

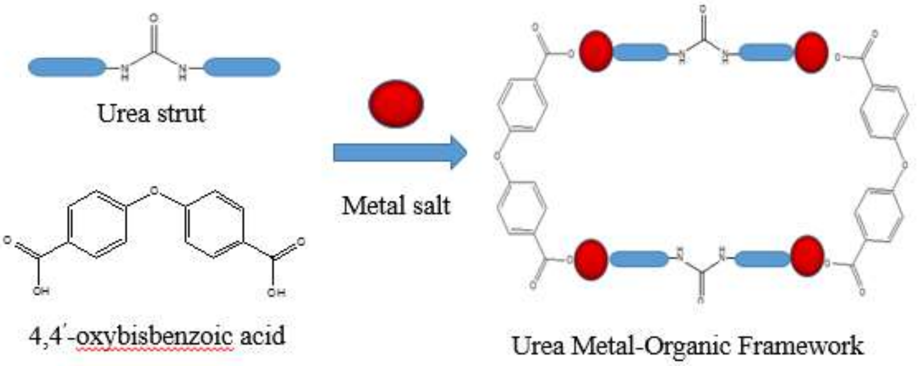

Fig.1. Synthesis of urea-containing metal-organic framework.

The productivity of the catalyst was evaluated by determination of the reaction selectivity for the conversion of styrene oxide to 2-methoxy-2-phenylethanol as the major product in our catalytic system. The prepared urea MOF catalyst was suspended in a MeOH (3mL) solution of epoxide (25 mg) and stirred at 60ºC. After 40 h reaction time, 95% selectivity was calculated for the above mentioned major product. When the reaction prolonged to 48 h, quantitative conversion of styrene oxide was obtained with 98% selectivity for 2-methoxy-2-phenylethanol that was characterized by GC and NMR.

Keywords: *Metal-Organic Framework, Methanolysis, Heterogeneous catalyst*

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Synthesis of 3,4-dihydropyrano[3,2-*c*]chromene using Fe_3O_4 nanoparticles-supported β-cyclodextrin-guanidine as an efficient and recyclable heterogeneous catalyst

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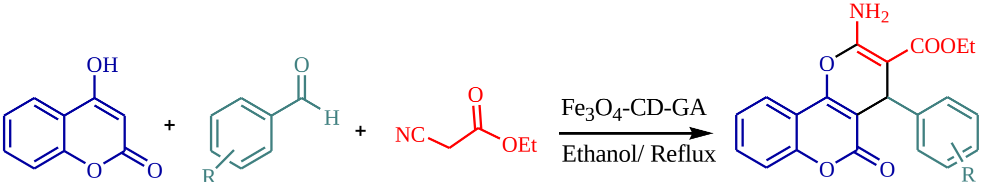
Dihydropyrano[3,2-c]chromene nucleus is a source of many biological properties and its derivatives show anti-microbial, anti-fungal, analgesic, anti-cytotoxic, anti-tuberculosis [1] and AChE inhibitory [2] activities. Therefore, the development of efficient methods for synthesis of these important heterocycles has attracted researchers' attention. Cyclodextrins show ability to encapsulate variety of guest molecules such as aliphatic and aromatic hydrocarbons, acids, amines, alcohols and small inorganic anions through host-guest interactions [3]. Immobilization of homogeneous organic catalysts on various support materials is sustainable method to recover and recycle catalysts. Owning unique structures and properties, magnetic nanoparticles can be serve as a highly efficient catalyst supports. Herein, considering the importance of chromenes and with a purpose of developing an efficient, reusable, heterogeneous, cost-effective and environment-friendly catalyst for synthesis of these compounds, amino-functionalized β-CD was prepared and grafted on Fe_3O_4 nanoparticles via the chemical co-precipitation approach. The prepared catalyst's efficiency was explored in synthesis of dihydropyrano[3,2-c]chromenes.



Scheme 1. *Synthesis of dihydropyrano[3, 2-c]chromene derivatives*

Keywords: *Multi-component, Dihydropyrano[3,2-c]chromene, Heterogeneous catalyst*

References

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Magnetization of urea-based ionic liquid and its application in synthesis of chalcones

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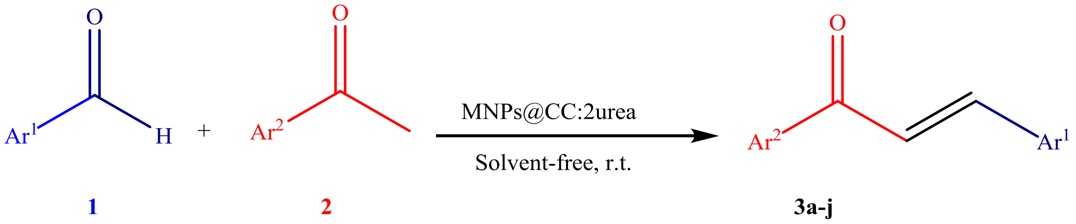
Abstract

Chalcones are an interesting target class of compounds which extensively investigated due to their biological, medical and industrial applications [1,2]. In this work, magnetite nanoparticles (MNPs) was prepared by co-precipitation of Fe^{2+} and Fe^{3+} salts in the presence of choline chloride (CC):2urea as a deep eutectic solvent (DES) [3,4]. Then MNPs was dispersed in CC:2urea to give the core-shell MNPs@CC:2urea. MNPs@CC:2urea was characterized by Fourier transform infrared (FT-IR), thermal gravimetric analysis (TGA), X-ray diffraction patterns (XRD), Brunauer–Emmett–Teller (BET), field-emission scanning electron microscopy (FESEM), and vibrating sample magnetometry (VSM). The synergic effects of DES and MNPs led to a high catalytic performance for MNPs@CC:2urea versus individual MNPs or CC:2urea in synthesis of chalcone derivatives. The advantages of the present method are short reaction time, easy separation of catalyst by an external magnet, efficiency, mild reaction conditions at room temperature, atom economy, and low loading of this recyclable hybrid catalyst.



Scheme 1. *Synthesis of chalcone derivatives*

Keywords: *Deep eutectic, magnetic, chalcone, solvent free*

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Preparation and application of magnetic nanocellulose for synthesis of dihydropyrimidinones

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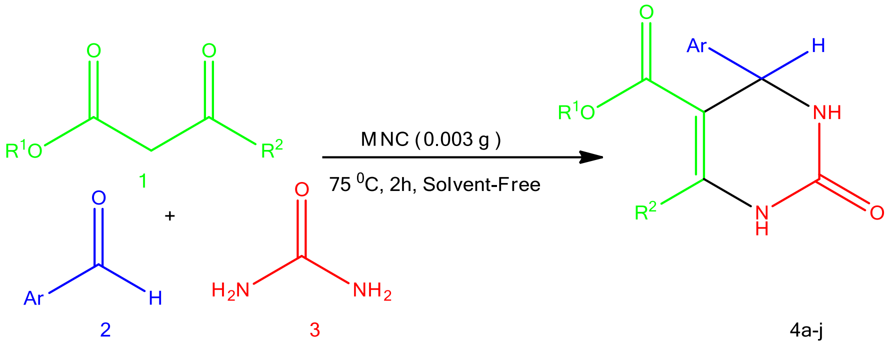
Abstract

In this work, magnetic nanocellulose (MNC) was prepared by cotton prewashing and hydrolysis in an alkaline medium together with coprecipitation of iron salts as Fe_3O_4 nano particles [1-3]. MNC is a safe, highly specific, low cost, biocompatible, and highly surface reactive catalyst [1,4]. MNC was characterized by Fourier transform infrared (FT-IR), thermal gravimetric analysis (TGA), X-ray diffraction patterns (XRD), Brunauer–Emmett–Teller (BET), field-emission scanning electron microscopy (FESEM), and vibrating sample magnetometry (VSM). Dihydropyrimidinones (DHPMs) are an interesting group of heterocycle compounds with broad spectrum of therapeutic and pharmaceutical properties [5]. The MNC was checked in synthesis of DHPMs in the absence of organic solvents exhibits a high performance for synthesis of various dihydropyrimidinones under solvent-free conditions. The advantages of the present method are deletion of organic and toxic solvents, short reaction time, easy separation of catalyst by an external magnet, low amount of catalyst, efficiency, and easy extraction of product from reaction mixture.



Scheme 1. *Synthesis of dihydropyrimidinnes derivatives*

Keywords: nanocellulose, magnetic, solvent free, dihydropyrimidinones

References

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Fe_3O_4@MCM-41@Pd-P2C: as high-efficient and magnetically recoverable Nanocatalyst for the stille coupling reaction

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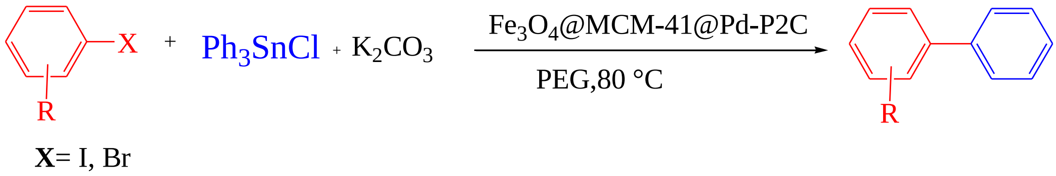
Carbon–carbon coupling reactions such as Stille reactions have been widely used as significant procedures in modern synthetic of organic chemistry for academic and industrial process including the pharmaceuticals, herbicides, agrochemicals, polymers, liquid crystal materials and hydrocarbons [1,2]. Mostly homogeneous palladium catalysts as efficient and active catalyst are used to catalyze the carbon–carbon couplings reactions as they offer high product yields, high selectivity and compatibility with many functional moieties [3].

Catalyzed reactions in homogeneous phase have many disadvantage e.g. their reusability and separation of catalysts from reaction mixture. These disadvantages are minimized by immobilization of homogenous catalysts on polymeric organic or inorganic supports such as magnetic iron oxide and mesoporous silica material (especially MCM-41)[4].

In this study, we synthesized Fe_3O_4@MCM-41@Pd-P2C by anchoring of Pd complexes to porous magnetic nanocomposite as catalyst supports. The catalyst was characterized by FT-IR spectroscopy, XRD, VSM, TEM, TGA, SEM, and ICP-OES techniques. It was used as an environmentally benign, excellent and reusable heterogeneous nano catalyst for still coupling reactions under mild experimental conditions. The given simple experimental procedure in this work, avoided the use of organic solvents which is in agreement with green chemistry principles, good reactivity to generate the corresponding products in good to excellent yields for reactions are the advantages of the present method. In addition, this catalyst was easily separable from the reaction mixture by external magnet and can be reused for several runs without any significant loss of stability and activity.



***Scheme 1**. Fe_3O_4@MCM-41@Pd-P2C catalysed Stille reaction*

Keywords: *Nanocatalyst, magnetic, still.*

References:

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Ni(II) Schiff base complex immobilized on Fe_3O_4@MCM-41 nanocomposites and study of its catalytic activity for the synthesis of 5- substituted 1*H*-tetrazoles

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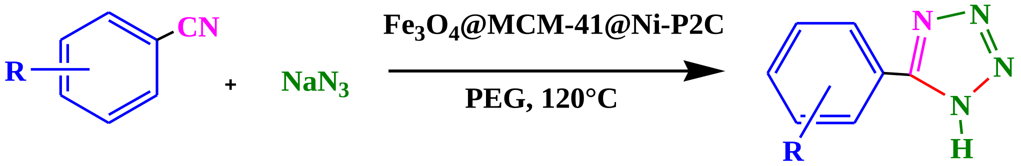
Immobilization of homogeneous catalysts on various solid supports with the advantage of catalysts separation and recycling is one strategy that developed in recent years [1]. Porous magnetic nanocomposites has been employed as useful and versatile solid support for homogeneous catalyst immobilization. These materials owing to its high thermal stability, high pore volume, high surface area, very narrow pore size distribution , and chemical and mechanical stability, are ideal to use as support[2]. Tetrazoles are one of the important and useful class of nitrogen-rich compounds that contain a wide range of applications, in the fields of catalysis technology, material sciences, organic synthesis, information recording systems, coordination chemistry, explosives, and especially in the synthesis of N-containing heterocycles[2-4].

In the present study, we prepared Schiff-base complexes of nickel anchored to magnetic nanoporous MCM-41 as a highly efficient and recoverable nanocatalyst for the synthesis of 5-substituted 1*H*-tetrazoles in PEG as green solvent. The catalyst was characterized by FT-IR spectroscopy, TGA, XRD, VSM, TEM, SEM and ICP-OES techniques The notable advantages of this procedure are simplicity in operation, mild reaction conditions, use of cheap and chemically stabile oxidant, short reaction times, and high yields of products. Also the catalyst can be easily separated from the reaction mixture by external magnet and reused several times without any significant loss of catalytic stability and activity.



Scheme 1. *Fe_3O_4@MCM-41@Ni-P2C catalysed the synthesis of 5-substituted 1H-tetrazoles*

Keywords: *Schiff-base, Nanocatalyst, 5- substituted 1H-tetrazoles.*

References:

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Fe-doped TiO_2 Electrospun Nanofibers as an Effective Visible-light-active Photocatalyst

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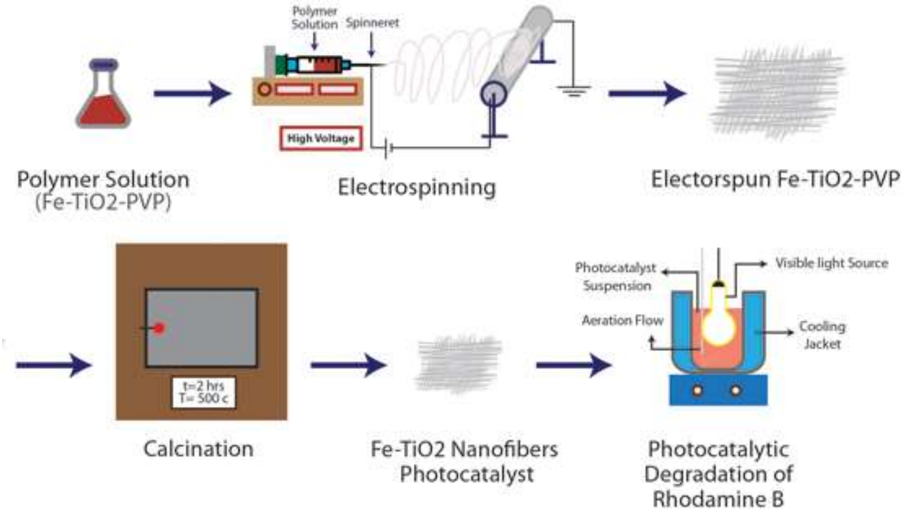
Transition metal dopants have been used to decrease the band gap energy of TiO_2 for visible light photocatalytic purposes [1]. Fe^{3+} is a good dopant candidate owing its unique half-filled electronic configuration, which can not only narrow the energy gap through the formation of new intermediate energy levels and but also help the separation of photogenerated electrons and holes [2]. Electrospun nanofibers have attracted much interest as a new form of photocatalyst due to their excellent properties, including a large surface to volume ratio, high porosity and interconnected pores [3]. Therefore, in this work, Fe-doped TiO_2 nanofibers have been fabricated using a sol–gel method and electrospinning technique with different Fe^{3+} contents. The effect of the Fe^{3+} concentration on the photocatalytic properties of these nanofibers have been investigated through the study of the degradation of a pollutant model (rhodamine B) using a visible light source. The experimental results demonstrate that the Fe-doped TiO_2 nanofibers exhibit significantly enhanced activity toward the rhodamine B degradation under visible light illumination in comparison with commercial TiO_2 powder(P-25) and undoped TiO_2 nanofibers. The maximum degradation which was observed for rhodamine B is 71% in 4 hours when the Fe^{3+} molar concentration was 1mol%. While this value was 51% and 53% for P-25 and undoped TiO_2 nanofibers, respectively.



Scheme 1. *Schematic illustration of the Fe-doped TiO2 nanofibers fabrication and experiments setup for photocatalytic degradation.*

Keywords: *Photocatalyst, Electrospinning, Fe-doped TiO_2, Visible light.*

References

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Visible-light-active Photocatalytic Microreactor with Fe-doped TiO_2 Electrospun Nanofibers Bed for Degradation of Dyes in Water

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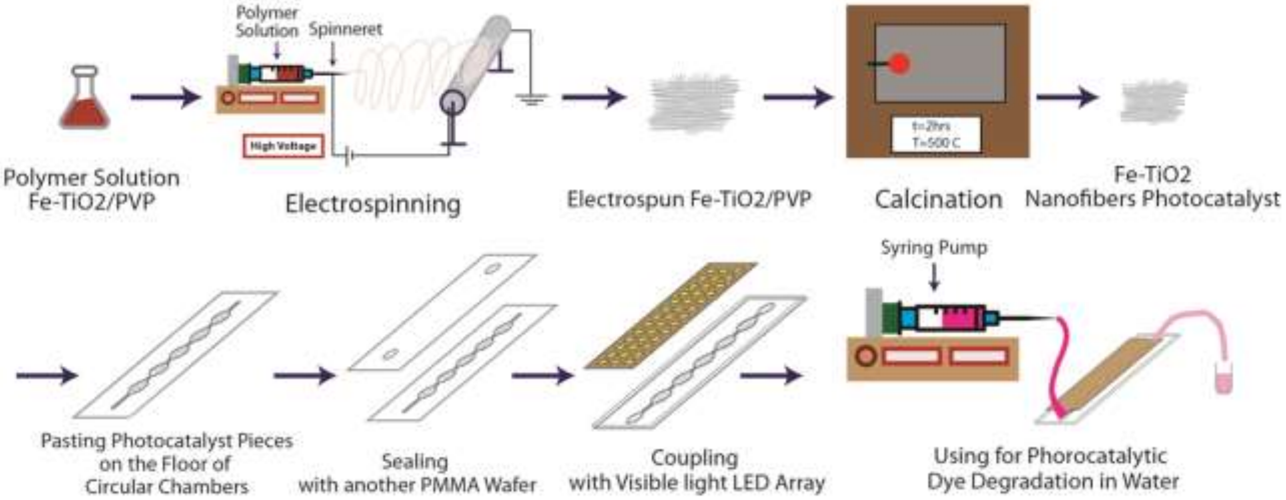
The development of microreactors for photocatalytic applications presents valuable advantages like fine control of light and fluids, large surface-area to volume ratio and uniform distribution of light onto the photocatalyst surface [1]. In this study, a low cost and simple photocatalytic microreactor was fabricated using laser engraving on polymethyl-methacrylate(PMMA) wafer. Fe-doped TiO_2 electrospun nanofibers were pasted on the floor of circular chambers as a photocatalytic bed. For evaluation of microreactor performance, the photocatalytic degradation of Rhodamine B(RhB) and Methylene Blue(MB) were investigated under visible light irradiation without any pH adjustment. The maximum photocatalytic degradation obtained in microreactor was 87% of 5 mg L^{-1} RhB for flow rate of 1 ml h^{-1}. While This value was 79% for MB.



Scheme 1. *Schematic illustration of the procedure for dye degradation in water using a photocatalytic microreactor under visible light irradiation.*

Keywords: *Microreactor, Photocatalyst, Electrospun Fe-doped TiO_2 nanofibers, Visible light.*

References

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Ionic liquid catalyzed three-component synthesis of imidazo[1,2-a]pyridines

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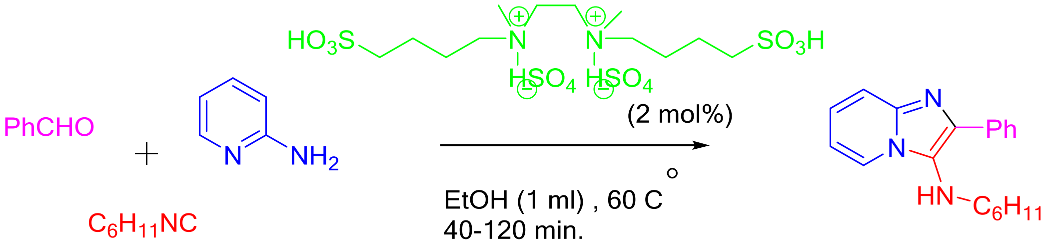
Imidazo [1, 2-a] pyridine is one of the most important nitrogen heterocycles, play an important role in contemporary chemical biology and medicinal research. New inventive approaches that make more efficient the synthesis of such important heterocycles are therefore highly desirable.
Among different types of multicomponent reaction strategy, a powerful strategy to prepare these imidazo [1, 2-a] pyridine derivatives involve the use of multicomponent reactions of aldehyde, isocyanide and 2-aminopyridine (MCRs) to form a single product. Some advantages of multicomponent reactions such as; non-required isolation of intermediates, atom-economic, simple work-up, safe, environmentally acceptable, and resource-effective, time saving, less waste and being performed in one pot manner made it fascinate considerable courtesy of synthetic organic chemists as an efficient tool especially in the synthesis of bioactive heterocycles [1].
Ionic liquids (ILs), being accepted as environmentally benign media as well as catalyst or dual catalyst–solvents in various transformations. Their remarkable characteristics are low volatility, low vapor pressure, reasonable thermal stability, recycling and reusability [2].
In summary, we presented a new protocol for the synthesis of imidazo [1,2-a]pyrimidine in the three-component reaction condition using acidic ionic liquid as a non-toxic and reusable catalyst, which offers considerable benefits such as simple work-up procedure, short reaction times, safe and clean conditions and recyclability of the acidic IL with eco-friendly approach.



***Scheme 1.** Synthesis of Imidazo[1,2-a]pyridines*

***Keywords:** Imidazo [1,2-a] pyridine, acidic ionic liquid, three-component reaction*

References

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Graphitic carbon nitride: a simple and reusable catalyst for one-pot synthesis of 1, 4-dihydropyridine derivatives

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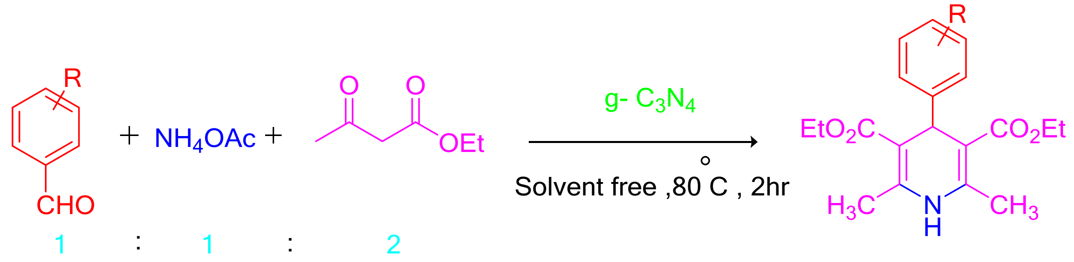
1, 4-Dihydropyridines (1,4-DHPs) are important bioactive heterocyclic compounds which possess analgesic, antiviral, antibacterial, and anti-inflammatory activities and represent an abundant structure found in Nature. 1,4-DHPs are generally synthesized using the classical Hantzsch method, through cyclocondensation of an aldehyde, β-ketoesters and ammonia either in acetic acid or in refluxing ethanol for long reaction times that this method typically leads to low yields [1].

Carbon catalysts, which include carbon nanotubes, graphite and graphene, have been used in many industries, including energy storage, the environment and as heterogeneous catalysts in organic reactions. One of the interesting materials that has attracted the attention of many scientists in recent years is carbon nitride, the presence of nitrogen atoms in the carbon framework has led to its high application in various fields of research. Carbon nitrides have several allotropes of which the graphitic phase is the most stable one. Its rich surface features have been attractive for applications in both energy and environment. [2]

In this protocol first graphitic carbon nitride nanosheets are prepared using inexpensive materials such as melamine and urea, and after identifid by using spectrscopy such as XRD, SEM, FTIR.

In summary, we developed a new protocol for the synthesis of various DHPs derivatives using graphitic carbon nitride as a highly efficient heterogeneous catalyst, which offers significant benefits such as simple work-up procedure, short reaction times, safe and clean conditions, and excellent yields with eco-friendly approach.



Scheme 1. *Synthesis of 1, 4-dihydropyridine derivatives*

Keywords: *Dihydropyridine, graphitic carbon nitride, Ionic liquid.*

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Pyridine-type Supported Pd(II) Complex on Fe_3O_4@SiO_2@SBA-15 for O-Arylation

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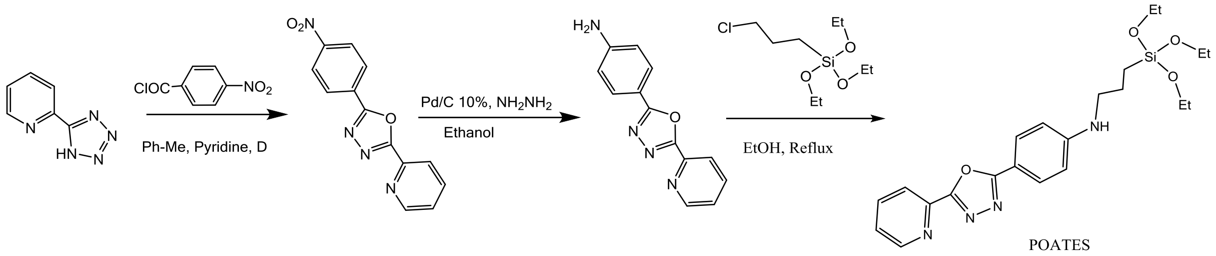
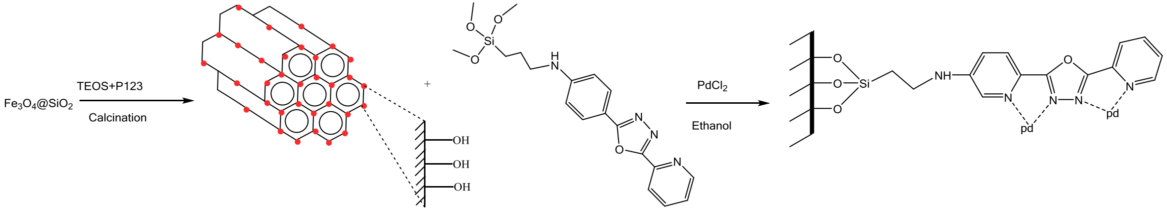
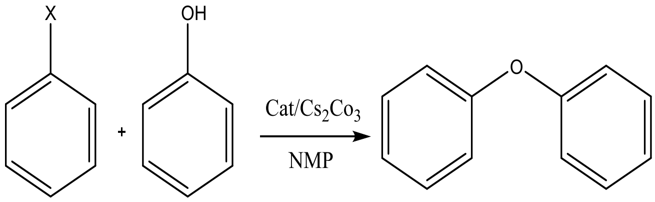
In this study, a ligand, 4-(5-(pyridine-2-yl)-1,3,4-oxadiazol-2-yl)anilineopropyltriethoxysilane (POATES) has been prepared in three steps starting from pyridine-2-carbonitrile, according to Scheme 1 [1-2]. Magnetite nanoparticles, obtained via co-precipitation method and covered by silica and mesoporous silica (SBA-15) layers, were silylated with POATES (Fe_3O_4@SiO_2@SBA-15-POATES) [3]. The core shells of the supported ligand were stirred in EtOH solution of Pd(II) to afford the supported Pd(II) complex, Scheme 2, which has been used as magnetically retrievable catalyst in *O*-arylation coupling reaction of aryl halides with phenol, Scheme 3 [4].



Scheme 1. *Synthesis of silylating ligand.*



Scheme 2. *Synthesis of supported Pd(II) complex.*



Scheme 3. *O-Arylation of phenols with aryl halides in the presence of Fe_3O_4@SBA-15-POATES*

Keywords: Pd(II)-nanoparticles, O-Arylation, coupling reaction, Magnetic catalyst

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Three_component synthesis of Pyrimido[1,2-a]benzimidazole in the presence of Fe_3O_4@SiO_2-$HClO_4$ as a novel magnetic catalysts

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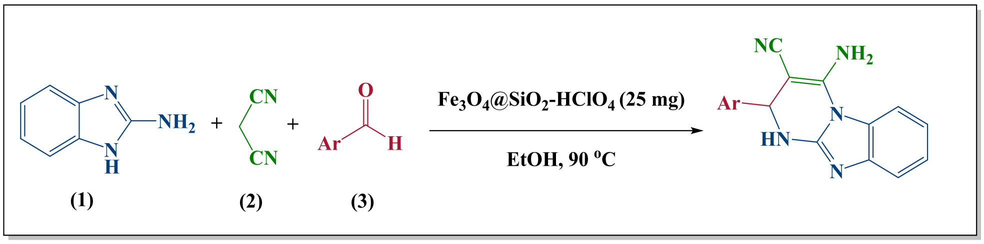
A mild, simple and efficient procedure for the preparation of Pyrimido[1,2-a]benzimidazole derivatives is described using Fe_3O_4@SiO_2-$HClO_4$ as a novel and reusable catalyst. . This catalyst was characterized using different types of methods, including Fourier transform infrared (FT-IR), X-ray powder diffraction (XRD), Thermogravimetric analysis (TGA), Transmission Electron Microscopy (TEM), Energy-dispersive X-ray spectroscopy (EDX) and Scanning electron microscopy (SEM). The catalyst was easily isolated from the reaction mixture by magnetic decantation using an external magnet and reused at least three times without significant degradation in the activity. The products are obtained in shorter times with excellent yields (75–97%) from the multicomponent reaction of 2-aminobenzimidazole (1), malononitrile (2), and Aldehydes (3).



Scheme 1. *Synthesis of Pyrimido[1,2-a]benzimidazole derivatives*

Keywords: *pyrimido[1, 2-a]benzimidazole, Magnetic nanoparticles, Reusable catalyst.*

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Benzene-1,3,5-tricarboxylic acid as an efficient ligand for different MOFs fabrication: synthesis, characterization and catalytic performance in biodiesel production

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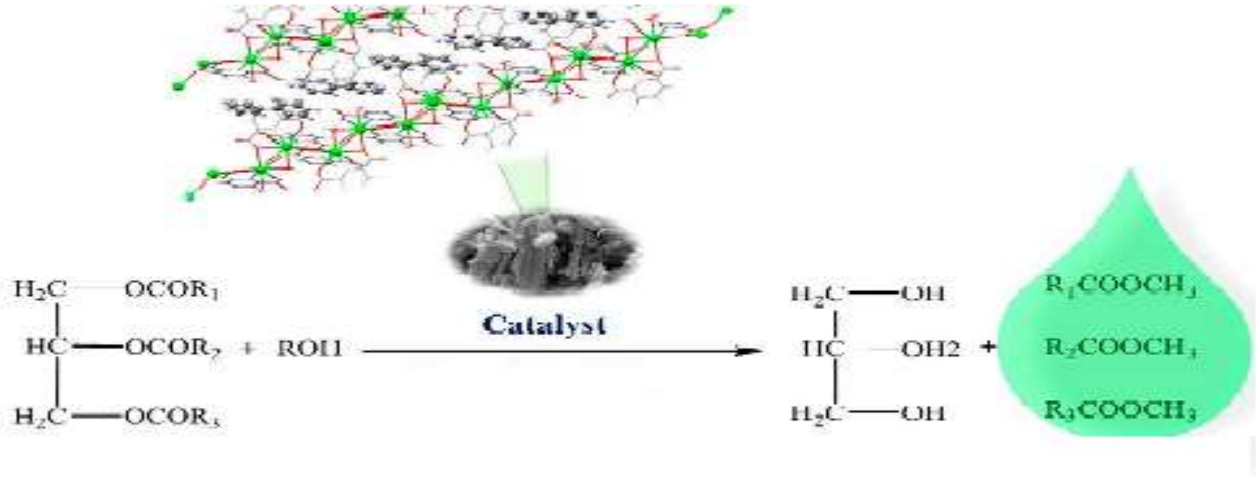
Metal-organic framework (MOFs) are modular porous materials synthesized from metal cluster nodes and organic linkers that connect these nodes. This rapidly expanding class of structure presents viable platforms for catalytic reactions because of its unique features such as high porosity, uniform and tunable pore size [1]. In this work, various type of MOFs with different metal nodes such as iron, chromium, vanadium and cobalt and benzene-1,3,5-tricarboxylic acid as organic linker are synthesized by hydrothermal method at 150°C, and were systemically characterized by XRD, FTIR, SEM.

The obtain highly porous and acidic catalysts were successfully used in esterification of oleic acid reaction that was carried out in an oil bath and finished in methanol at 70°C, and to determine and quantify the influence of the reaction times, molar ration of methanol: oil, catalyst dosage, reaction temperature and oil composition on the conversion (or yield) of triglycerides to biodiesel The gas chromatograph equipped with a flame ionization detector is used [2]. The result of this study confirmed that among this MOFs with different nodes Co-MOF exhibits the most catalytic activity for transesterification of oleic acid with methanol after that respectively Fe-MOF, Cr-MOF, V-MOF had the highest conversion percentages.



Scheme 1. *Model process of esterification for the production of biodiesel*

Keywords: *Metal-organic framework 1, Heterogeneous catalyst 2, Biodiesel 3.*

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Synthesis and modification of ZSM-22 and immobilization of transition metals such as Cr, Cu, Fe and Ni in order to increasing the efficiency of bio-diesel production from oleic acid oil

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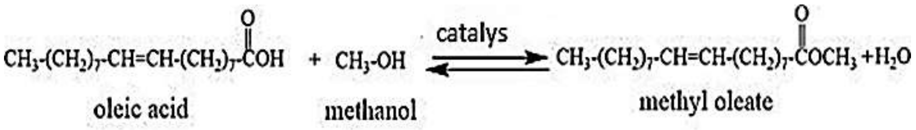
Zeolites are a wide range of minerals that are composed mainly of aluminosilicate and their major commercial use in industrial applications are as adsorbents and catalysts. Having a well-defined structure, selectivity, active sites, modifying cationic components, easy synthesis, convenient access and affordable prices, are great features for choosing zeolites as catalysts. They are promising catalysts for the transesterification reaction of vegetable oils for biodiesel production. ZSM-22 is a good candidate for a solid base catalyst from an economical point of view.

In the present work, we reviewed ZSM-22 catalyst for oleic acid transesterification to produce biodiesel. A series of ZSM-22s with different Si / Al ratios was prepared by hydrothermal method. In these structures, some metals such as Fe, Ni, Cu and Cr were placed in active sites to improve the performance of the catalyst [1-2]. Scheme 1. shows the process of esterification for the production of biodiesel from oleic acid.

Different compounds of ZSM-22 were optimized through various reaction parameter such as: amount of catalyst, molar ratio of oil to alcohol, reaction time and temperature. According to the results of the analyzes, Fe was more active than other metals. After Fe, Cu, Ni and finally Cr were active respectively (Fe>Cu>Ni>Cr).

The best performance of catalyst was achieved with methanol to oil ratio of 10:1(mmol), 11wt % (0.3g) of catalyst loading, at 70 ℃ reaction temperatures for 48 h of reaction time. Catalysts were characterized by several spectroscopic and analytical techniques like XRD, EDAX, FT-IR, BET, GC, GC-Mass, TPD NH3 and FE-SEM. A major part of the research has been dedicated to the proper synthesis of catalyst to increase the production efficiency of biodiesel. The purpose of this study is to improve catalytic properties, improve the structure and synthesis method, in order to increase the production efficiency of biodiesel. The synthesized catalyst used in the process of optimal biodiesel production of oleic acid are used and the production efficiency and selectivity are calculated and compared.



$$\mathrm{CH_3\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}\overset{\overset{O}{\|}}{C}OH} + \mathrm{CH_3\text{-}OH} \underset{}{\overset{\text{catalys}}{\rightleftarrows}} \mathrm{CH_3\text{-}(CH_2)_7\text{-}CH{=}CH\text{-}(CH_2)_7\text{-}\overset{\overset{O}{\|}}{C}OCH_3} + \mathrm{H_2O}$$

***Scheme 1.** Process of esterification for the production of biodiesel from oleic acid*

***Keywords:** biodiesel1, zeolite2, catalysis3, oleic acid4.*

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Synthesis, Characterization and Electrocatalytic Properties of Titanate Nanostructures

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Abstract

The remarkable physicochemical properties of ferroelectric compounds have attracted sustained scientific and technological interests. Lead titanate ($PbTiO_3$) is a typical perovskite ferroelectric material with a high Curie temperature and low dielectric constant and these properties make them suitable for multilayer capacitors, piezoelectric actuators and sensors [1-3]. In this work, the preparation of $PbTiO_3$ nanoceramics using sol-gel method and their structural and electrocatalytic characterizations are reported. The structural properties of the nanoparticles were studied via Fourier transform infrared spectroscopy, X-ray diffraction and transmission electron microscopy. Using the techniques crystallization process, morphology and particle size of the calcined powders were characterized. The results showed that $PbTiO_3$ nanoceramics with an average size ranging from 35-50 nm could be obtained after calcining of the dried gel at 550 °C for 2 h. Further, the electrocatalytic sensing behavior of $PbTiO_3$ nanoparticles was investigated by electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) techniques in the presence of $[Fe(CN)_6]^{3-/4-}$ redox couple. For achieving the purpose a $PbTiO_3$ nanoceramics modified carbon paste electrode was designed (PTN/CPE). Then the oxidative behavior of the probe redox couple has been investigated by EIS and CV at the surface of the nano-structured modified electrode. Using the proposed method, the PTN/CPE showed an excellent electrocatalytic activity for the $[Fe(CN)_6]^{3-/4-}$ redox couple, and accelerated electron transfer between the electrode and analyte. Therefore, the electrochemical sensing experiments suggest that the $PbTiO_3$ nanoceramics will become a potential candidate in the field of nanostructured electrochemical sensors.

Keywords: *$PbTiO_3$ Nanoceramics, Sol-gel Method, Structural Characterizations, Electrocatalytic Properties*

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Facile Synthesis of Chalcopyrite Nanostructures and Its Electrocatalytic Properties

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Abstract

Nanostructures of inorganic magnetic and semiconductor materials have been the subject of intense research since 1990's. The primary motivation for this increased activity is the size dependent properties of these materials. The I-III-VI_2 compounds (chalcopyrite) exhibit strongly size dependent properties that may find wide variety of applications including catalyst, optical parametric oscillation, second harmonic generation, up conversion, down conversion, detectors, LEDs, solar cells, various optoelectronic and sensors [1-3]. In the present study, chalcopyrite ternary semiconductor $CuAlS_2$ (CAS) nanocrystals were synthesized via facile method. The sol-gel process was used for synthesize of $CuAlS_2$ nanoparticles. Characterizations of the obtained powders were carried out by means of X-ray diffraction, energy dispersive X-ray spectroscopy, scanning electron microscopy and transmission electron microscopy. Then, a modified carbon paste electrode was prepared using $CuAlS_2$ nanoparticles (CASN/CPE). The electrochemical behaviour of the nano-structured modified electrode was investigated by means of electrochemical impedance spectroscopy and cyclic voltammetry techniques using $[Fe(CN)_6]^{3-/4-}$ redox couple. Using the techniques the electrocatalytic activity of the CASN/CPE was confirmed. The results showed that $CuAlS_2$ nanocrystals accelerate electronic transmission rate between the modified electrode and $[Fe(CN)_6]^{3-/4-}$ redox couple. Therefore, $CuAlS_2$ nanoparticles are proper candidate for electrochemical detection of various analytes.

Keywords: *$CuAlS_2$ nanocrystals, Semiconductor, Sol-gel process, Electrocatalyst*

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Desulfurization of Petroleum Products Using Nano Polyoxometalete/Titanium dioxide Catalytic System

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Petroleum products contain significant amounts of organic sulphur, such as mercaptanes, benzothiophenes, poly sulphons, disulphides and etc. Sulphur combustion, cause conversion of them to sulphoxides and results problems to human and environment health [1].

Oxidative desulphurization (ODS) method leads to proper sulphur conversions at low temperature and pressure, and relatively easily combinable with separation processes [2].

Nowadays, we investigate heterogeneous polyoxometalates/Titanium dioxide (POMs/TiO_2) catalysts. Various types of Nano POMs; (Molybdophosphoric acid, tungstophosphoric acid, tungstomolybdophosphoric acid) were synthesized; and POMs/TiO_2 nano composites obtained via bottom-up method [3]. Prepared catalysts were characterized by Fourier transform infrared (FTIR), powder X-ray diffraction (XRD), scanning electron microscopy (SEM).

The catalysts activities were measured by the total sulphur content of petroleum products before and after desulphurization. The effects of kinds of POMs, amount of catalyst loading, reaction time, oxidized content, temperature, pH value, and sulfoxide separator material were investigated. Results showed that POM/TiO2 has the higher catalytic activities than that of pure nano TiO_2 and nano POMs. Among various synthesized nano composites, HPW/TiO_2 nano-composite was found to be the best sulphur removal catalyst. Desulfurization increased on the pH value (2-3) and the best results were obtained on the temperature 105 °C. The sulfoxide can be readily separated from the end production using extractor, without changing their properties.

Keywords: *Polyoxometalate, Photocatalyst, Nano composites.*

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Study on the Photocatalytic Effect of Heteroplyacid-Titania Nanocomposites On methylene blue degradation

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Today industrial development and environmental contamination need greatest concerns and should be removed for environmental and human health protection [1]. One of the big environmental problems is wastewaters containing various types of pollutants such as organic dyes which produced by pesticides, petrochemicals and etc. so they have high toxicity, slow biodegradation and potential carcinogenicity [2].

At present several industrial techniques such as oxidation, adsorption, precipitation, degradation and so on have been used which cost much money and create another type of pollutions. Photocatalysts as an effective techniques have potential in this area [3].

Titanium dioxide (TiO_2) in combination with heteropolyacids (HPA) as semiconductor nano composite under UV irradiation could effectively concerns for pollution reduction [4-6].

Some HPAs, (Molybdophosphoric acid, tungstophosphoric acid, silicotungstic acid) and HPA/TiO_2 nano composites were synthesized as a green, cheap and solid acid catalyst by impregnation method. Nano composites were characterized by Fourier transform infrared (FTIR), powder X-ray diffraction (XRD), scanning electron microscopy (SEM). We designed a UV illumination box to degrade methylene blue as a common azo dye pollutant in the environment. The photocatalytic degradation was investigated under UV, visible and dark illumination. The special effects of dye concentration, HPA loadings, catalyst dose, temperature and pH value were investigated. Heterogeneous HPA/TiO_2 nano composites showed good photo-degradation of methylene blue under UV irradiation and room temperature with 98% yield. Nano composites can be separated and recovery from reaction media.

Keywords: *Heteropolyacid, nano composites, photocatalyst.*

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Pt nanoparticles supporting on polyaniline: a catalytic anode for methanol fuel cell

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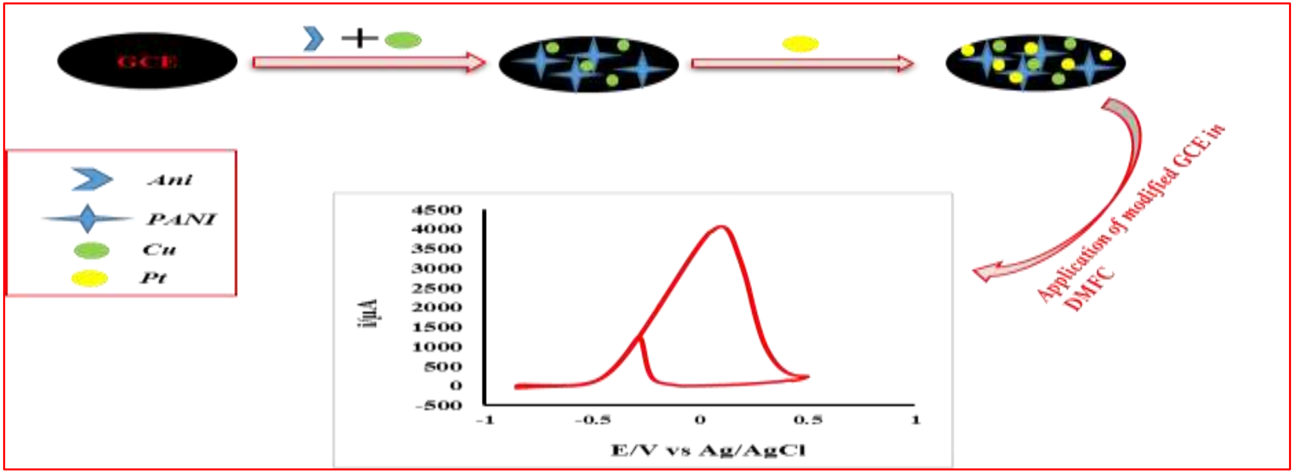
Direct methanol fuel cell (DMFC) has become a significant power source due to unique properties such as high energy density and low pollution emission. One of the most important parameters for prosperous performance of DMFC is the electro-catalytic activity of the utilized anode. Pt-based catalysts are used as the most popular catalyst in DMFC. High cost, low abundance, and high poisoning of these catalysts have established challenges to the production of new types of catalytic materials. Making use of appropriate support materials for the construction of Pt-based catalysts alleviate their defects. In this regard, conductive polymers are desirable supporting materials. In this work, in reply to the mentioned challenges, we propound the synthetic method for the production of a new Pt-based catalyst by using the polyaniline (PANI) as the support. PANI is a conductive polymer with low-cost synthesis, high stability, and reversible redox properties. Herein, aniline (Ani) was used as the polymer precursor and a polymerization reaction was performed in the presence of Copper (Cu) ions as the oxidant agents. So, in this process a polymeric layer, a layer with Cu nanoparticles, a transition metal, was synthesized. The existence of Cu nanoparticles cause the excellent electro-catalytic activity. Then, electrodeposition of platinum (Pt) nanoparticles was performed by 40 consecutive cycles at a sweep rate of 50 mV.s^{-1} in the potential range of -0.4V to 1V *vs.* Ag/ AgCl in H_2PtCl_6 solution as the precursor. The electro-chemical performance of synthesized catalyst on the glassy carbon electrode (Pt/ Cu-PANI/ GCE) was investigated by cyclic voltammetry (CV) and chronoampherometric (CA) methods. The obtained catalytic activity and durability exhibit Pt/ Cu-PANI is a superior candidate for modification of electrode surface in methanol fuel cell.



Scheme 1. *The synthetic route of Pt/ Cu-PANI composite.*

Keywords: *methanol, polyaniline, catalytic-durability.*

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A non-noble metal polymeric composite as the cost-effective catalyst in methanol fuel cell

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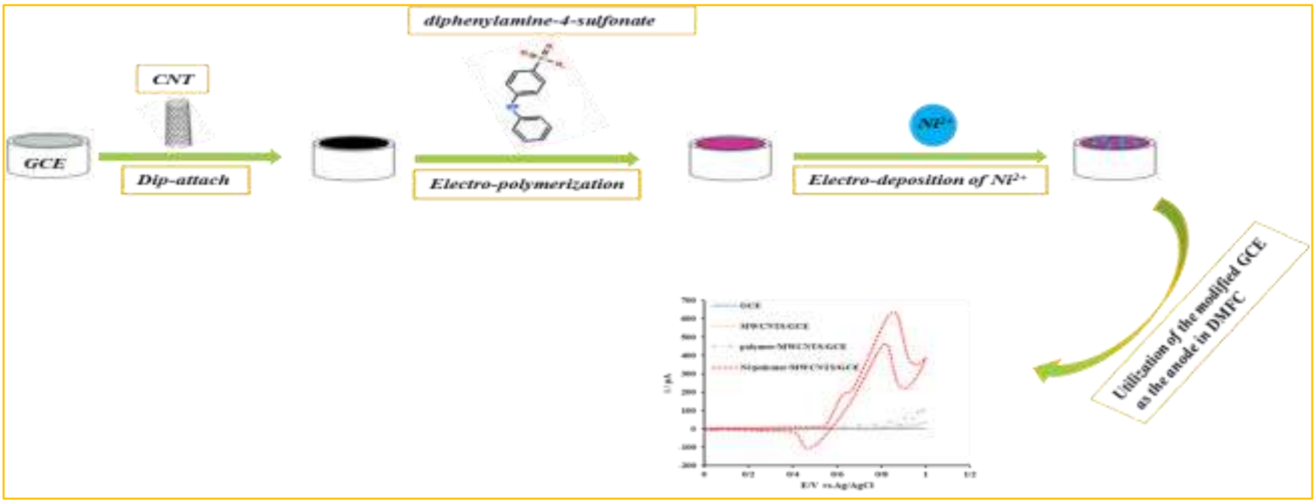
In the modern world, the novel, ecological, economical, and renewable energy sources are the essential requirements. In this aspect, direct methanol fuel cell (DMFC) is an acceptable alternative. The poisoning of the anode that cause poor kinetics of methanol oxidation is a barrier in the DMFC spread employing. The modification of the anode surface is preferential treatment. In this aspect, the development of modified anodes with polymeric composite, non-noble metal with the controlled morphology and size distribution embedded in a conducting polymer matrix, due to high electrical conductivity, porosity, and chemical stability are effective remedies. In this work, we covered the glassy carbon electrode (GCE) surface up with the carbon nanotube (CNT) for the production of a useful substrate for polymeric layer. The polymeric film was formed by 15 consecutive cycles at a sweep rate of 50 mV.s^{-1} in the potential range of -0.5-1.5 V *vs.* Ag/ AgCl in the sodium diphenylamine-4-sulfonate (DPA) solution as the precursor. To the incorporation of Ni ions and formation of the polymeric composite, 15 repeated cyclic voltammetry at the sweep rate of 100 mV.s^{-1} in the potential range of 0-1 V *vs.* Ag/ AgCl were performed in the $NiSO_4$ solution. Surface characterization of synthesized electrocatalyst (Ni-p-DPA/ CNT/ GCE) were investigated by Field Emission Scanning Electron Microscopy (FESEM) and energy-dispersive X-ray spectra (EDS). Electrochemical performance of Ni-p-DPA/ CNT/ GCE in the alkaline media indicates improvement modified GCE towards methanol oxidation. The catalyst stability was studied by chronoamperometry, and highly stable response of catalyst in methanol fuel cell was concluded. This study proposes Ni-p-DPA/ CNT/ GCE as the appropriate anode in methanol fuel cell.



Scheme 1. *Schematic diagram of synthesis stages of Ni-pDPA/ CNT/ GCE.*

Keywords: *direct methanol fuel cell (DMFC), polymeric composite, electrocatalyst.*

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A facile and practical synthesis of triazolo(4,3-*a*)pyrimidines using γ–Fe_2O_3 based nanocatalyst

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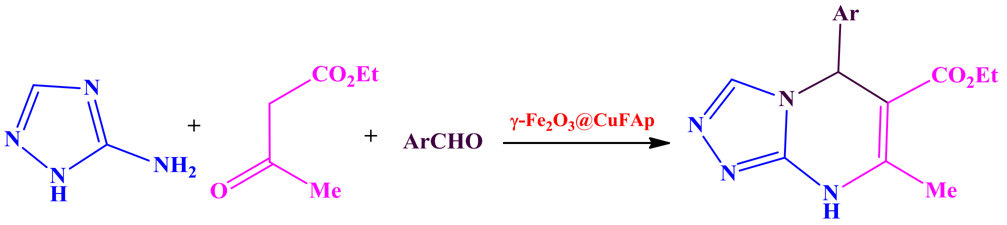
Aminoazoles have been recognized as excellent building blocks for MCRs due to the presence of several nucleophilic centers with different reactivity [1]. Particularly, 3-aminotriazoles and 5-aminotetrazoles have been extensively explored as substrates for various MCRs.
On the other hand, triazole derivatives have been the object of intense investigations in medicinal chemistry and belong to a major class of natural heterocyclic compounds, because of their remarkable activity. For example, 1,2,3-triazoles have found widespread use in pharmaceuticals and agrochemicals [2]. In addition, based on the extensive researches, it has also been observed that triazole derivatives include significant biological activities such as aticancer [3], antitubercular [4], antifungal, antibacterial, anti-HIV [5], anti-inflammatory, antimalarial and antioxidant activity [6].

Owing to the important applications of triazole derivatives in synthetic and medicinal chemistry, and our continued interests for the synthesis of biologically important products [7-9], herein, we report a new and practical method for the synthesis of triazolo(4,3-*a*)pyrimidine derivatives by the reaction of 3-amino-1,2,4-triazole, ethyl acetoacetate and aryl aldehydes in the presence of γ–Fe_2O_3@CuFAp nanocatalyst (Scheme 1). This new method furnished the desired triazolopyrimidines in excellent yields and short reaction times. All products were characterized by IR, ^1H NMR and ^{13}C NMR analyses.



Scheme 1. *Synthesis of triazolo(4,3-a)pyrimidine derivatives*

Keywords: *3-Aminotriazole, ethyl acetoacetate, triazolopyrimidine, nanocatalyst.*

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Atom Transfer Radical Polymerization of Methyl Methacrylate by supported CuBr/2-(Aminophenyldiphenylphosphinete) Catalyst on Nano Silica

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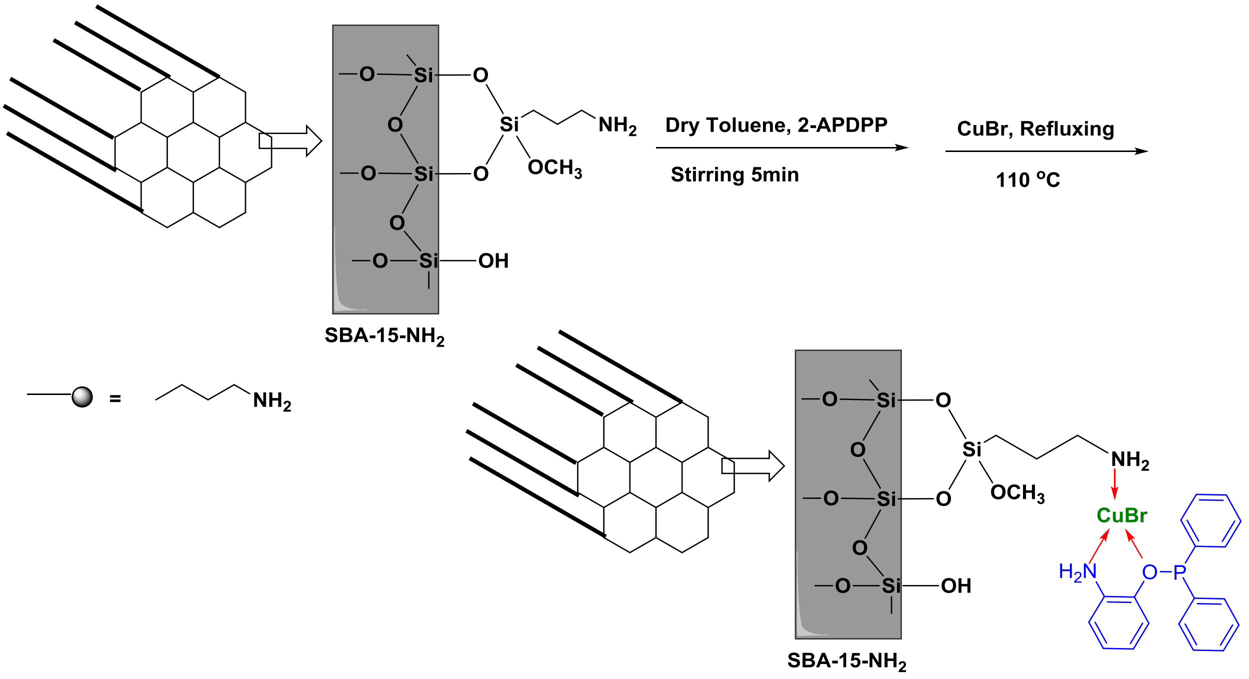
Abstract:

A nano silica supported catalyst was used for Atom transfer radical polymerization of methyl methacrylate. Firstly, 2-Aminophenyl Diphenylphosphinite ligand was synthesized and then this ligand and CuBr were attached to NH_2-modified SBA-15. Finally, this prepared catalyst was used as a catalysis for polymerization process. The FT-IR, 1H-NMR and ^{13}C-NMR techniques were used for characterization of products.



***Scheme 1.** synthesis of CuBr/2-APDPP/SBA15-NH2.*

***Keywords:** methyl methacrylate; ATRP; CuBr; SBA-15; 2-Aminophenyl Diphenylphosphinite.*

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A novel and practical method for the selective synthesis of sulfons from sulfides using Metal Oxide-Metal nanocatalyst

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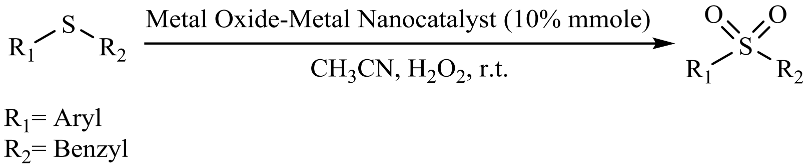
Developing versatile and eco-friendly methodologies that make easy the synthesis of biologically active organic compounds is in great demand. Oxidation of organic sulfides is the most utilized method to produce sulfones, which is drawing continuous attention in chemical research and development due to the importance of these products [1].

Nanostructured metal oxide-metal synthesized in a one-pot redox reaction is used as an effective and chemoselective nanocatalyst for direct conversion of sulfides to sulfones. 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 oxidation of sulfides to sulfones using nanostructured metal oxide-metal in the presence of H_2O_2 as a green oxidant at room temperature (Scheme 1).



Scheme 1. *Oxidation of sulfides to sulfones using metal oxide-metal nanocatalyst in the presence of* H_2O_2

Keywords: *Nanostructured metal oxide-metal, Hydrogen Peroxide, Sulfide, Sulfone.*

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Boehmite-Ligand- palladium (0): Novel, effective and reusable heterogeneous catalyst for O-arylation and N-arylation via Ullmann coupling

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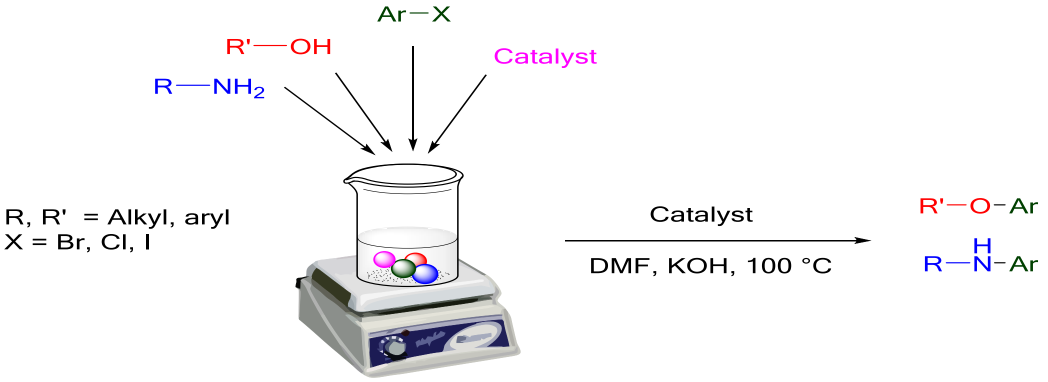
Palladium-catalysed cross-coupling reactions have been found a special place in organic reactions.[1] Within the previous couple of decades, various economical heterogeneous and homogenous palladium catalysts have been used for cross-coupling reactions, particularly, C-N and C-O Ullmann-type coupling reactions.[2]

One of the most stable and inexpensive solid support is boehmite. Boehmite is an orthorhombic structure of aluminum oxide hydroxide (γ-AlOOH).

It is notable that, boehmite nanoparticles were prepared in a green solvent (H_2O) at room temperature while not the necessity for an inert atmosphere.

Boehmite has some attractive features such as: thermal, chemical and mechanical stability, non-toxicity, not air or wetness sensitive, large specific surface area and easily available and eco-friendly. Biaryl ethers have wide applications in polymer industries and are useful ligands in metal-catalyzed organic reactions.[3]

Therefore, during this content, we have a tendency to introduce the boehmite modified with Ligand containing palladium (0)-catalyzed C-N and C-O cross-coupling reactions of varied aryl halides with phenols and different amines in high to excellent yields (Scheme 1).



***Scheme 1.** Synthesis of biaryl ethers and biaryl amines*

***Keywords:** Boehmite, Biaryl rthers, Biaryl amines*

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Three-component synthesis of ferrocene containing 3,4-dihydroquinoxalin-2-amines from 1,2-phenylenediamine, ferrocene carboxaldehyde and isocyanides in the presence of *p*-toluenesulfonic acid

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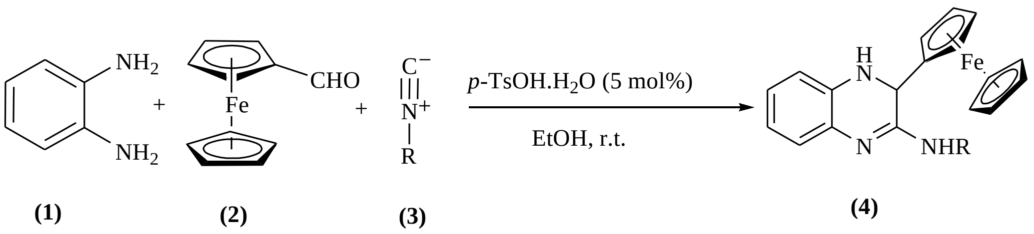
Abstract: Quinoxaline is one of the heterocyclic compounds containing nitrogen atom which shows a wide ranging of biological and pharmacological activities such as fungicide, antibacterial, antimalarial, antidepressant. Several methods have been reported in the literature for the synthesis of quinoxaline derivatives. These methods are multistep in nature. In this research, we report the synthesis of some new quinoxaline derivatives containing a ferrocene unit by using a three-component reaction between 1,2-phenylenediamine, ferrocene-carboxaldehyde, and isocyanides in the presence of a catalytic amount of *p*-toluenesulfonic acid. This approach is an effective, easy and high-yield procedure.



Scheme 1. *Three-component reaction of 1,2-phenylenediamine, ferrocene carboxaldehyde, and isocyanides.*

Keywords: *Multicomponent reactions, Heterocyclic compounds, 3,4-Dihydroquinoxalin-2-amine*.

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Rhodium-Catalyzed Asymmetric Arylation of Benzophenone Derivatives

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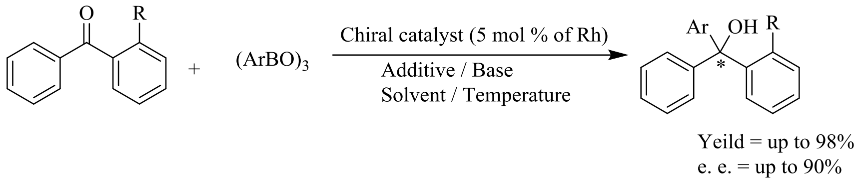
Rhodium-catalyzed asymmetric arylation reactions provide one of the most straightforward and powerful ways to introduce aryl fragments in an enantioselective manner. In principle, any reaction that involves Rh-catalyzed asymmetric addition of an aryl group to a double or triple bond is called “Rh-catalyzed asymmetric arylation” (RCAA). Due to because special reactivity and selectivity of rhodium complexes compared to other catalytic systems, significant attention has been paid to the use of rhodium catalysts in the formation of C−C bonds. In this kind of reactions, highly efficient asymmetric catalysis has been achieved by employing a chiral ligand. [1-3]

Asymmetric addition of aryl group to diaryl carbonyl compounds is a best method to afford chiral benzylic alcohol. In this work, the addition of various aryl groups to benzophenone derivatives took place in the presence of different rhodium/chiral diene ligand catalysts and the chiral alcohols were produced in high yields with high enantioselectivity (Scheme 1).



Scheme1. *Asymmetric addition of aryl groups to benzophenone in presence of rhodium/chiral diene ligands.*

Keywords: *Asymmetric addition, Rhodium/Chiral diene ligand, Benzophenone .*

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CuO Encapsulated in Mesoporous Silica SBA-15 Used as Heterogeneous Catalyst for Synthesis of Aldimines

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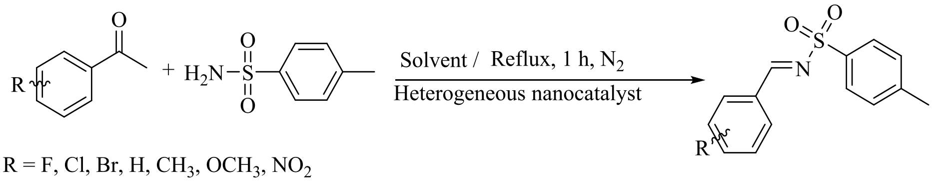
Today, the importance of electron deficient imines such as sulfonyl imines is well known as a key intermediate in various chemical reactions. The applicability as anticancer agent, anti-inflammatory nature, antifungal and antibacterial behavior, affirm the importance of their biological rule also. The electrophilic nature, relative stability and reactivity of these electron deficient imines give rise to use them for preparation of various nitrogen containing compounds. So, the significance of designing the fruitful methods for producing imines has attracted a great deal of attention in recent years [1].

Other side, supported nanometals are one of the most important categories of heterogeneous catalysts with broad applications in the industry. According to the literature, some materials, such as SBA-15, MCM-41 and zeolite were applied for preparation of metal nanoparticles [2,3].

Here in, different nanomaterial such as CuO, SBA-15, and CuO-SBA-15 were synthesized in different ways, and then in a simple, clean and efficient process, aldimines were afforded by reaction of diverse aldehydes and sulfonamide in presence of prepared heterogeneous nanocatalysts under reflux condition (Scheme 1). The desired products were produced in high yields. After each reaction, the heterogeneous catalyst was separated and reused in other reaction cycles.



Scheme1. *Preparation of aromatic aldimines in presence of heterogeneous nanocatalysts.*

Keywords: *Aromatic Aldimines, Heterogeneous nanocatalysts.*

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Synthesis, Characterization and Catalytic Features and Crystal Structure of Mn(II) Complex With a tetradentate Salen ligand

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Abstract: The Schiff bases and their complexes have played an important role in the development of coordination chemistry biological and material science. Schiff base ligands stabilize different metal ions to yield metal complexes with a variety of properties and applications. For instance, the chelating salen, is known by the ability to significantly decrease the redox potentials, and the resulting complexes constitute suitable systems to catalyse multiple redox reactions such as asymmetric epoxidation of unfunctionalized olefins, catalase reaction [1,2], water photolysis[3],Diels-Alder cycloaddition, enantioselective cyclopropanation of styrene and ring opening of epoxides [4-7]. In this work, we describe the synthesis of a new mononuclear complex of manganese (II),viz,$[MnL(OAc)_2].3H_2O$ containing the corresponding N-donor Schiff base ligand. A mononuclear Mn (II) Complex, $[MnL(OAc)_2].3H_2O$ has been derived tetra dentate salen, N,N'-bis(phenyl(pyridine-2-yl)methylene)ethane-1,2-diamine (L) . The molecule was characterized by elemental analysis, FT-IR, and single-crystal X-ray crystallography. The complex crystallized in the monoclinic space group C2/c with unit cell dimensions a=24.4771(6) Å, b=8.0621(2) Å, c=30.5018(8) Å, $\alpha = 90^\circ$, $\beta = 97.437(2)^\circ$, $\gamma = 90^\circ$,V= 5968.5(3) $Å^3$, Z = 8, $R_1 = 0.0336$, and $wR_2 = 0.0404$. In the crystal structure of complex the Mn (II) with four coordinated nitrogen atoms and two acetate ions has a distorted cubic geometry. Three water molecule are also incorporated in the crystal network. Several hydrogen bonds present in the crystal structure. Oxidation reactions carried out on styrene and revealed that the complex compound was good and effective catalyst for styrene oxidation. Comparison between neat and complex catalyzed reactions proves that the oxidation reactions using catalysts give higher conversions than their corresponding neat reactions.

Keywords: Manganese (II) Complex, Catalytic Activity, X-Ray Crystal Structure

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One-Pot and Chemoselective Synthesis of 6-Bromo-2-Oxo-2H-Chromene-4-Carboxylate Catalyzed by Nano Silica Powder

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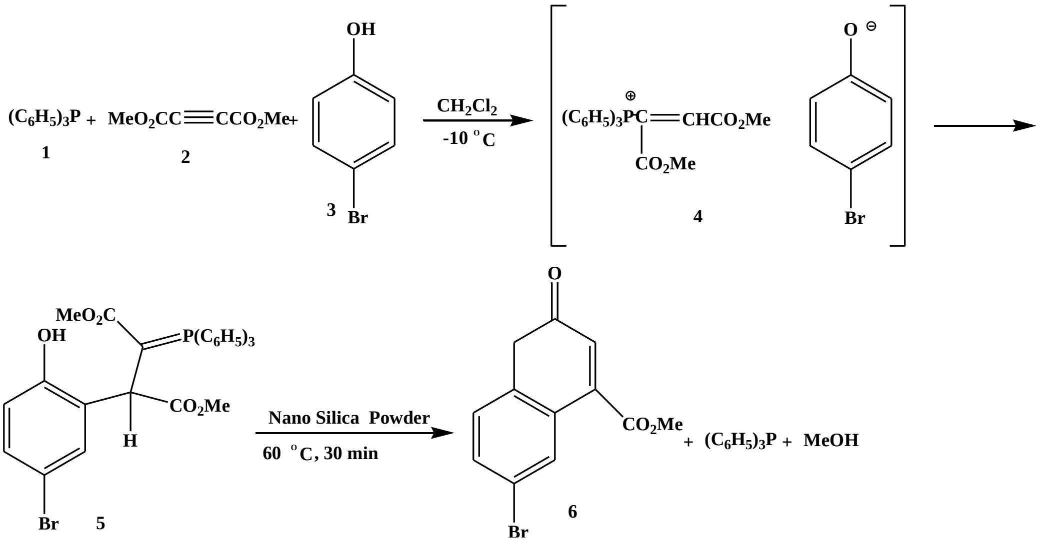
Coumarin derivatives are important chemicals in the perfume, cosmetic, agricultural and pharmaceutical industries [1]. However, the conventional methods for coumarin synthesis require drastic conditions. For example, 4-methyl-7-hydroxycoumarin has been prepared by stirring a mixture of resorcinol and ethyl acetoacetate in concd H_2SO_4 for 12–24 h. The development of alternative environmentally friendly synthetic methods of coumarins is strongly requested [2]. Here, we report a simple and efficient synthesis of coumarins via catalytic action of nano silica powder in the conversion of dimethyl2-(5-bromo-2-hydroxyphenyl)3-(triphenylphosphoranylidene) butanedioate to methyl 6-bromo-2-oxo-2H-chromene-4-carboxylate in solvent-free conditions at 60°C in fairly high yield (Scheme 1).



Scheme 1. *Synthesis of 6-bromo-2-oxo-2H-chromene-4-carboxylate*

Protonation of the highly reactive 1:1 intermediates, produced in the reaction between triphenylphosphine and dimethyl acetylenedicarboxylate, by 4-bromophenol leads to vinyltriphenylphosphonium salt, which undergoes aromatic electrophilic substitution reaction with conjugate base to produce dimethyl2-(5-bromo-2-hydroxyphenyl)3-(triphenylphosphoranylidene) butanedioate. Nano Silica Powder was found to catalyze conversion of dimethyl 2-(5-bromo-2-hydroxyphenyl)-3(triphenylphosphoranylidene)butanedioate to methyl 6-bromo-2-oxo2H-chromene-4-carboxylate in solvent-free conditions at 60°C in fairly high yield. In summary, we have found that nano silica powder is able to catalyze conversion of ylide 5 to compound 6 in solvent-free conditions.

Keywords: 4-Bromophenol; Nano silica powder; vinyltriphenylphosphonium salt

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Nano Silica Powder Catalyzed STEREOSELECTIVE C-Vinylation of Diphenylacetonitril

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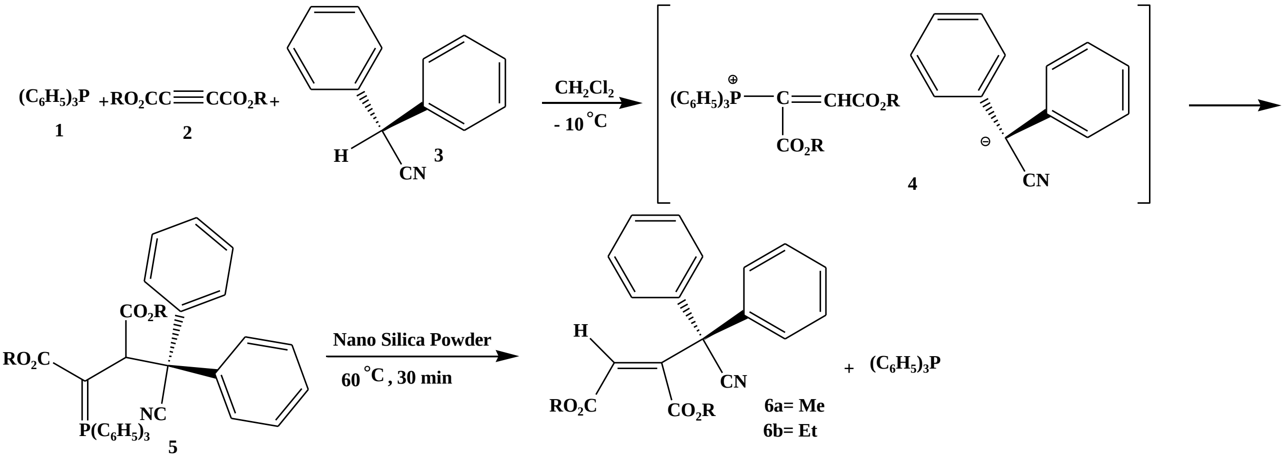
β-Addition of nucleophiles to the vinyl group of vinilic phosphonium salt leading to the formation of new alkylidene phosphoran has attracted much attention as a very convenient and synthetically useful method in organic synthesis. In recent years, we have established a convenient, one-pot method for preparation of the phosphonium salt 1 . In this article, we report facial one-pot stereoselective synthesis of dialkyl(Z)-2[cyano(diphenyl)methyl]-2-butenedioates in fairly high yields under thermal and microwave conditions in solvent-less system (SCHEME 1).



Scheme 1. *Synthesis of Dialkyl(Z)-2[cyano(diphenyl)methyl]-2-butenedioate*

The ylide 5 may result from initial addition of triphenylphosphine 1 to the acetylenic ester 2 and concomitant protonation of the 1:1 adduct, followed by the electrophilic attack of the vinyltriphenylphosphonium cation to the carbanion 4 (SCHEME 1). TLC indicated formation of ylides 5 in CH_2Cl_2 .Nano Silica powder was found to catalyze conversion of the stabilized phosphorus ylides 5 to dialkyl(Z)-2-[cyano(diphenyl)methyl]-2-butenedioates 6 under thermal conditions in solvent-less system.

Keywords: *diphenylacetonitrile, C-Vinylation, Dialkyl(Z)-2[cyano(diphenyl)methyl]-2-butenedioate*.

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Functionalized graphene oxide anchored to Ni complex as an effective recyclable heterogeneous catalyst for Sonogashira coupling reactions

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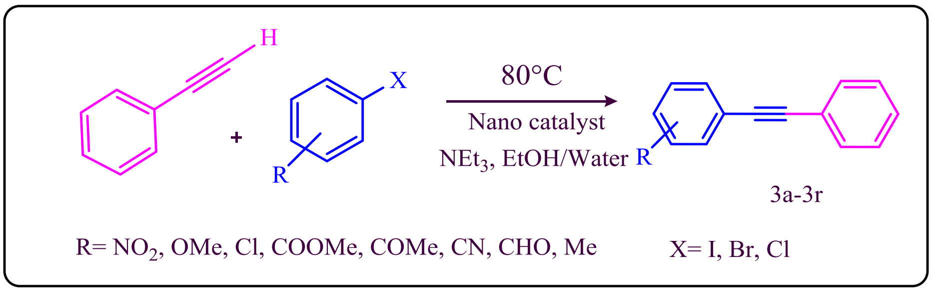
The Sonogashira cross coupling reaction between alkynes and aryl halides is blooming as a general methodology for the construction of C(sp)-C(sp^2) bonds [1]. Diarylethynes are versatile compounds in organic chemistry, and therefore, several procedure for their synthesis have been investigated [2]. Carbon-carbon triple bonds are very useful in the chemical industry such as new drugs and polymers, because they can be simply functionalized through multiple addition reactions. In chemical science, polyalkyne derivatives are applied to preparation carbon-rich materials, new carbon allotropes and organic LEDs [3,4].

The Sonogashira cross coupling reaction is an applied method used to prepare diarylethynes from readily available aryl halide derivatives and phenyl acetylene. The coupling reaction using N, N'-Bis(2-hydroxyethyl)ethylenediamine on to core shell graphene oxide (GO@SiO_2-BHED-Ni) as catalyst was studied in this research. The catalyst showed good thermal stability and recyclability in the reaction. Moreover the catalyst is simply separated and can be reused several times without significant loss of catalytic activity. A wide range of aryl halides was coupled successfully under palladium and phosphine free conditions. The use of this catalyst led to the formation of substituted aromatic alkynes in excellent yields and short reaction times.



Scheme 1. *Synthesis of diarylethynes derivatives*

Keywords: *Coupling reaction, Diarylethynes, Heterogonous catalyst, Nickel chloride, Graphene oxide.*

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Synthesis of intermediate multi-functional imidoyl chlorides for preparation of PCN ligands

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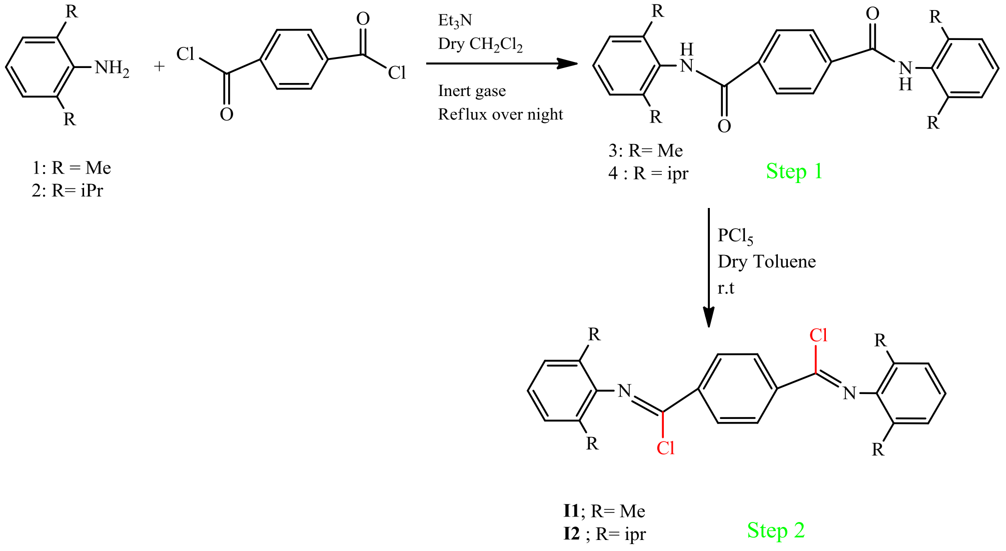
The reaction of amides with variety of halogenating agents such as PCl_5, $SOCl_2$ produces imidoyl halides. Imidoyl halides contain active carbon - halogen bond provide appropriate situation to form C- P bond from trivalent phosphine reagents. It is worth noting that C - P bond is used extensively for synthesis of organophosphorous ligands with P, N and C donor groups. The nature of PCN donor ligands plays fundamental role in determination the performance of chromium catalyst that strongly affected in activity and selectivity of tri/tetramerization of ethylene in selective oligomerization [1 -3]. In the present work amide is prepared by Schiff base condensation of amine and carbonyl group. Chlorination of amide with PCl_5 provides new imidoyl chlorides (**I1** and **I2**) as intermediate for PCN ligands preparation. First the appropriate amide was obtained by the reaction of aniline drive and terephthaloyl chloride in basic condition to produce N- aryl benzenediamide. Then the imidoyl chloride synthesized by the reaction of N- aryl benzenediamide and PCl_5. The procedure for synthesis of **I1** and **I2** are shown in **Scheme 1**.



***Scheme 1**; Synthetic route for preparation of imidoyl chloride **I1** and **I2**.*

Keywords; amid group, Imidoyl chlorides.

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Design of new multidendate PCN ligands to improve Philips catalyst system in selective oligomerization of ethylene

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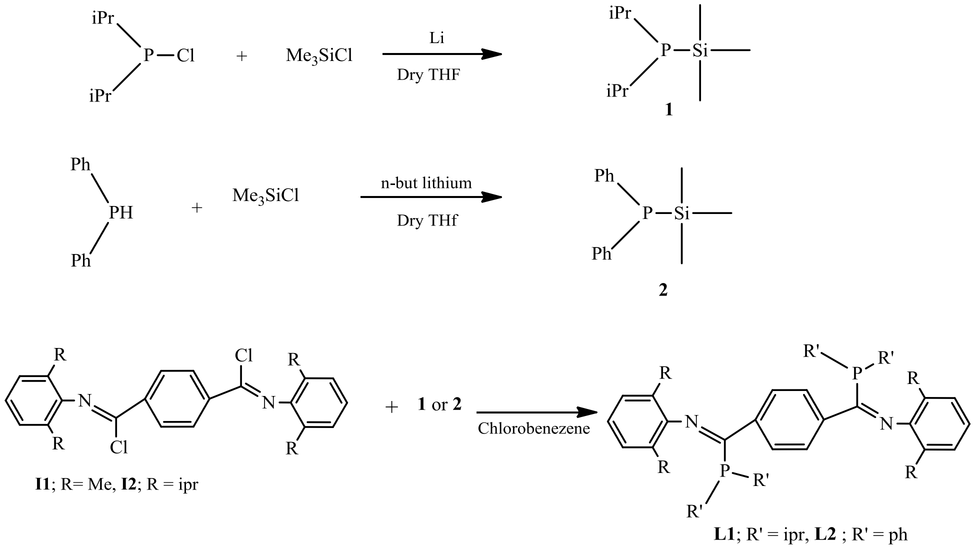
To the development of systems for selective tri/tetramerization of ethylene to 1- hexene and 1-octene in ethylene oligomerization, various changes on Philips catalyst systems as pioneer industrial method have been done by design of organophophorous systems. Different type of multidentate ligands with N, P, C and S donors are capable to stabilize chromium cycle in catalyst process [1]. The ability of 1- phosphanyl methanimine type ligand in improving selectivity and activity of catalyst for prodution high yield of 1- hexene and 1- octene have been investigated and get considerable attention by researcher [2-3]. In this work PCN ligands are designed by nucleophilic substitution of trivalent phosphorous in trimethylsilylphosphines with chloride in electrophilic iminium carbon bond (-Cl-C=N-) to form desire C-P bond. Different aliphatic and aromatic phosphines were selected to investigate the electronic and steric effect of phosphine functional groups on catalyst behavior. The appropriate trimethylsilyl phosphines are synthesized with deals of phosphines with trimethylsilyl chloride in the present of alkaline metals. Subsequently the reaction of imidoyl chloride with trimethylsilyl phosphine gives **L1** and **L2**. General synthetic route for preparation of trimethylsilylphosphines and ligands **L1** and **L1** are shown in **Scheme 1**.



Scheme 1*; Synthetic procedure for preparation of* ***L1*** *and* ***L2*** *as PCN ligands for ethylene oligomerization.*

Keywords; selective tri/tetramerization, PCN ligands, multidendate

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Selective photocatalytic oxidation of alcohols to aldehydes and ketones by nitromethane on titanium dioxide under light irradiation

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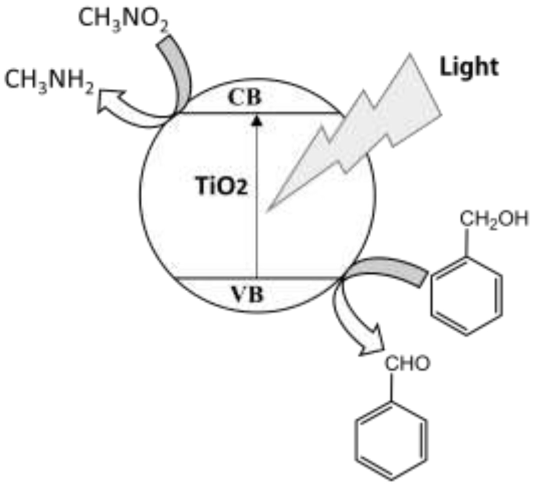
The oxidation of alcohols to aldehydes and ketones is one of the most important transformations in organic chemistry both in laboratory and industrial scale, because the corresponding carbonyl compounds are valuable compounds such as pharmaceuticals, agricultural chemicals and fine chemicals[1-2]. Photocatalytic reactions using semiconductor nanomaterials have attracted much attention. One of the most promising semiconductors for photocatalytic applications is titanium dioxide. The reasons for its widespread are due to its low price, chemical and thermal stability, large commercially availability [3].

In this study, for the first time, nitroalkanes, especially nitromethane, have been used as an electron acceptor for the oxidation of alcohols in the presence of TiO_2 photocatalyst. The reactions showed excellent selectivity for production of aldehydes. In the case of the use of larger nitroalkanes, the imine product, which is the result of the reaction of aldehyde with aliphatic amine, is also produced and TiO_2 showed high reusability in this reaction.



Scheme 1. *photocatalytic oxidation of benzyl alcohol on TiO2 in the presence of nitromethane under light irradiation*

Keywords: *TiO_2, nitromethane, Photooxidation*

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An efficient synthesis of diarylmethylamine by copper catalyst

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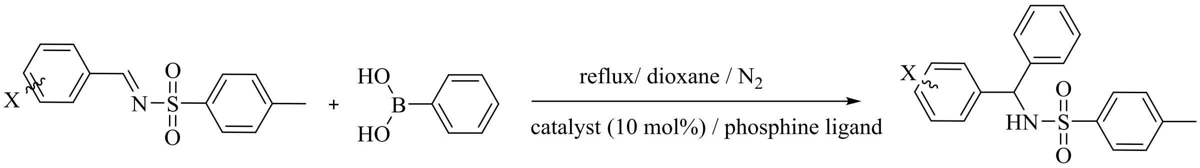
Amines are important building blocks of pharmaceutical and agrochemical compounds which are also used as ligand and base in organic reactions [1].This type of structure is of interest for preparing natural product, bioorganic and drugs that can mention as cetirizine (antihistaminic) to treat allergic, sertraline and tianeptine (anti-depression), letrozole (treat cancer) and many other medications [2,3]. Arylation of activated aldimines is a superior route for the synthesis of α-arylmethylamines. Due to the application of these compounds, the use of various transition metal catalysts, substrates and aryl donor groups have been developed to improve the catalytic activity, scope of substrates and other variables. However some of these methods were used toxic and expensive reagents [4].
Herein we have designed an arylation reaction on imines to synthesis of aryl amines. A wide range of aryl amines were afforded by addition of aryl boronic acid to different aldimines in presence of non-expensive copper metal and phosphine ligands. The desired products were produced in good yield and were characterized by IR, ^{1}HNMR and ^{13}CNMR.



Scheme 1. *Copper catalyzed arylation of activated aldimines.*

Keywords: *Arylation reaction, Copper catalyzed, Aldimine.*

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Electrochemical Oxidation of Benzylic C-H Bonds

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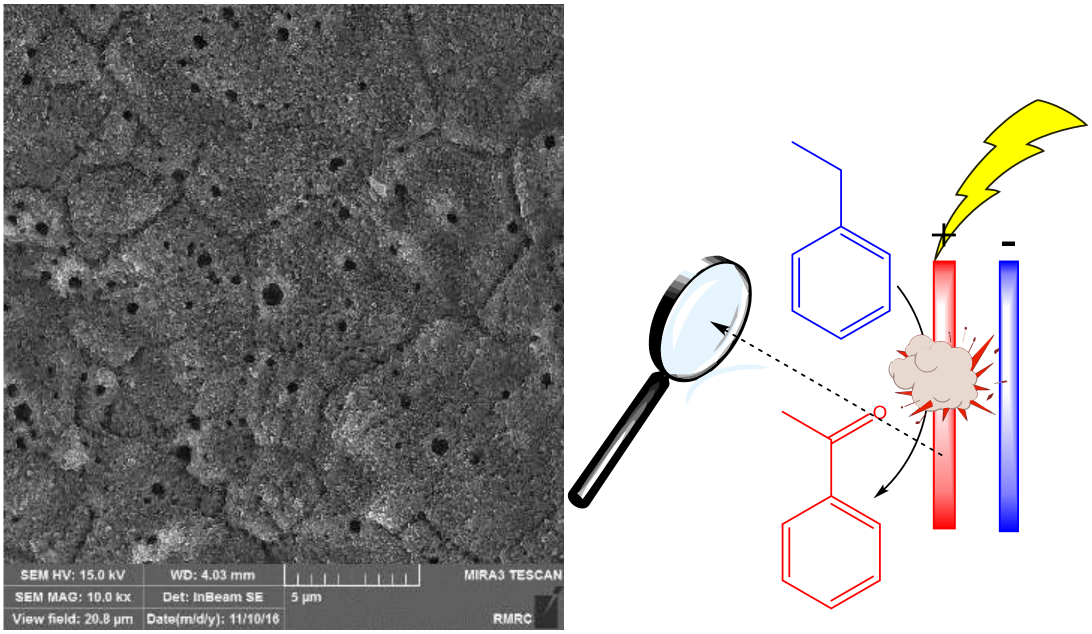
Various catalytic procedures based on transition metals have been developed for the oxidation of organic compounds. Especially, new methods and strategies for the direct functionalization of C–H bonds are of current interest in retrosynthetic analysis, affecting the synthesis of natural products, medicines, and materials [1]. In the past decades, the most reported methods for the activation of C-H bonds used highly toxic or expensive catalysts (such as ruthenium, iridium, iron) [2]. Herein, we report an electrochemical method that can emerge as a useful tool for C-H oxidation using. We used different metal and carbon-based electrodes and the optimal conditions contain solvent, electrolyte and potential. The best reaction was performed in the presence of two nickel-based electrodes and 95% of ketone was formed. The developed method is simple, inexpensive, accessible and reusable.



Scheme 1. *Oxidation benzylic C-H bond*

Keywords: Electrochemistry, nickel electrode, C-H bond oxidation

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An Abinitio Study on the structure, Energetics and Spectra of Phthalimido-Prolineamide as Chiral Catalyst for Aldol Reactions

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Phthalimido-prolinamide (PP) was prepared from N-Boc-proline and N-aminophthalimide. It was developed for organocatalytic enantioselective direct aldol reactions of various aldehydes with ketones [1]. The use of 5 mol% of water accelerated the reaction and the α-hydroxy carbonyl product could be attained in high yields and high stereoselectivities. In this work, the structure, energetics and infra-red (IR) spectrum of PP were studied by ab initio electronic structure methods, namely, Møller–Plesset second-order perturbation theory (MP2) correlated consistent, aug-cc-pvDZ basis functions. Figure 1 and 2 represent the optimized structure and IR spectrum of the catalyst, respectivally. The longest peak in figure 2 refers to asymmetric stretch of the two carbony groups in the phthalimide part of the molecule. The active sites of molecule can be defined by analyzing the partial atomic charges. The mulliken charge of the oxygen in carbonyl group of proline component have been estimated -0.967 which is the highest negative value and the maximum posetive value refers to C atom in that carbonyl group. Molecules such as PP has several sites to accept proton. Proton transfer to these sites can lead to the production of stable protonated ions which may accelerate the reaction. In cases where there are more than one protonated ion, the concept of topical proton affinity (PA) arises. Topical PA as the negative of the enthalpy change of the proton transfer reaction were calculated at the DFT (B3LYP) level of theory with 6-311++G(g,p) basis set because of the extremely time consuming method of MP2 in this case. Gas phase basicity (GB) as the negative of the Gibbs free energy change of the proton transfer reaction is defined at the same level of theory. All of the computations were performed with Gaussian 09 package. The ionization energy and electron affinity can refer to vertical and adiabatic quantities. Vertical ionization energy (VIE) and vertical electron affinity (VEA) are calculated as electronic energy difference between the ground state of the neutral molecule and its cation and anion at the equilibrium geometry of neutral molecule, respectably. Adiabatic ionization energy (AIE) and adiabatic electron affinity (AEA) are defined as the energy difference between neutral molecules and referred ions in their relaxed geometry [2]. These values were estimated at the B3LYP/6-311++G(d,p) level of theory. The information of the amount of mentioned properties can be helpful in finding of the role of catalyst in mechanism of the reactions.

Figure 1. optimized structure of phthalimido-prolinamide at MP2/aug-cc-pvDZ

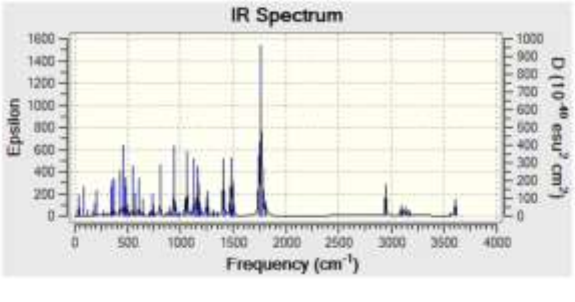

Figure 2. IR spectrum of phthalimido-prolinamide at MP2/aug-cc-pvDZ level of theory

Keywords: *ab initio, Phthalimido-prolinamide,catalyst.*

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Synthesis of Amines by Nucleophilic 1‹2-Addition of Organo Boron Reagents to the C-N Double Bond of Aldimines

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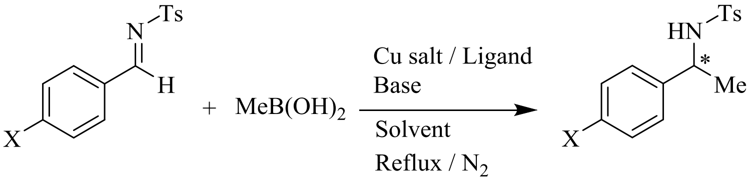
Chiral amines are essential precursor to preparation of pharmaceuticals and natural products. Hence, the methods for synthesis of these compounds have been considerable interest. Among methods for the synthesis of amines, the catalytic addition of dialkalzinc reactants on the imines and catalytic ethylation of imines by using different catalysts has been reported. Wei-Ming Huang and Biing-Jiun Uang used amino alcohol as ligands for the addition of dialkylzinc to imines[1]. Methylation of imines reported by Tamioka and colleagues using dimethylzinc reagent in the presence of amidophosphin-copper catalysts [2]. Hayashi and co-workers reported the first example of methylation of imines by using trimethylboroxine in the presence of rhodium catalyst[3].

In this project, we tried to prepare methyl amines by addition of methylboronic acid to aromatic aldimines in the presence of phosphine ligands and various copper salts (Scheme 1). The desired products were produced in good yield and were characterized by IR, ^{1}H NMR and ^{13}C NMR.



Scheme 1. *Methylation of aldimine derivatives by using methyl boronic acid in presence of copper catalysts.*

Keywords: *Copper catalyst, Methylation reaction, Methyl boronic acid.*

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Mn (salen) complexs on graphene oxide as highly efficient Catalyst for Epoxidation of Styrene

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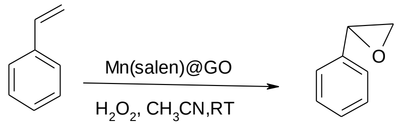
Graphene oxide and its derivative have attracted extensive interests in many fields, including catalytic chemistry, organic synthesis, and electrochemistry, recently. Transition metal complexes are one of the most useful and powerful catalysts for industrial processes. However, the practical applications of homogeneous metal complexes are hampered by their high costs with problems of separating from the reaction mixtures. Therefore, designing heterogenized metal complex catalysts is of great interest for economic and environmental reasons in recent years [1-5]. Catalytic epoxidation [6] of styrene is an important practical reaction for producing styrene oxide which is an important industrial organic intermediate and is used in the synthesis of fine chemicals and pharmaceuticals [7].A Mn (salen) complex has been homogeneously immobilized on a modified graphene oxide (GrO) support via covalent bonding. The loading of Mn (salen) complex on GrO nanosheets was monitored by FTIR, TG-DTA, and elemental analyses. The catalytic properties of Mn (salen) - Graphene oxide compound in the oxidation of styrene with H_2O_2 as oxidant were investigated and compared with the properties of their homogeneous analogues. It was found that both heterogeneous Mn (salen) catalysts were more active than their homogeneous analogues and that the product selectivity varied in cases of different oxidants. The supported Mn (salen) complex showed high yield of styrene oxide (86.0%) and good recoverability when using air as oxidant.



Scheme 1. *Epoxidation of Styrene*

Keywords: *graphene oxide, heterogeneous catalyst, epoxidation*

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Modeling of Selective Catalytic Reduction of NO with NH_3 Process using Cu/ZSM-5 Nanocatalyst

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Nitrogen oxides have been reported as one of the most serious pollutants. Selective catalytic reduction (SCR) of NO_x by NH_3 is an effective technology for reducing nitrogen oxide emissions. Despite the wide use of NO_x reduction by SCR process, many aspects concerning the reaction mechanism are still not well understood [1]. The objective of our current research is to develop a reaction kinetic model of the proposed mechanism for the SCR of NO by NH_3 over Cu/ZSM-5 nanocatalyst. The Cu/ZSM-5 nanocatalyst prepared via impregnation method then catalytic tests were carried out in a fixed bed reactor at different temperatures of 100 to 400˚C.

An objective of the modelling was to estimate the kinetic parameters based on the experimental results. For parameter fitting purposes the Arrhenius equation was reformulated as:

$$k_i = A_i \exp[\frac{-E_{ai}}{R}(\frac{1}{T} - \frac{1}{Tm})] \qquad (1)$$

The model of the reactor was adopted from a heterogeneous model in which the reaction was assumed to occur in the solid catalytic bed. In this model, the space time of the feed (W/F_{Feed}) is considered as independent variable and the weight fractions (ω_i) of chemical species is considered as dependent ones [2].

$$\frac{d\omega_i}{d(W/F_{Feed})} = \sum_{j=1}^{n} \mathrm{r_j} \qquad i = 1,2,\ldots, number\ of\ components \quad (2)$$

All reactions are assumed elementary and depending on each reaction it would be first, second or third order.

$$\mathrm{r_j} = k_j \prod_{i=1}^{m} \omega_i \qquad j = 1,2,\ldots, number\ of\ reactions \qquad (3)$$

where k_j is the kinetic parameter of jth reaction. The method for estimation of the kinetic parameters was consisted of solving mass conservation equations for each component. By means of equation (2), the mass gradient relations can be written for each component. The differential equations corresponding to the mass conservation equation of each chemical species were solved and the kinetic parameters were estimated using hybrid genetic algorithm. The objective function which was used to minimize the deviation between experimental and calculated weight fractions of chemical species is according to the equation (4)

$$OF = \sum_{i=1}^{m} \sum_{j=1}^{p} \left(\omega_{i,j} - \omega_{i,j(\,calc.)}\right)^2 \qquad (4)$$

Figure 1 represent the products distribution versus space time of reactor at reaction temperature 300℃. In this Figure, the experimental and calculated values were shown by points and lines respectively. As observed in the Figure, the results indicates a good agreement between experimental and calculated data obtained from kinetic model.

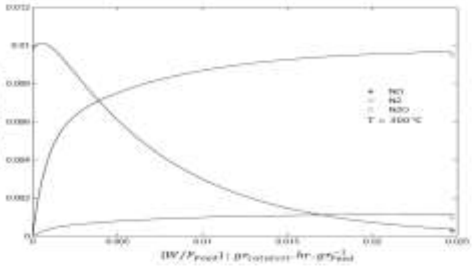

Figure 1- Weight fractions of main components versus space time of reactions for T=300 ℃

Keywords: *NO reduction*, *Cu/ZSM-5, Kinetic Modeling.*

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Kinetic Study of the 3-hydroxytyraminium in the Presence N-hydroxy-phenylacetamide as catalyst

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Abstract

We study the electrocatalytic oxidation of 3-hydroxytyraminium using N-hydroxy-phenylacetamide as catalyst with cyclic voltammetry, chronoamperometry, and differential pulse voltammetry (DPV). First, the electrochemical behavior of the modified electrode was investigated in buffer solution. Then the diffusion coefficient, electrocatalytic rate constant, and electron‐transfer coefficient for 3-hydroxytyraminium oxidation were determined using electrochemical approaches. This method was also used for the determination of 3-hydroxytyraminium in a pharmaceutical preparation using the standard addition method. The homogeneous rate constants (k_{obs}) were estimated by comparing the experimental cyclic voltammograms with the digitally simulated voltammograms based on EC mechanism.

Keywords: *: Electrocatalys; Oxidation; 3-hydroxytyraminium; N-hydroxy-phenylacetamide.*

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Cu^{II} immobilized on aminated Fe_3O_4@ cellulose nanofibers (Fe_3O_4@ cellulose nanofibers -NH_2-Cu^{II} NPs): a novel, bio-based and magnetic nanocatalyst for the synthesis of benzimidazole derivatives

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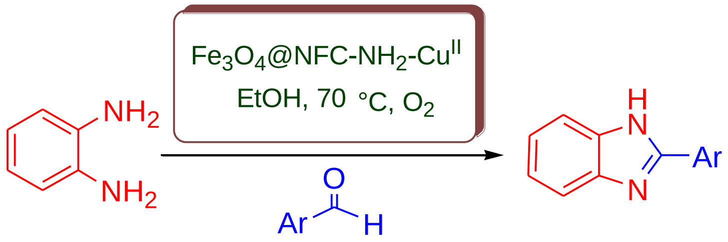
From the point of view of green chemistry magnetically recoverable catalysts have appeared as a powerful and persuasive option, due to their ability like excellent catalytic performance and easy separation and recovery from the reaction mixture [1]. Aggregation/ oxidation of metal particles and reduction in catalytic activity which are kinetic problems often caused by highly active surface atoms can be solved by a well-chosen stabilizer [2]. Such a stabilizer is able to control the size of particles, improve the chemical stability, shape the magnetic features of the hybrid materials, avoid the agglomeration and also obtain the catalyst aim. cellulose nanofibers (CNFs) is of excellent interest due to properties such as nontoxicity, earth abundance, biodegradability, broad chemical-modifying capacity and fine chemical stability [3].

Synthesis privileged of benzimidazoles through an economical and environmentally friendly method is always desirable because benzimidazoles and its derivatives have received extensive attention in medicinal chemistry and show a wide spectrum of pharmacological activities [4].

In this study we report the synthesis of a novel heterogeneous Cu nano-particles bio-supported based magnetic nanomaterials catalyst (Fe_3O_4@ CNPs- NH_2-Cu^{II} NPs) and its identification by various techniques like FTIR, TGA, SEM, TEM, EDX, ICP-AES and VSM.

The applicability of the constructed heterogeneous nanocatalyst was explored in the synthesis of benzimidazoles through the cyclization reaction of 2-amino anilines with benzaldehyde derivatives using O_2 as an oxidant in ethanol as a green solvent at 70 °C. The catalyst could be easily separated by an external magnet and reused for at least five times without any appreciable loss of its catalytic reactivity



Scheme 1. *Synthesis of benzimidazoles catalyzed by Fe_3O_4CNPs- NH_2-Cu^{II} NPs*

Keywords: *benzoimidazoles, cellulose nanofibers, Fe_3O_4@ CNPs- NH_2-Cu^{II} NPs*

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Epoxidation reaction catalyzed heterogeneously by Mn complex - polyoxometalate compound

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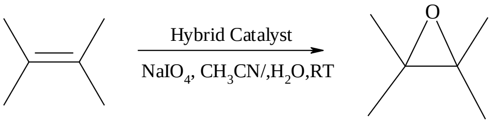
Organoimido substituted POMs as valuable building blocks can construct novel nanostructured organic–inorganic hybrid molecular materials in well-developed common organic synthesis methods, such as Pd-catalyzed carbon–carbon coupling , esterification and epoxidation. Nowadays, inorganic–organic hybrid materials based on polyoxometalates (POMs) are extensively attracted because of theirpotential applications in catalysis, gas storage, magnetism, photochemistry and electrochemistry [1-5]**.** Their features of an oxygen-rich surface, high charge density and controllable size mean POMs are becoming popular inorganic building blocks. A hybrid complex based on covalent interaction between of 1, 2-bis (p-aminophenylthio) ethane (BAPTE), and a Lindqvist type polyoxometalate, $Mo_6O_{19}{}^{2-}$, was prepared. This new hybrid catalyst, Mn (II) complex -POM, was characterized by ^1H NMR, FT- IR, and UV-Vis spectroscopic methods and cyclic voltammetry. The catalytic activity of Mn(II) complex -POM hybrid material was investigated for epoxidation reaction were produced in good to excellent yield. The reusability of this catalyst was also investigated.



Scheme 1. *Epoxidation of olfins*

Keywords: *organic–inorganic hybrid, epoxidation, polyoxometalates*

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Synthesis and Characterization of Organic−Inorganic Modified Silica Hollow Nanoparticles for the Oxidation of Alcohols to Aldehydes and Ketones

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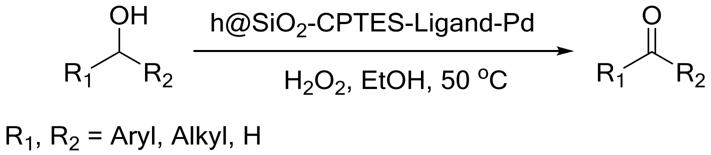
We demonstrate the preparation and characterization of novel organic−inorganic hybrid palladium nanocatalyst fabricated via the covalent grafting of Pyr-ligand on chlorfunctionalized silica-hollow nanoparticles, followed by its metallation with palladium acetate for the selective oxidation of primary 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 carbon nanospheres as templates. Acting as seeds, carbon nanospheres were then wrapped with a silica shell by the modified Stöber method [2]. After calcination at 600℃, uniform spheres with a thin shell of silica and hollow interior structures were synthesized. The synthesized substrates are in a spherical morphology and uniform size distribution. The nanostructure and properties of nanocatalyst were studied by TEM, SEM, XRD, TGA, and FT-IR characterizations.



Scheme. 1 Oxidation of alcohols by using H_2O_2 in the presence of ethanol at 50°C.

Keywords: *Modified Silica Hollow Nanoparticles, Palladium Nanocatalyst, Oxidation.*

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Kinetic Study of the Catechols in the Presence of diethyl phosphite using N-hydroxyphthalimide as catalyst

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Abstract

The electrocatalytic oxidation of catechols in the presence of diethyl phosphite was performed using N-hydroxyphthalimide as catalysts. Initially, the oxidation- reduction of n-hydroxyphthalimide was investigated and the voltammetric results confirmed the production of relatively stable radical under electrochemical oxidation. Thereafter, the reactivity and electrocatalytic performances of generated radicals were investigated toward the various Catechols derivatives at different pH values. Based on these results the best electrocatalytic activity was observed at acetate buffer. The mechanism of electrochemical oxidation of catechols using N-hydroxyphthalimide as catalysts have been studied in the presence of diethyl phosphite as a nucleophile in aqueous solution. Voltammetric studies indicate that the quinones derived from catechols, and its derivatives, participate in michael addition reaction with diethyl phosphite. The reaction mechanism consists of electron transfer followed by a chemical reaction which is named as an EC mechanism. The homogeneous rate constants (k_{obs}) were estimated by comparing the experimental cyclic voltammograms with the digitally simulated voltammograms based on ec mechanism. Also the effects of nucleophile concentration and substituted group of catechols on voltammetric behavior and the rate constants of chemical reactions were examined.The abstract should be typewritten for A4 format paper, maximum one page for all contributions.

Keywords: *: Electrocatalys; Oxidation; N-hydroxyphthalimide; catecohol.*

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Halloysite Nanoclay containing Ionic-liquid and Cuprous Sulfite: Efficient Catalyst for Click Reaction

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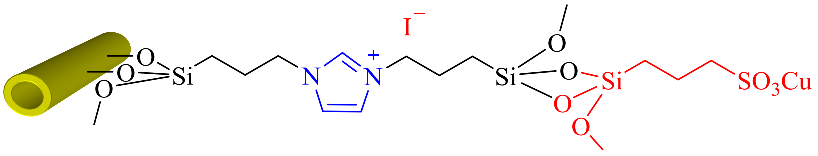
A novel heterogeneous catalyst, Hal-IMI-SO_3Cu, was designed and synthesized based on functionalization of Halloysite nanotubes with ionic liquid. It was prepared and fully characterized by applying TEM, BET, SEM/EDS, ICP-AES, XRD, TGA, and FTIR spectroscopy. Hal-IMI-SO_3Cu exhibited excellent catalytic activity for Click reaction under mild and eco-friendly condition. The comparison of the catalytic activities the catalyst without sulfur(Hal-IMI-Cu), the catalyst without IL(Hal-SO_3HCu), the catalyst in which –SH was not oxidized to –SO_3H(Hal-IMI-SCu) , the catalyst without copper(Hal-IMI-SO_3H), with that of the catalyst confirmed that copper played the dominant role in the catalysis. Moreover, the contribution of sulfur species and IL, to the catalysis was confirmed. It was also proved that the presence of –SO_3H was more favorable than –SH. Notably, the catalyst could be recovered and reused for ten reaction runs with slight loss of the catalytic activity and copper leaching.



***Scheme 1**.structure of catalyst*

Keywords: Halloysite; Ionic liquid; Click reaction; Heterogeneous catalyst; CuI.

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Green bio-based synthesis of starch-halloysite hybrid: An efficient heterogeneous catalyst for C–C coupling reactions

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Using halloysite nanoclay (Hal) as support and its multi-functionalization, Pd@Hal-SA, containing amine-functionalized starch with Cl-halloysite nanoclay, followed by coordination of Pd (II) acetate Pd@Hal-SA. The catalyst was characterized by using SEM/EDS, FTIR, XRD, BET, ICP-AES, TGA and DTGA. It was used as a novel heterogeneous catalyst for coupling reactions under mild reaction condition. The comparison of the catalytic activity of Pd-Hal(the catalyst without SA), Pd-SA (the catalyst without Hal)and Pd@Hal-SA confirmed the superior performance of the latter, indicating the contribution of two components, SA and Hal to the catalysis. Moreover, the catalytic activity of Pd@Hal-SA was higher than that of Pd@Hal+SA, implying that the use of hybrid system was more efficient that use of individual components in a separated form, due to the synergism between SA and Hal.

The catalyst could be successfully recycled for several consecutive reaction times with slight loss of the catalytic activity.

Keywords: *Halloysite nanoclay; Starch; Pd nanoparticles; Heterogeneous catalyst.*

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Supported liquid metals: high-technology catalysts in chemical synthesis

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The development of high-technology catalysts which combine selectivity, productivity, robustness and ease of processing at the highest possible level is the ultimate goal in the catalytic chemistry. One such system involves supported liquid metal catalysts which benefits from the simultaneous metallic and liquid natures of the liquid metals[1,2]. Unlike traditional heterogeneous catalysts, the catalytic process of the highly dynamic supported liquid metal catalysts does not proceed at the surface of the metal nanoparticles, but presumably at homogeneously distributed metal atoms at the surface of a liquid metallic phase. Indeed, supporting a dissolved catalytic active metal in a metallic solution merges some features of heterogeneous catalysis, particularly, easy product separation, with features of homogeneous catalysis, particularly, electronic–steric control, because of the formation of isolated metal sites in a certain metal matrix, which in turn presents different electronic features caused by the inter metallic interactions[3]. The existence of a liquid metal catalytically active phase in a catalyst seems to offer a number of very important features[4]: (a) A higher activity/selectivity because of the special nature of the atomically isolated active sites created in a liquid metal environment; (b) Resistance to active metal agglomeration; (c) Self-healing properties and insensitivity to coking because of the high dynamics of the liquid interface. In fact, by dissolving the active metal in a liquid metallic environment, uniform catalytic sites can be created that provide electronic and steric properties different from those of the supported solid metal nanoparticles. Here we review some supported liquid metal catalysts as the high-technology catalysts for some of the catalytic important reactions such as formic acid dehydrogenation[5], alkane dehydrogenation[4], methane conversion to hydrogen and separable carbon[6] and so on. Also we survey the processing technologies for the preparation of our investigated supported liquid metal catalysts. We believe that this opens a wide field of new catalytic materials, which could provide a highly interesting research field for theoretical, fundamental and applied studies.

Keywords: Liquid metals, High-technology catalysts, Chemical synthesis, Metallic and liquid natures

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APTPOSS and Cyclodextrin Nanosponge Hybrid as an Efficient Pd-immobilized Nanomagnetic Catalyst for Ligand and Copper Free C-C Coupling Reactions

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To promote our previously reported effort on developing new heterogeneous Pd immobilized catalyst using cyclodextrin nanonosponge (CDNS) [1], a hybrid of octakis [3-(3-aminopropyltriethoxysilane) propyl]octasilsesquioxane (APTPOSS) and CDNS was used as a support to embed Fe_3O_4/Pd nanoparticles. The obtained catalyst, Fe_3O_4/Pd@CDNS-APTPOSS could promote ligand and copper free Sonogashira and Heck coupling reactions and different characteristic methods, including FTIR, TGA, XRD, SEM/EDS, TEM, ICP/AES and BET were applied to characterize the obtained catalyst. Although APTPOSS potential for catalytic activity has been proved [2,3], the catalytic activity of Pd@CDNS-APTPOSS was superior compared to that of Pd@APTPOSS and Pd@CDNS, indicating the synergism between CDNS and APTPOSS and the catalyst was recyclable with slight Pd leaching and loss of the catalytic activity after several reaction runs.

Keywords: *APTPOSS 1, Cyclodextrin Nanosponges 2, Pd Nanoparticles 3, C-C Coupling Reactions 4*.

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Magnetic nobel metal-based nanocatalysts in reduction of the priority pollutant 4-nitrophenol

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The nanocatalyst technology in organic synthesis has become a subject of intense investigation. In particular, magnetic nanoparticles (MNPs) as non-toxic, readily accessible, and retrievable nanoparticles offer many advantages in clean and sustainable chemistry. The use of MNPs as catalysts in chemical synthesis has been extensively studied in recent years. The recovery of expensive catalysts after their use is one of their most noticeable features in the sustainable process development. Additionally, the activity and selectivity of magnetic nanocatalysts can be manipulated by their surface modification[1] .

Noble metal nanoparticles have attracted considerable attention because of their distinctive physicochemical properties and their potential applications as a new class of efficient catalysts [2]. 4-Nitrophenol (4-NP) as an important industrial crude material has been extensively used in industrial processes such as those concerned with wood protection, explosives, herbicides, dyes, etc [1–3]. This compound is one of the most common waste pollutants because of its high solubility and stability in water. The reduction of 4-NP has become an important topic in recent years because the product, 4-aminophenol (4-AP) is an extremely useful intermediate for the preparation of analgesic and antipyretic drugs including acetaminophen and paracetamol. Various methods including chemical oxidation, biodegradation, photocatalytic degradation and solvent extraction have been employed to remove 4-NP from wastewater. Among these approaches, catalytic reduction is useful due to its being of cost, green and economically efficient[۳] .

To effective conversion of the 4-NP, many nanosized metal catalysts such as Au, Ag, Ru, Ir and Pd have been investigated, and represented superior catalytic activity and stability .

Since the excessive cost and scarcity of nobel metals are big obstacles for their industrial applications , therefore, the utilization efficiency and recovery yield of Pt nanocatalysts are very important challenges in the design of nobel metal-based catalysts .

Here we review some magnetic nobel metal-based nanocatalysts as the recoverable and reusable nanocatalysts for the highly efficient reduction of 4-NP Also we survey some of effective factors such as temperature, catalysts amounts reducing agents and pH on the reaction times and yields in our investigated magnetic nobel metal-based nanocatalysts[4].

Keywords: *"Magnetic nanoparticles", "nobel metal-based catalysts", "4-nitrophenol", "catalytic reduction"*

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Microwave assisted the synthesis of benzo[a]pyrano-[2,3-c]phenazine derivatives catalyzed by Multisulfonate hyperbranched polyglycerol functionalized graphene oxide as a novel and reusable catalyst

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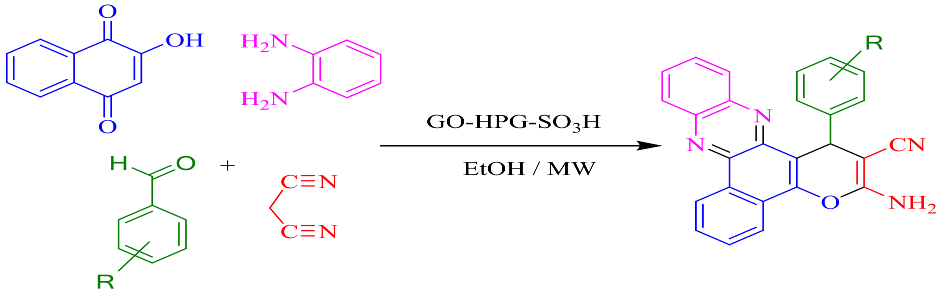
In recent years, designs of multi-component reactions (MCRs) because of their advantages in comparison with multi-step reactions according to environmental and economic considerations have received significant attention for the synthesis of biologically interesting compounds [1]. Also, microwave -assisted organic synthesis applied as an eco-friendly and powerful synthetic approach to accelerate organic reactions. Recently, carbon based nanostructures such as graphene oxide have used as substrate for polymer matrices [2]. Hyperbranched polyglycerols belong to a group of macromolecules have attracted considerable attention over the past few years due to their unique molecular structure and properties [3]. A class of hyperbranched polymers are the aliphatic polyether polyols named polyglycerol with tree-like structure that have wide range of new properties, and thus a greater area of applications [4]. Phenazines are nitrogen-containing heterocycles that exist in natural and synthetic products .They are structural components of diverse kinds of bacteria species. They have been demonstrated various pharmaceutical activities. Moreover, chromenes as an important class of compounds have been showed remarkable effects as pharmaceuticals such as antifungal and antimicrobial activities. Although molecules with phenazines and chromenes moieties have attracted a lot of attention in drug discovery but functionalized benzo[a]pyrano[2,3-c]phenazine derivatives have seldom been described. Herein, we would like to report the synthesis of multisulfonate hyperbranched polyglycerol modified graphene oxide (GO-HPG-SO_3H) as highly efficient and reusable catalysts for the preparation of benzo[a]pyrano[2,3-c]phenazine derivatives *via* a four-component reaction of 2-hydroxynaphthalene-1,4- dione, o-phenylenediamine, aldehydes, and malononitrile under Microwave irradiation.



Scheme 1. *Synthesis of benzo[a]pyrano[2,3-c]phenazine derivatives*

Keywords: *Microwave, Graphene oxide, Hyperbranched polyglycerol, Sulfonate, Catalyst, Benzo[a]pyrano[2,3-c]phenazine.*

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Kinetic Study of the Catechols in the Presence of diethyl phosphite using N-hydroxyphthalimide as catalyst

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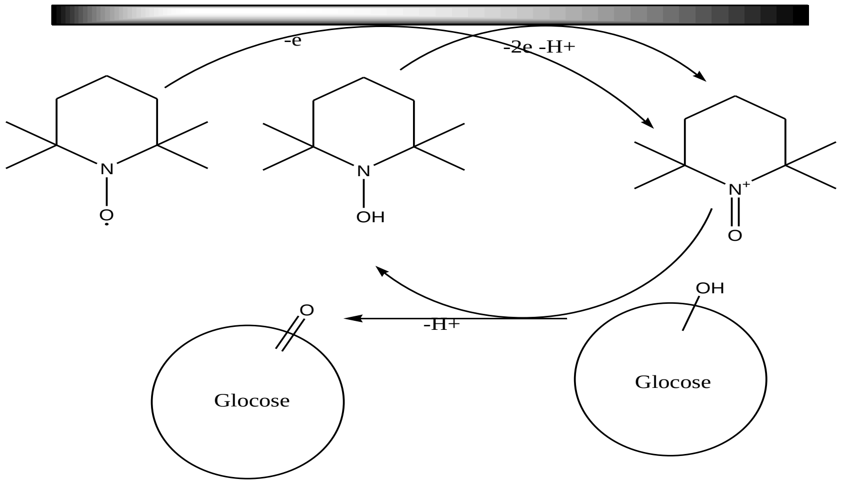
Abstract

The electrocatalytic oxidation of catechols in the presence of diethyl phosphite was performed using N-hydroxyphthalimide as catalysts. Initially, the oxidation- reduction of n-hydroxyphthalimide was investigated and the voltammetric results confirmed the production of relatively stable radical under electrochemical oxidation. Thereafter, the reactivity and electrocatalytic performances of generated radicals were investigated toward the various Catechols derivatives at different pH values. Based on these results the best electrocatalytic activity was observed at acetate buffer. The mechanism of electrochemical oxidation of catechols using N-hydroxyphthalimide as catalysts have been studied in the presence of diethyl phosphite as a nucleophile in aqueous solution. Voltammetric studies indicate that the quinones derived from catechols, and its derivatives, participate in michael addition reaction with diethyl phosphite. The reaction mechanism consists of electron transfer followed by a chemical reaction which is named as an EC mechanism. The homogeneous rate constants (k_{obs}) were estimated by comparing the experimental cyclic voltammograms with the digitally simulated voltammograms based on ec mechanism. Also the effects of nucleophile concentration and substituted group of catechols on voltammetric behavior and the rate constants of chemical reactions were examined.The abstract should be typewritten for A4 format paper, maximum one page for all contributions.



Keywords: *: Electrocatalys; Oxidation; N-hydroxyphthalimide; catecohol.*

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Preparation and characterization of cobalt oxide nanoparticles as catalyst for synthesis of xanthene derivatives under ultrasonic conditions

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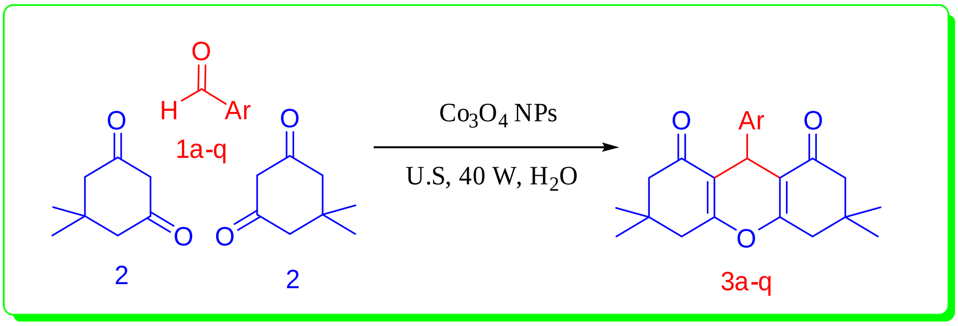
Nanomaterials and Nanotechnologies attract tremendous attention in recent researches. Nanomaterials in the size range of 3–50 nm have received increased attention in the last few decades because they exhibit physical properties that are intermediate to those of individual molecules and bulk materials [1].

Cobalt (II, III) oxide (Co_3O_4) is a technologically important material with applications in lithium-ion batteries, heterogeneous catalysts, gas sensing, ceramic pigments, and electrochemical devices. This transition metal oxide, when falling in the nanosized regime, is expected to lead to even more attractive applications in the conjunction of their traditional area and nanotechnology [2]. The present investigation reports, the synthesis and characterization of cobalt (II, III) oxide (Co_3O_4) nanoparticles using co-precipitation and using as catalyst for synthesis of xanthenes.

Xanthene is pharmacologically important oxygen-containing as heterocyclic moiety exhibiting an array of potent biological activities like antibacterial, antiviral, anti-inflammatory, antitumor, antioxidant, anti-plasmodial etc. Also this review gives the method for the construction of xanthenes by cobalt oxide nanoparticle as catalyst [3]. Many of the reported methods involve the use of various harsh catalysts/reagents that are not environmentally benign, produce a large amount of waste and need longer reaction times. Among various chemical methods for preparing cobalt oxide nanoparticles, in this research the co-precipitation method is used to the process simplicity.

In this research, the synthesis of cobalt oxide nanoparticles was investigated and used as a heterogeneous catalyst, also as an efficient in the synthesis of xanthene derivatives as developing new eco-friendly, efficient and economical valuable method.



Scheme 1. *Synthesis of xanthene derivatives by using cobalt oxide nanoparticles*

Keywords: *Nanomaterials, Cobalt oxide, Xanthene.*

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One-Pot and Chemoselective Synthesis of Alkyl 3-Oxo-3H-Benzo[f]Chromene-1-Carboxylates Derivatives Catalyzed by Nano Silica Powder

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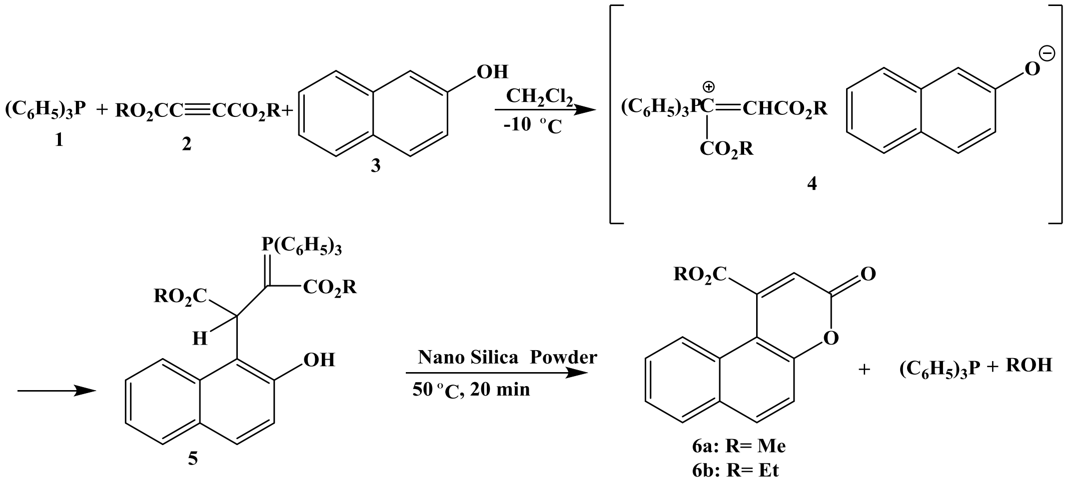
Chromene skeleton compounds occupy an important place in therealm of natural and synthetic organic chemistry. They are used as anticoagulants, additives in food and cosmetics, and in the preparation of insecticides, optical brighteners, and dispersed fluorescent and laser dyes.
In this article, we report on the catalytic activity of Nano Silica Powder in the conversion of dialkyl 2-(1-hydroxy-2-naphthyl)-3-(1,1,1-triphenyl-λ5 -phosphanylidene) succinates to alkyl 3-oxo-3H-benzo[f]chromene-1-carboxylates in solvent-free conditions at 50°C in fairly good yields (Scheme 1).



Scheme 1. *Synthesis of alkyl 3-oxo-3h-benzo[f]chromene-1-carboxylates*

The ylide (5) may result from initial addition of triphenylphosphine to the acetylenic ester 2 and concomitant protonation of the 1:1 adduct, followed by the electrophilic attack of the vinyltriphenylphosphonium cation on the aromatic ring at ortho α-position relative to the strong activating group (Scheme 1). TLC indicated formation of ylides 5 in CH_2Cl_2 . Silica gel powder was found to catalyze conversion of ylides 5 to alkyl 3-oxo-3H-benzo[f]chromene-1-carboxylates (6a–b) in solvent free conditions at 50°C in fairly good yields (Scheme 1). TLC indicated that the reaction was completed after 20 min.

Keywords: *2-hydroxynaphthalene, vinyltriphenylphosphonium salt, Nano Silica Powder.*

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One-Pot and Chemoselective Synthesis of Alkyl 2-Oxo-2H-Benzo[h]Chromene-4-Carboxylates Derivatives Catalyzed by Nano Silica Powder

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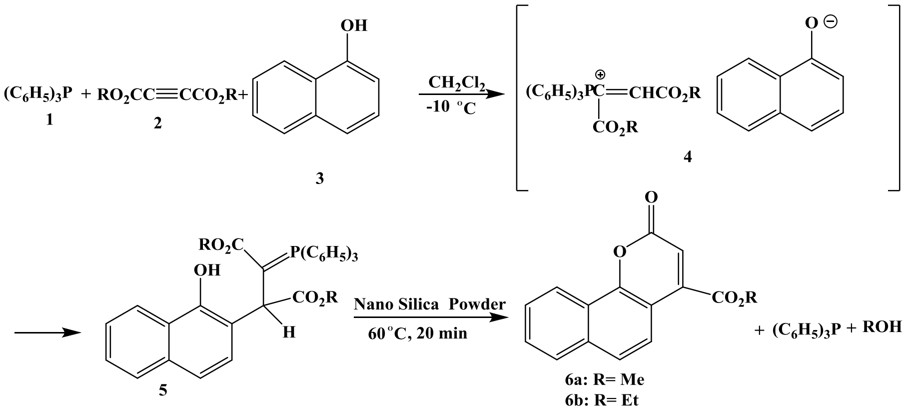
While chromene skeleton compounds have been long studiedin recent years they have attracted a greater growing interest, some having been found to possess properties of considerable pharmacological or industrial significance[1,2]. In this article, we report on the catalytic activity of nano silica powder in the conversion of dialkyl 2-(1-hydroxy-2-naphthyl)-3-(triphenylphosphoranylidene)butanedioates to alkyl 2-oxo-2H-benzo[h]chromene-4-carboxylates in solvent-free conditions at 60°C in fairly good yields (Scheme 1).



Scheme 1. *Synthesis of alkyl 2-oxo-2h-benzo[h]chromene-4-carboxylates*

The ylide (5) may result from initial addition of triphenylphosphine 1 to the acetylenic ester 2 and concomitant protonation of the 1:1 adduct, followed by the electrophilic attack of the vinyltriphenylphosphonium cation on the aromatic ring at ortho β-position relative to the strong activating group (Scheme 1). TLC indicated formation of ylides 5 in CH_2Cl_2. Nano silica powder was found to catalyze conversion of ylides 5 to alkyl 2-oxo-2H-benzo[h]chromene-4-carboxylates (6) in solvent-free conditions at 60°C in fairly good yields (Scheme 1). TLC indicated that the reaction was completed after 20 min.

Keywords: *chromene, Nano silica powder, 1-hydroxynaphthalene*.

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NiFe$_2$O$_4$@SiO$_2$@amino glucose magnetic nanoparticle as a new, green, effective and magnetically seperable catalyst for the synthesis of benzoimidazo[1,2-a]pyrimidine

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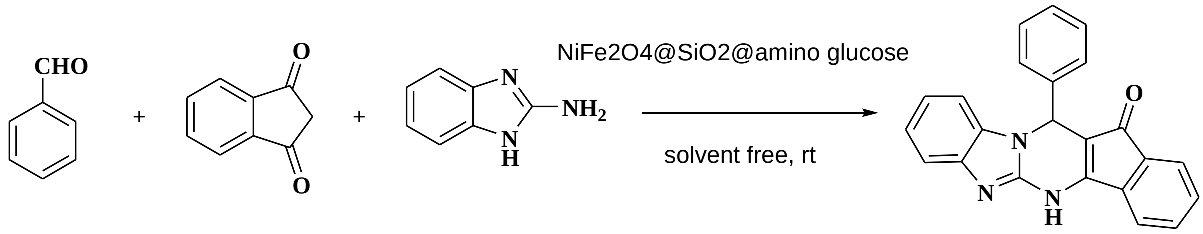
Imidazopyrimidines are important scaffolds in medicinal chemistry, as they exhibit a broad spectrum of biological activity such as anticancer, antitubercular, antiviral, antimicrobial, antifungal , anti-inflammatory, Parasiticidal activity, calcium channel blockers, benzodiazepine receptor agonists, and potent P38 MAP kinase inhibitors [1].

Nanoparticles due to their high surface area, high activity and selectivity, easy separation and isolation of products from the reaction mixture have been developed as suitable replacements for conventional heterogeneous catalysts [2]. Besides, using magnetic nanoparticles as catalysts is associated with other advantages including easy synthesis and functionalization, low toxicity and low cost. However, magnetic nanoparticles can easily aggregate into larger clusters because of their anisotropic dipolar attraction.

In continuation of our works, to synthesize heterocyclic and biologically active compounds [3], hererin, we wish to report our trial for the synthesize benzoimidazo[1,2-a]pyrimidine using three component synthesis of aldehyde, indanedione and 2-aminoimidazol using NiFe$_2$O$_4$@SiO$_2$@amino glucose magnetic nanoparticle under solvent free condition.



Scheme 1. *Synthesis of benzoimidazo[1,2-a]pyrimidine*

Keywords: *benzoimidazo[1,2-a]pyrimidine, indandione, solvent free*

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Laccase on graphene oxide: Immobilization and use as a novel biocatalyst for phenol degradation

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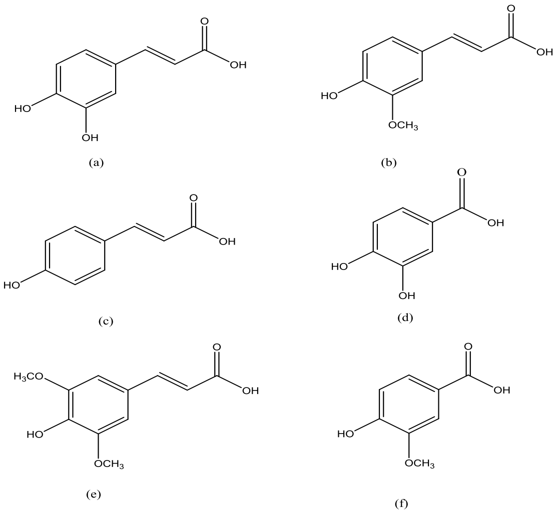
Laccases (E.C. 1.10.3.2, *p*-diphenyl: dioxygen oxidoreductase) belong to the so-called blue-copper family of oxidases[1], this enzyme has a high biotechnological interest as demonstrated by several studies reporting its use for green processes [2], such as bioremediation. Laccase from *Myceliophthora thermophile* (Novozym 51003) was immobilized on graphene oxide as a novel method of covalent immobilization by nucleophilic attack of amino groups of laccase to oxygen groups of the support. The enzyme loading on the support was about 94 mg/g under the optimum conditions (pH 4.5, 100 min). The effect of pH, temperature and organic solvent on immobilized enzyme activity was determined and compared with those of free enzyme. In general the immobilized enzyme was found to be stabilized compared to the free enzyme. The immobilized laccase was used for the oxidation of a mixture of six phenolic compounds (caffeic acid, ferulic acid, *p*-coumaric acid, protocatechuic acid, sinapic acid and vanillic acid) chosen among those present in olive mill wastewaters (OMWs) (scheme 1). Reaction yield observed for the oxidation of the examined phenolic compounds were different after 2 h (Table 1).

Table 1.The removal efficiency of phenolic compounds.

Compound	Removal efficiency
Caffeic acid	93%
Ferulic acid	97%
p-Coumaric acid	95%
Protocatechuic acid	55%
Sinapic acid	98%
Vanillic acid	68%



***Scheme 1.** The phenolic compound: (a)caffeic acid, (b)ferulic acid, (c)p-coumaric acid, (d)protocatechuic acid, (e)sinapic acid and (f)vanillic acid*

***Keywords:** Laccase, biocatalyst, phenol degradation.*

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Synthesis of magnetic Ni nanoparticles anchored on cellulose and its application towards reduction of 4-nitrophenol

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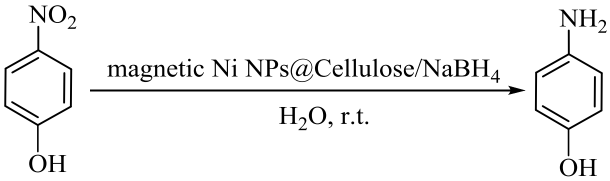
4-nitrophenol (4-NP) is among the most common organic pollutants in industrial and agricultural wastewaters. It can damage the central nervous system, liver, kidney and blood of humans and animals [1]. Thus reduction of 4-NP to nondangerous product, 4-aminophenol (4-AP), is very useful and important in many applications that include analgesic and antipyretic drugs, photographic developers, corrosion inhibitors, anticorrosion lubricants, and so on [2]. 4-NP reduction using metal NPs has recently received much attention [3]. Among various metal nanoparticles, nickel nanoparticles (Ni NPs) have received great attention owing to their high catalytic activity, inexpensive nature, readily preparation, the ability to replace noble metal nanoparticles, and magnetic property which make them to be effective and easily separated from the reaction mixture by use of external magnet [4]. In the current work, we synthesis the magnetic Ni nanoparticles supported on cellulose (magnetic Ni NPs@Cellulose). The prepared nanocomposite was found to be highly efficient catalyst in the reduction of 4-NP to 4-AP with excess amounts of $NaBH_4$ in water at room temperature (Scheme 1). Furthermore, the nanocomposite could be easily separated from the reaction media by an external magnet and reused four times without significant loss of activity.



Scheme 1. *The reduction of 4-NP to 4-AP using magnetic Ni NPs@Cellulose nanocomposite*

Keywords: *Cellulose, Metal nanoparticles, 4-Nitrophenol.*

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Cu-EDA complex anchored onto magnetic cellulose: As an efficient and recyclable nanocatalyst for the reduction of 4-nitrophenol

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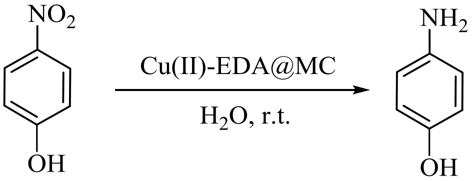
Nitroarene compounds such as 4-nitrophenol (4-NP) are persistent organic contaminants commonly found in various industrial effluents released from pesticides, plasticizers, dyes and pharmaceutical industries [1]. Besides, 4-NP is highly toxic and owing to its mutagenic effects and potential carcinogenicity has been listed as one of the main industrial pollutants by US environmental protection agency [2]. Therefore, it is necessary to find the effective methods to remove this contaminant. In this regard, the catalytic reduction of 4-NP to 4-aminophenol (4-AP) has gained significant interest since it usually occurs in the aqueous phase without the production of by-products, and the product 4-AP is potentially used in the production of analgesic, antipyretic drugs, anticorrosion lubricants. However, this process cannot proceed without catalyst [3]. In this work, the fabrication of a highly efficient magnetically separable nanocatalyst has been reported by immobilizing the Cu(II) over ethylenediamine (EDA) functionalized magnetic cellulose (Cu(II)-EDA@MC) and applied for the reduction of 4-NP by $NaBH_4$ in water at room temperature (Scheme 1).



Scheme 1. *The reduction of 4-NP to 4-AP using Cu(II)-EDA@MC*

Keywords: *Cellulose, 4-Nitrophenol, Water.*

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Urea functionalized magnetic graphene oxide: A novel adsorbent for Cu(II) remediation and study of catalytic activity of the resulting complex in *p*-nitrophenol reduction

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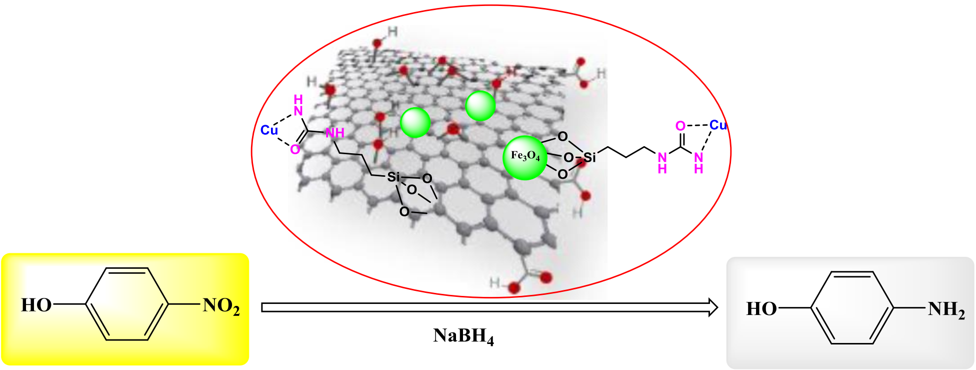
Through the continuous growth of industrialization, water contamination of heavy metals has been a worldwide problem nowadays. Thereinto, copper (Cu(II)) is regarded as one of the important and hazardous inorganic contaminants [1] that can be accumulated in human bodies and cause various diseases [2]. Therefore, it is of great importance to eliminate Cu^{2+} ions from wastewater. So far, many methods have been employed to eliminate Cu^{2+} from wastewater including ion exchange, chemical precipitation, electrochemical separation process, solid phase extraction, membrane separation, and adsorption [3]. Among these methods, the adsorption technique is one of the most preferred methods for its easy operation, high efficiency, and cost-effectiveness [4]. Also, adsorbent is a very important step in the adsorption procedure. In this work, the urea functionalized magnetic graphene oxide (mGO@Urea) was fabricated and examined as a novel adsorbent for the removal of Cu^{2+} ions from aqueous solutions. After the adsorption process, the adsorbent was magnetically separated and applied as an efficient catalyst for the reduction of *p*-nitrophenol with $NaBH_4$ (Scheme 1).



Scheme 1. *Reduction of p-nitrophenol with NaBH4*

Keywords: *Cu^{2+} ions; Magnetic graphene oxide; p-nitrophenol.*

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Photocatalytic degradation of rhodamine B by surface modification of magnetic TiO_2 with copper (II) porphyrin under blue LED light irradiation

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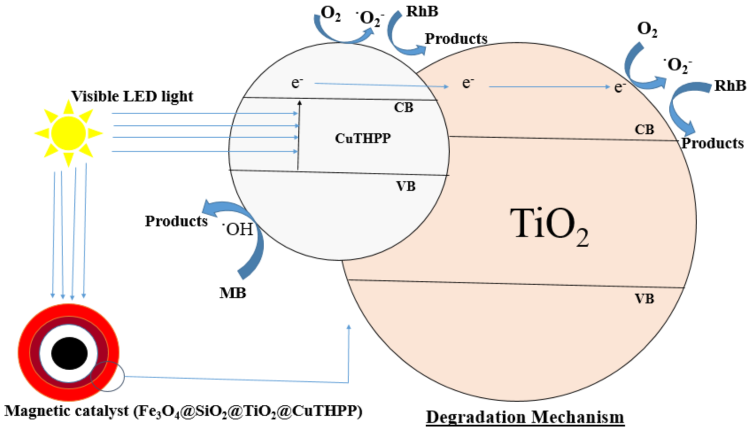
Recently, the degradation of organic pollutant in waste water has drawn much attention. Photodegradation is one of the most ideal methods to solve this problem due to its inexpensive, highly efficient, and environmental friendly [1]. TiO_2 is widely used as photocatalyst in degrading pollutant water because of its nontoxic, insoluble, and inexpensive. Metalloporphyrin derivatives are prominent photosensitizers because their high activity of harvesting visible light. The TiO_2 is successfully sensitized by metalloporphyrin for its visible light photosensitivity and semi-conductivity, which leads to its widely use as photocatalyst [2]. The LED sources have several advantages, such as high electricity to-light yield with minimal heating, their low energy consumption, long lifetime, and small size. An efficient magnetic TiO_2-CuTHPP composite photocatalyst have been obtained by impregnating the CuTHPP onto the surface of TiO_2 at room temperature. The results of SEM, EDS, XRD and FT-IR spectra proved that CuTHPP has combined with TiO_2 successfully and did not change the crystal structure of the TiO_2. Photocatalytic activity of the photocatalyst was evaluated under blue-LED irradiation by the use of rhodamine B dye as a model compound.



Scheme 1. *The proposed mechanism for photocatalytic degradation of rhodamine B on magnetic TiO_2-CuTHPP under blue-LED light irradiation*

Keywords: *TiO2, Rhodamine B, Porphyrin.*

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Electrocatalytic Activity of Vitamin D in the Present N-Hydroxy-N-Phenylacetamide as Electrocatalist

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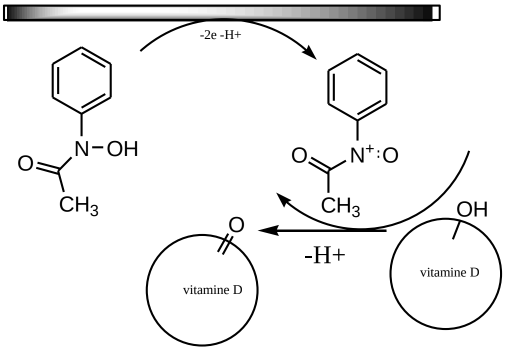
Abstract

Electrocatalytic activities and mechanism of vitamin D in the present N-hydroxy-N-phenylacetamide as electrocatalist have been studied by cyclic voltametry. We performed a complementary study of the electrocatalytic performances of N-hydroxy-N-phenylacetamide using voltammetry as a versatile and informative technique. N-hydroxy-N-phenylacetamide exhibited a good and well-defined electrocatalytic activity in aqueous solution. Investigations of the efficacy of the reaction conditions revealed that the catalytic performance is greatly affected by the pH of the solution—and that there is a fundamental difference in reactivity between these apparently similar systems. New kinetic data were obtained by means of voltammetric analyses and digital simulations of the cyclic voltammograms [1-5].



Scheme. 1 Electrocatalytic oxidation vitamin D

Keywords: *Electrocatalysis; Oxidation; N-hydroxy-N-Phenylacetamide; vitamin D*

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Synthesis, characterization and sonocatalytic degradation of an azo dye on Europium doped CdSe nanoparticles

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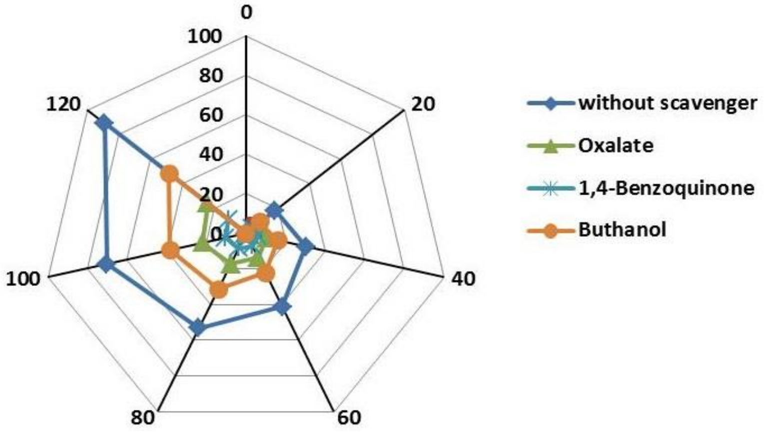
In this study, Eu-doped CdSe nanoparticles with variable Eu^{3+} content were synthesized by a simple sonochemical method. Eu^{3+} substitution into the structure of CdSe resulted in a material with new physical properties, composition and morphology. The synthesized nanoparticles were characterized by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Brunauer–Emmett–Teller (BET) and UV-Vis diffuse reflectance spectroscopy techniques. The sonocatalytic efficiency of pure and $Eu_xCd_{1-x}Se$ samples was evaluated by monitoring the decolorization of RRed 43 in aqueous solution under visible light irradiation. The BET specific surface area and pore volume of me/soporous europium doped CdSe greatly exceeds in comparison to undoped CdSe samples. Among the different amounts of dopant, 8% Eu-doped CdSe showed the highest sonocatalytic activity. The effects of various parameters such as initial dye concentration, catalyst loading, ultrasonic power, and the presence of radical scavengers were investigated. The addition of benzoquinone (BQ) results in remarkably inhibited degradation and the addition of ammonium oxalate reduced the removal percentage to 24%. Superoxide radicals and photogenerated holes were detected as the main oxidative spices. As a consequence, the Eu-doped CdSe materials have potential applications as an efficient catalyst in wastewater treatment.



Scheme 1. *Effect of different scavengers on decolorization of Reactive Red43, [Dye] = 20 mg/L, [Catalyst] = 1 g/L, [Scavengre] = 5 mM*

Keywords: *Europium, Sonocatalytic degradation, Nanomaterials.*

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Evaluation of catalytic properties of two new Fluorinated Metal-Organic Frameworks (F-MOFs) Generated by Mechanosynthesis

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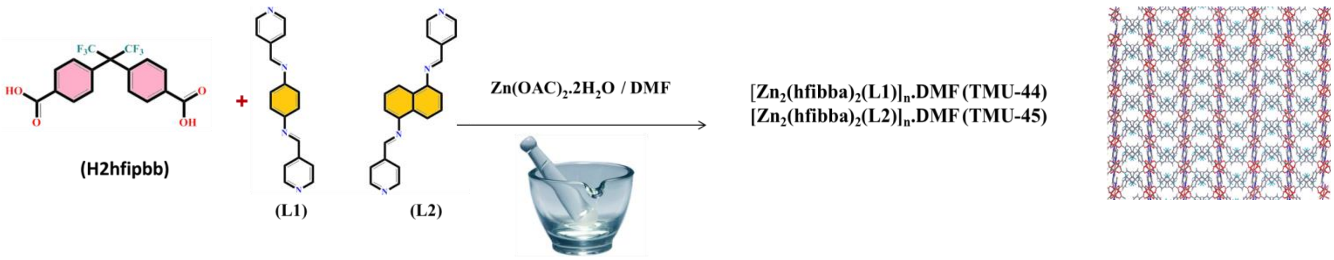
Two new fluorinated metal−organic frameworks (F-MOFs), namely, $[Zn_2(hfibba)_2(L1)]_n$.DMF (TMU-44) and $[Zn_2(hfibba)_2(L2)]_n$.DMF (TMU-45) were successfully synthesized by the mechanochemical method. These isoreticular MOFs have been characterized by different spectroscopic techniques such as FT-IR spectroscopy, powder X-ray diffraction (PXRD) and thermal gravimetric analysis (TGA).

The catalytic activity of these isoreticular F-MOFs as efficient heterogeneous catalysts toward Henry reaction was tested and compared to each other. TMU-44 and TMU-45 exhibited good catalytic activity in methanol media with excellent conversions. These catalysts maintain their crystalline frameworks after the reaction and are easily recovered and reused at least three cycles without significant loss in their catalytic activity and the conversion of benzaldehyde can be kept over 95%.



Scheme 1. *Chemical structure of the H_2hfipbb, L1, and L2 ligands used for the construction of Fluorinated Metal-Organic Frameworks*

Keywords: *Heterogeneous catalyst, F-MOFs, Henry reaction, Mechanosynthesis.*

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Green synthesis of nano zinc ferrite using chicken feet extract and its use as catalyst for the synthesis of 1,3,5-triaryl-4,5-dihydro-1*H*-pyrazoles

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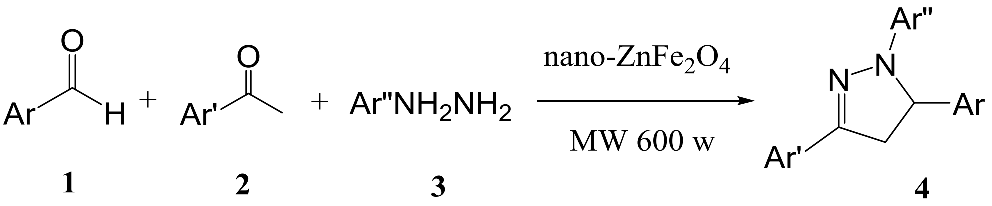
Zinc ferrite type of magnetic nanoparticles (MNPs) could catalyze organic reactions in a mild and environment friendly manner [1-3]. This work described a green and useful method for the preparation of $ZnFe_2O_4$ nanoparticles using chicken feet extract. This nano particles used as an efficient nanocatalyst for the synthesis of 1,3,5-triaryl-4,5-dihydro-1*H*-pyrazoles. The synthesis was carried out *via* a simple three-component reaction between arylaldehydes, arylmethylketones, and arylhydrazines in good to excellent yields in the precense of nano $ZnFe_2O_4$ in solvent-free conditions (Scheme 1).

General procedure for the synthesis of 1,3,5-triaryl-1*H*-pyrazoles **4a**. The reaction was carried out by first mixing benzaldehyde **1** (1 mmol, 0.106 g), acetophenon **2** (1 mmol, 0.120 g), and NaOH (1 mmol, 0.040 g) in the presence of $ZnFe_2O_4$ magnetic nanoparticles (0.010 mmol, 0.002 g), then phenylhydrazine **3** (1 mmol, 108 g) added to the reaction mixture. After then heating them under microwave irradiation at 600 watts for 1 minute in solvent-free condition. Reaction monitoring by TLC clearly indicated formation of the corresponding 1,3,5-triphenyl-4,5-dihydro-1*H*-pyrazole **4a**. Then ethanol (3 mL) was added to the reaction mixture and then $ZnFe_2O_4$ magnetic nanoparticles were separated by a magnet. After that, the product was separated as a light yellow crystalin solution. The solvent was removed and the product was recrystallized from ethanol. The isolated yield was 90%..

In conclusion, We have developed a simple and green method for the synthesis of 1,3,5-triphenyl-4,5-dihydro-1*H*-pyrazoles in the presence of $ZnFe_2O_4$ magnetic nanoparticles under microwave irradiation and Solvent-free conditions. Short reaction times, excellent yields of products, and mild reaction conditions, inexpensive and readily available starting chemicals and catalyst, Eco friendly, use of simple chemicals, and high atomic economy are the main advantages of this method.



Scheme 1. *Three-component synthesis of 1,3,5-triphenyl-4,5-dihydro-1H-pyrazole* ***4*** *using* $ZnFe_2O_4$ *magnetic nanoparticles under solvent-free and microwave irradiation conditions.*

Keywords: *Nano* $ZnFe_2O_4$*, Microwave, chicken feet extract, Solvent-free.*

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Efficient synthesis of $ZnFe_2O_4$ nanoparticles using grape juice and its use as catalyst for the synthesis of methylenebisamides

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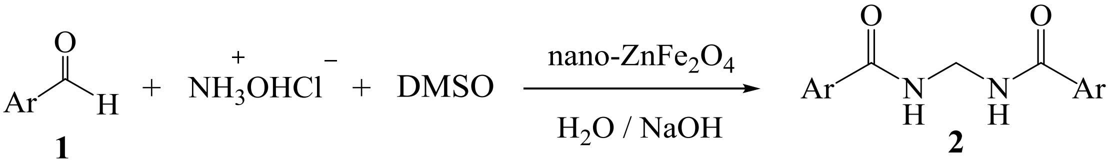
Nano zinc ferrite type of magnetic nanoparticles (MNPs) could catalyze organic reactions in a mild and environment friendly manner [1-3]. This work described a green and useful method for the preparation of $ZnFe_2O_4$ nanoparticles using chicken feet extract. This nano particles used as an efficient nanocatalyst for the synthesis of 1,3,5-triaryl-4,5-dihydro-1*H*-pyrazoles. The synthesis was carried out *via* a simple three-component reaction between arylaldehydes, arylmethylketones, and arylhydrazines in good to excellent yields in the precense of nano $ZnFe_2O_4$ in solvent-free conditions (Scheme 1).

The reaction were carried out by first mixing benzaldehyde **1a** (1 mmol), hydroxylamine hydrochloride (1 mmol), sodium hydroxide (1 mmol), nano $ZnFe_2O_4$ (0.15 mmol) (Nano zinc ferrite were synthesis via sol gel method using grape juice) and DMSO 3mL in 5 mL water as a one-pot reaction. Then the reaction mixture was stirred at 80 °C for 1 hour. The TLC monitoring of the reaction mixture clearly indicated the formation of *N,N'*-methylenedibenzamide **2a** in excellent yield. Afterward the residue was filtered and recrystallized in ethanol and then the product **2a** was obtained. In conclusion, we have developed a practical, simple and efficient reaction for the synthesis of bisamides using nano zinc ferrite. The method has several advantages, including high yields of products, easy experimental work-up, and use of simple and available starting materials, high atom economy, eco-friendly and mild reaction conditions without the use of any catalyst and organic solvents.



Scheme 1. *Multi component synthesis of methylenebisamides**2***

Keywords: *Nano $ZnFe_2O_4$, Methylenebisamides, Grape juice, Green.*

References

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Ru nanoparticles supported on magnetic porous carbon and their photocatalytic activity in organic reactions

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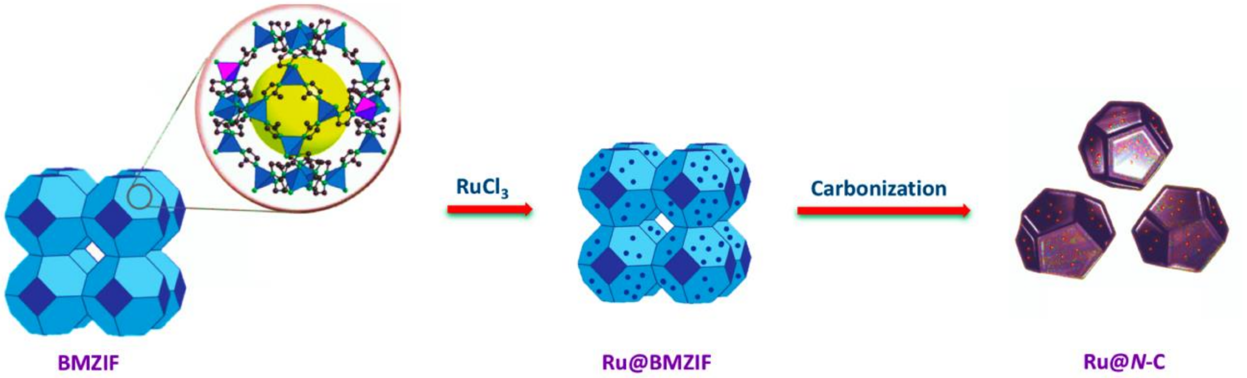
A novel nitrogen doped carbon photocatalyst was successfully prepared from the carbonization of ruthenium on/in bimetallic zeolitic imidazolate framework (BMZIF) hybrid. The weight percent 1% and 5% of Ru@*N*-C showed low photocatalytic activity in the reduction of *p*-nitrophenol, while the weight ratio 2.5% demonstrated the high photocatalytic activity. Carbonized catalysts derived from either Ru@ZIF-67 or Ru@ZIF-8 exhibit poor activity.



Scheme 1. *Schematic illustration of the formation procedure of Ru@N-C*

Keywords: *Photocatalyst, Reduction, Ruthenium, Zeolitic imidazolate framework, Carbonization*

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One-pot solvent-free synthesis of pyrido[2,3-d:6,5-d′]-dipyrimidines catalyzed by $MgFe_2O_4$ magnetic nanoparticles under microwave irradiation

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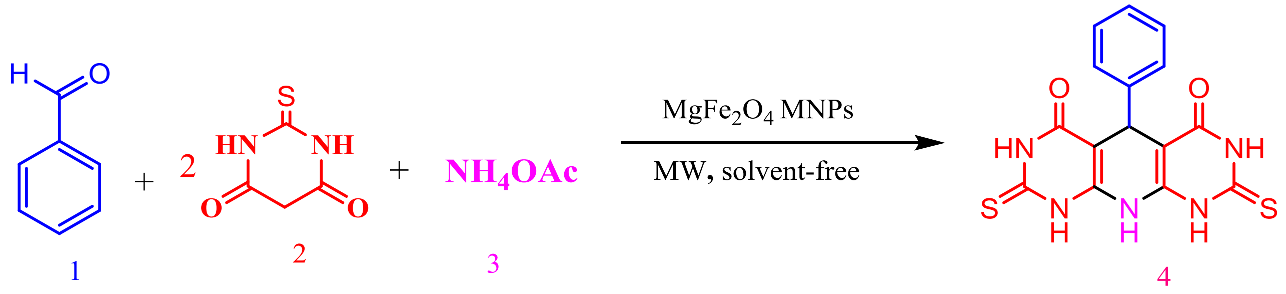
The development of multi-component reactions (MCRs) to produce biologically active compounds has become an important area of research in organic, combinatorial, and medicinal chemistry. MCRs leading attractive heterocyclic scaffolds are particularly useful for the creation of diverse chemical libraries of “drug-like” molecules, because, the combination of three or more small-molecular-weight building blocks in a single operation leads to high combinatorial efficacy in creating diversity [1].
The pyridopyrimidine scaffold is extensively described as heterocycles in many natural and synthetic biologically active compounds, as well as in different drug discovery programs. The properties of pyridopyrimidine depend on the position of the nitrogen atom in the fused ring scaffold. Pyrido[2,3-d:6,5-d′]pyrimidines occupy a special place in four possible isomeric structures and their structure has been the subject of medical research, because this scaffold is associated with a wide range of pharmacological properties and biological activities, such as dihydrofolate reductase inhibitory activity, antimicrobial activity, antitumor activity, anti-inflammatory, tyrosine kinase inhibition, calcium channel antagonists and fibroblast growth factor receptor inhibition. Some of the pharmaceutically important compounds containing pyrido[2,3-d]pyrimidine nucleus such as adenosine kinase inhibitor (I) and cyclin-dependent kinase inhibitors (II) [2-5].
In this project, a facile one-pot and four-component economical synthesis of pyrido[2,3-d:6,5-d]dipyrimidines using aldehyde, 2-thiobarbituric acid and ammonium acetate in the presence of $MgFe_2O_4$ NPs as magnetically heterogeneous catalyst in solvent free conditions under microwave irradiation is described. The current synthesis displays attractive characteristics such as; the use of magnetically recoverable and reusable catalyst, convenient one-pot operation, short reaction periods, high to excellent yields, solvent free conditions and is considered to be relatively environmentally benign.



Scheme 1. *Synthesis of pyrido[2,3-d:6,5-d']dipyrimidine derivatives*

Keywords: *Green synthesis, Solvent-free, Thiobarbituric acid, $MgFe_2O_4$ nanoparticles*

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Biosynthesis of lanthanum oxychloride nanoparticles as a photocatalyst

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Lanthanide compound nanostructures such as oxides and hydroxides, lanthanum oxyfluoride, fluorides, and phosphates have received broad attention because of their outstanding magnetic, catalytical and optical properties arising from the 4f electron configuration of the lanthanides [1,2]. Among these materials lanthanum oxychloride (LaOCl) is of great interest because of their attractive properties and tremendous applications such as catalyst supports, luminescent materials, conversion of alkanes to alkyl chlorides, gas sensors and can be doped with rare-earth ions for special applications, such as bioimaging probes [3]. In addition, LaOCl is known for the high chemical stability, nontoxicity, the low maximum phonon cutoff energy, and ability to promote efficient phonon energy transfer (ET) to dopant ions, which are originated from the low phonon vibrational energy and high ionicity of the bond between rare earth and chlorine [4,5].

In this study, LaOCl nanoparticles of tetragonal structure were successfully synthesized by a facile sol-gel method using tragacanth gel. This method has many benefit such as nontoxic, economic viability, ease to scale up, less time consuming and environmental friendly method for the synthesis of LaOCl nanoparticles without using any organic chemicals. The sample was investigated by energy dispersive X-ray analysis (EDX), powder X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), Fourier transforms infrared spectroscopy (FTIR). In addition, the photocatalytic degradation activity of LaOCl nanoparticles were evaluated using reactive blue 21 dye as organic contaminant irradiated only with visible light from fluorescent lamp. Catalytic reactions were monitored by using UV–Vis spectrophotometer.

Keywords: *LaOCl nanoparticles, Biosynthesis, degradation of dye.*

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Synthesis of fatty acid derivatives of curcumin as new lipophilic prodrugs

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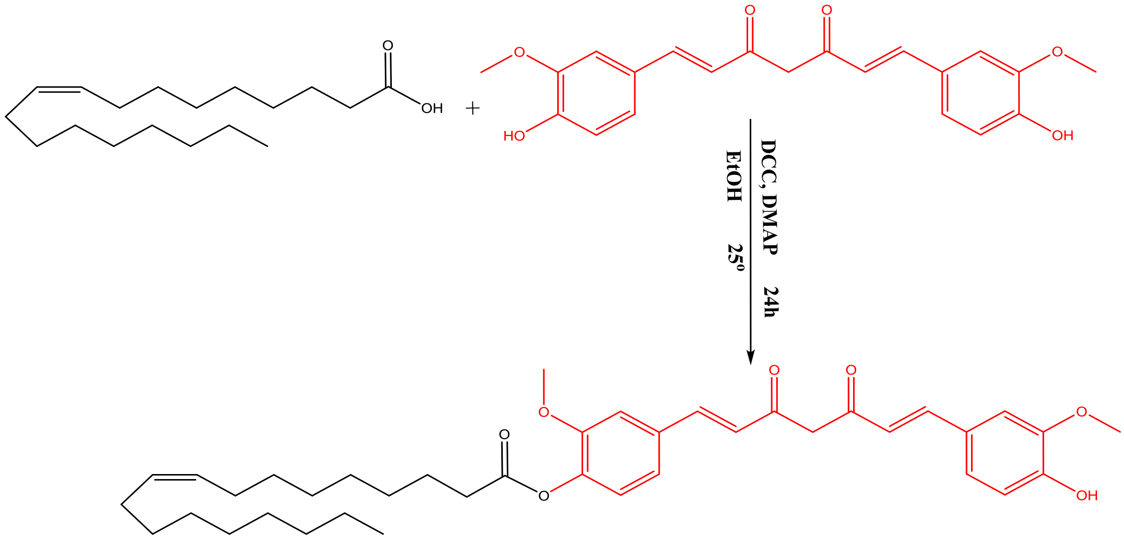
Today, the use of lipophilic prodrugs is one of the important issues in drug delivery. Lipophilic prodrugs can have an important role in improving bioavailability, passing biological membranes, Facilitating drug transfer, targeting drugs and treatment of cancer. The ultimate goal in prodrugs design is to overcome the different limitations of drugs, and access to pharmacokinetics of drugs. Curcumin, which is derived from Curcuma longa, has a wide range of therapeutic activities, such as anti-tumor activity, antioxidant. The purpose of this study was to design and produce lipophilic curcumin prodrug based on Oleic acid. A mixture of Oleic acid, DCC and catalytic amount of 4-dimethylaminopyridine (DMAP) in ethanol as a solvent, then (0.5 mmol) of curcumin was added at room temperature under magnetic stirring conditions until the reaction was complete. Eventually, the N, N–dicyclohexylurea was filtered off and the solvent was removed under reduced pressure to give the product which was chromatographed over a column of silica gel using methanol as eluent. In this study, a lipophilic curcumin prodrug was synthesized during the esterification reaction between the carboxylic acid of Oleic acid and the hydroxyl groups of curcumin. The synthesized prodrug was characterized using IR, ^{1}H-NMR and ^{13}C-NMR spectroscopy. An appropriate method for esterification reactions of curcumin and Oleic acid was developed. Derivatives lipophilic prodrug curcumin were successfully synthesized in order to improve the bioavailability and also characterized the compound structures [1-3].



Scheme 1. *Synthesis of derivatives lipophilic Prodrug curcumin*

Keywords: *Prodrug, Curcumin, Conjugation, lipophilic*

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Green synthesis of 1,2,4-triazole-3-thione derivatives in natural deep eutectic solvents

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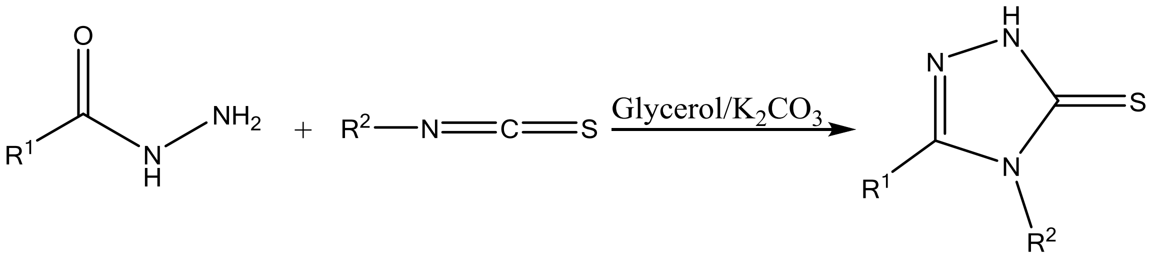
Heterocyclic compounds containing heteroatoms N, S and O represents important place in medical chemistry. Triazole ring is present in many natural products and biologically active compounds. For example, triazole derivatives were considered as antifungal and antiviral agants [1,2].

Deep eutectic solvents play an essential key in green chemistry. They are nontoxic, reusable, eco-friendly and environmentally organic compounds. Deep eutectic solvents act as catalysts in many reactions [3].

In this project, various hydrazide derivatives were reacted with alkyl or aryl isothiocyanates under optimized conditions in a deep eutectic solvents including glycerol-potassium carbonate to afford novel 1,2,4-triazole-3-thione derivatives (scheme. 1). The progress of the reaction was checked by TLC. The chemical structures of all compounds were confirmed by IR and ^{1}H NMR and ^{13}C NMR spectral data. Simple work-up, mild reaction conditions, short reaction times, use of a green eutectic solvent, and excellent product yields are advantages of this method.



Scheme 1. *Synthesis of 1,2,4-triazole-3-thione derivatives*

Keywords: *Deep eutectic solvents, Green synthesis, 1,2,4-triazole-3-thione derivatives.*

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Green synthesis of $CoFe_2O_4$ nanoparticles using *H.rawanium* and their use as a green catalyst for the synthesis of polyhydroquinoline derivatives

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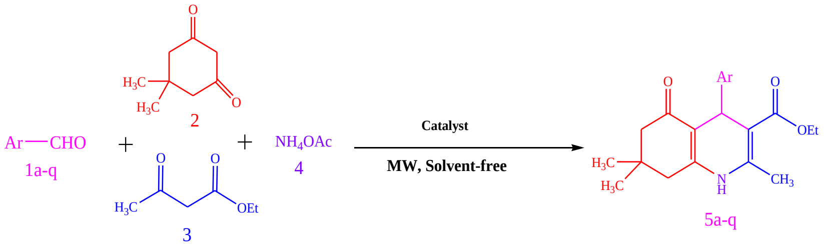
Here we represent green and efficient synthesis of $CoFe_2O_4$ nanoparticles (NPs) [1] by *Heracleum rawanium* fruit extract as non-toxic reducing agent and stabilizer without adding any surfactant. The extraction of fruit of this plant with water is described by maceration. The natural products found in plants have an important role in synthesis of nanoparticles [2,3]. FT-IR spectroscopy, X-ray diffraction (XRD) pattern and field emission scanning electron microscopy (FESEM) have been used in the characterization of the nanoparticles thus prepared. The results showing that MNPs synthesized by *H.rawanium* extract have high purity and the average particle size is 33 nm. In addition, Cobalt ferrite nanoparticles as an efficient catalyst were used for the synthesis of polyhydroquinoline derivatives via multi-component reactions under microwave irradiation. This method have several advantages such as short reaction time, excellent products yields (86-94), simple work and use of recoverable catalyst.



Scheme 1. *Synthesis of polyhydroquinoline derivatives*

Keywords: *Cobalt ferrite, Polyhydroquinoline, Microwave Irradiation*

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An efficient and green one-pot synthesis of 6-Amino-5cyano-4-phenyl-2-mercapto pyrimidine via three-component reaction of aldehyde ،malononitrile and urea using $CoAl_2O_4$ nanoparticles as catalyst

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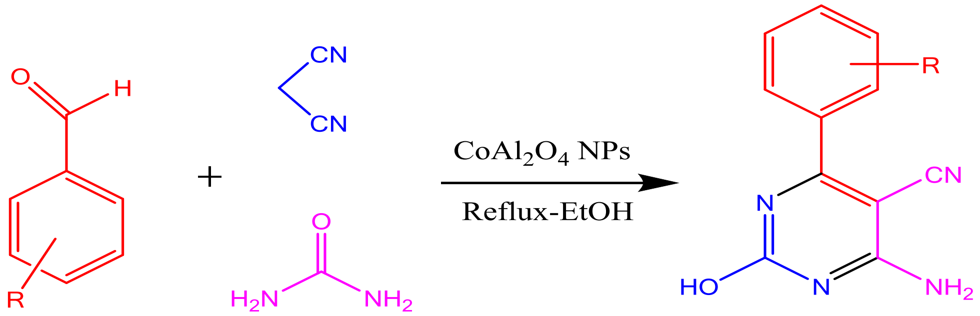
Heterocyclic molecules are of biological interest due to their potential physical and chemical properties. Among these the pyrimidine compounds occupy a unique position in pharmaceutical chemistry, as they are components of nucleic acids. The important pyrimidine compounds have diverse applications as bactericidal, fungicidal, analgesics, anti-inflammatory and anti-tumor agents [1,2]. Nowadays, the one step methods involving three component condensation using different reagents and catalysts are popular in synthetic organic chemistry for the synthesis of heterocyclic compounds. These single step methods are more convenient as compared with two step strategies as they require shorter reaction times, product isolation easy and give higher yields and recoveries of the product [3].

As part of our interest in the synthesis of heterocyclic compounds and green chemistry, we report a simple mild and high efficient procedure for one pot three component synthesis of 6-Amino-5cyano-4-phenyl-2-mercapto pyrimidine derivatives. The reaction was performed in ethanol using aryl aldehyde ،malononitrile and urea in the presence of $CoAl_2O_4$ NPs as a green high efficient catalyst (Scheme 1). Operational simplicity, use of readily available and safe reagents, easy work-up and high yields are some of the positive attributes of this method.



Scheme 1. *Synthesis of 6-Amino-5cyano-4-phenyl-2-mercapto pyrimidine*

Keywords: *$CoAl_2O_4$ nanoparticles, Pyrimidine derivatives, Three-component reaction.*

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Green synthesis of $NiFe_2O_4$@a-Al_2O_3 nanoparticles as a magnetically separable photocatalyst for the degradation of organic dye

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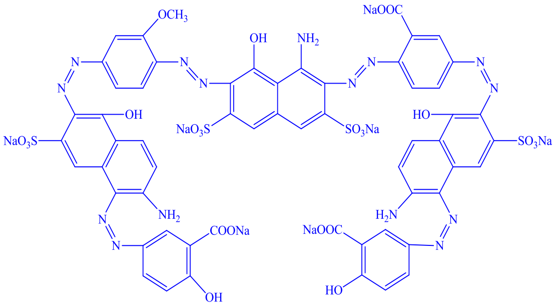
Over the past decades, nanoparticles have attracted much attention owing to their lately discovered characteristics and extensive usage in a variety of fields such as in sensors, catalysis, recording heads, and magnetic drug delivery [1,2].
In the present study, a sol-gel procedure has been applied for the synthesis of $NiFe_2O_4$@a-Al_2O_3 nanoparticles using tragacanth gel which is eco-friendly, inexpensive, cost effective, and simple. The photocatalytic efficiency of $NiFe_2O_4$@a-Al_2O_3 MNPs has been assessed for direct black 122 (DB122) dye degradation as an environment polluting model under visible light irradiation. The structure and characterization of DB122 dye are presented in Table 1.

Table 1 *The chemical structure and characteristics of DB122*

Molecular Structure	Multi-azo class
Molecular Formula	$C_{58}H_{34}N_{15}Na_7O_{24}S_4$
Molecular Weight	1614.17 g/mol
CAS Registry Number	16894-32-9
λ_{max}	519 nm
Structure	

$NiFe_2O_4$@a-Al_2O_3 magnetic nanoparticles was characterized using Fourier transform infrared spectroscopy (FTIR), X-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM), and vibrating sample magnetometer (VSM). XRD result demonstrated the formation of single phase cubic spinel structure. The photocatalytic activity of catalyst was measured with changing factors including photocatalyst dosage, initial dye concentration, and contact time. The results presented that $NiFe_2O_4$@a-Al_2O_3 MNPs could degrade 94% of the DB122.

Keywords: *nanoparticles, photocatalyst, degradation.*

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Green synthesis of $La_2O_2CO_3$ nanoparticles using tragacanth gel and its use as photocatalyst in the degradation of Black WNN dye

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Lanthanum oxide is used to make optical glasses, which increases their density, refractive index, and hardness. In combination with oxides of tungsten, tantalum, and thorium, La_2O_3 improves the resistance of the glass against alkali compounds and is known as one of the ingredients for production of piezoelectric and thermoelectric materials. It is also used as a catalyst for the oxidative coupling of methane. Owing to its excellent physical and chemical properties, $La(OH)_3$ has been extensively used as high-potential oxide ceramic, hydrogen storage materials, superconductive materials and, etc. Until quite recently, the catalytic and sorbet properties of $La(OH)_3$ have been concerned intensively for their potential applications. Different metal oxides, hydroxides and carbonates were examined as photocatalysts for wastewater treatment. The effluents of textile and dye industries are the main pollutants in wastewater. This causes serious environmental problems such as increase of toxicity of environment, chemical oxygen demand (COD), biochemical oxygen demand (BOD), bad smell, and color of the wastewater. The colored organic dyes are heavily polluted the water system. The complete remediation of these dyes into less harmful chemicals is required to overcome these problems. Among various dye remediation process, the heterogeneous photocatalytic process is well known method for the decomposition of hazardous waste materials especially organic compounds into less harmful chemicals [1-4].

The use of natural gel is generating interest of researchers toward cost effective, nontoxic, economic viability and eco-friendly green synthesis of nanoparticles. In this work, lanthanum oxy-carbonate nanoparticles were synthesized using tragacanth gel as biotemplate by the sol–gel method without using any organic chemicals. The sample was characterized by powder X-ray diffraction, fourier transform infrared spectroscopy and scanning electron microscopy. Thereupon, $La_2O_2CO_3$ NPs as an efficient photocatalyst was used for the degradation of Black WNN dye under visible light irradiation. The results display that the catalyst could remove *ca.* 90% of the Black WNN dye. The effects of initial dye concentration, photocatalyst dose, and visible light irradiation on dye degradation were evaluated.

Keywords: *lanthanum oxy-carbonate nanoparticles, Black WNN dye, Photocatalysis.*

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Biocatalytic Application of Immobilized Laccase on Epoxy-Functionalized Silica in Biodegradation of Phenolic Compounds

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A novel method of laccase immobilization on epoxy-functionalized silica particles was developed. Laccase from *Myceliophthora thermophila* was covalently immobilized onto epoxy-functionalized matrix by nucleophilic attack of amino groups of laccase to epoxy groups of the support. The enzyme loading on the support was about 30 mg/g under the optimum conditions (pH 4.5, 24 h).

The effect of pH, temperature and organic solvent on immobilized enzyme activity was determined and compared with those of free enzyme. In general the immobilized enzyme was found to be stabilized compared to the free enzyme. Lineweaver-Burk plots were used to calculate kineticparameters for ABTS oxidation. K_M values were 24.0 and 25.3 μM while v_{max} values were 10.0 and 1.6 μM min_{-1} for free and immobilized laccase, respectively. The performance of the biocatalyst was evaluated by the degradation of phenolic compounds including phenol, *p*chlorophenol and catechol. The removal efficiency of catechol by immobilized laccase was about 95% after 2 h.

Keywords: *Laccase, Immobilization, Phenol biodegradation.*

Preparation of Biocatalyst by Immobilization of Eversa on Chitosan Beads for Production of Biodiesel from Palm Oil

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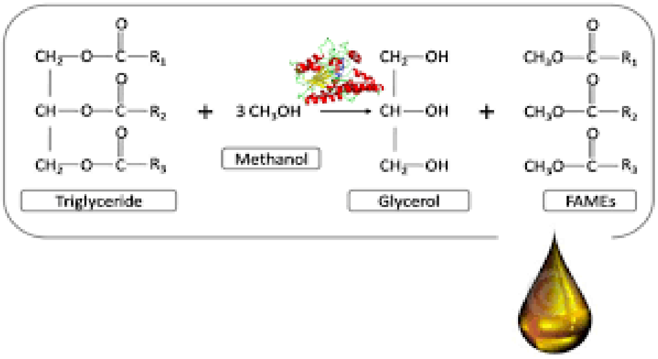
Biodiesels or fatty acid methyl esters (FAMEs), which are derived from triglycerides by trans-esterification with methanol, have attracted considerable attention during the past decade as a renewable, biodegradable, and nontoxic fuels [1]. Enzymatic production of biodiesel has been considered a promising alternative since the early 1990s in the scientific community. Recently, however, this potential can been realized with the official launches of Novozymes Eversa Transform in Dec 2014, followed by the more thermostable enzyme, Eversa Transform 2.0 in May 2016. Eversa Transform 2.0 (Genetically modified *Aspergillus oryzae* lipase) is a free liquid lipase, with properties developed for the specific use in biodiesel application [2]. In this study, enzymatic production of biodiesel was performed from reaction of palm oil and methanol by using immobilized Eversa (as a biocatalyst) on chitosan beads by three component reaction. Chitosan, a deacetylated form of chitin, is one of the natural polymers which was used in bead shape as support. The Eversa loading on the support was about 231 mg/g under the optimum conditions (pH 7, 24 h). Also it was found, *t*-butanol as a co-solvent was affected on reaction yield. The influences of six principal variables, molar ratio of methanol to oil, weight percent of biocatalyst to oil, *t*-butanol to oil, temperature and time of reaction, on the yield of biodiesel reaction were investigated. Finally the optimum condition was found at 3:1, 19.5%, 10% (w/w), 50ºC and 48 hours respectively.



Scheme 1. *Synthesis of Biodiesels (FAMEs)*

Keywords: *Biodiesel, trans-Esterification, Palm oil, Eversa, Chitosan beads, Ugi reaction.*

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Synthesis, spectroscopic characterization and catalytic activity of UO_2 with a tridentate Schiff base ligand

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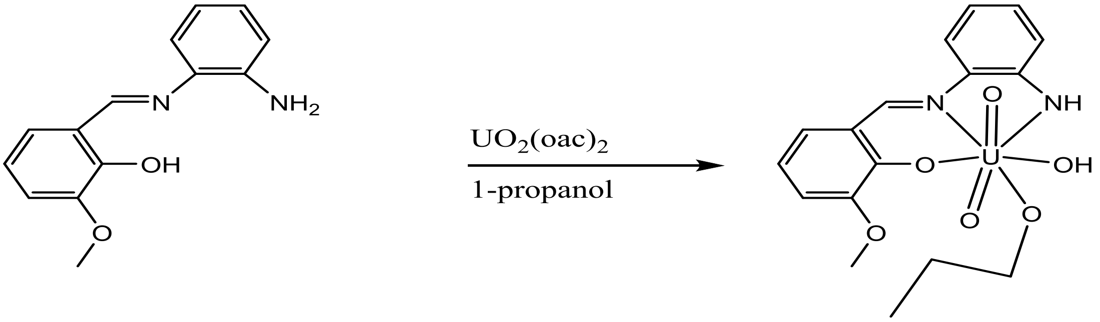
Schiff base and related complexes cover a wide range of application in catalytic fields and they are great research interest. Due to the formation of stable complexes with transition metal ions and participation of azomethine linkage in the chelation process, Schiff bases are considered as a model compound and play active role in the development of coordination chemistry [1]. Schiff base complexes possess high stability in different oxidation states resulting in a wide range of application for these complexes, such as bio catalytic [2] and catalytic activities [3].

A tridentate Schiff base ligand, (E)-2-(((2-aminophenyl)imino)methyl)-6-methoxyphenol (H_2L), and its uranyl(VI) complex [UO_2(L)(PrOH)], have been synthesized and characterized using physicochemical and spectroscopic methods such as molar conductivity, elemental analysis, ^{1}HNMR, UV-Vis and FT-IR. The prepared compound was also screened for catalytic activities. The catalytic activities were investigated on the multicomponent reactions of malononitrile and aromatic aldehydes.



Scheme 1. *Synthesis of [UO2(L)(PrOH)]*

Key words**:** *Schiff base complex. Catalytic activates, .X ray crystallography*

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Metalloporphyrin as Effective Catalysts for the Aerial Oxidation of Bisnaphthols to Spirodienones

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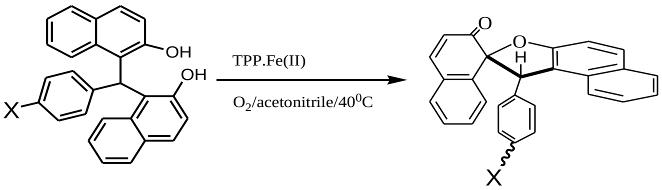
Porphyrins are cyclic ligands composed of four pyrrole units connected through CH bridges. Porphyrines and Metalloporphyrins are found in important biological systems, for example porphyrin is the basic building block of hemoglobin and myoglobin (an oxygen molecules carrier in blood) called heme. The Metal cation of heme is Fe^{2+} to which oxygen molecule is attached. Porphyrins and metalloporphyrins are also used as effective catalysts in a number of chemical and photochemical process (such as PDT).[1] Porphyrins and metalloporphyrins[2] have been prepared in our laboratory by refluxing pyrrole and benzaldehyde in the presence of concentrated HCl and *N*-hydroxyphthalimide in dimethylformamide. NMR data confirm the structure of these compounds. The synthesized metalloporphyrins were then used as effective catalysts for the aerial oxidation of bisnaphthols to spirodienones Scheme 1. The latter compounds are obtained in two diasteromeric forms which are easily characterized by their NMR spectral data. Reaction times, yields and melting points of all products are shown in Table 1.



1, X= H
1a, X= 4-$CH_3C_6H_4$
1b, X= 4-ClC_6H_4
1c, X= 3 -$OCH_3C_6H_4$
1d, X= 2 -$OCH_3C_6H_4$
1e, X= 4 -$OCH_3C_6H_4$
1f, X= 2 -ClC_6H_4

2, X= H
3a, X= 4-$CH_3C_6H_4$
3b, X= 4-ClC_6H_4
3c, X= 3 -$OCH_3C_6H_4$
3d, X= 2 -$OCH_3C_6H_4$
3e, X= 4 -$OCH_3C_6H_4$
3f, X= 2 -ClC_6H_4

Scheme 1. *Aerial oxidation of 1 mmol 4-methylphenyl bisnaphthole*

Table 1*. Reaction time, yield and melting point of product*

Entry	Product	Time (h)	Yield (%)[a]	M.P. °C
1	2	4	68	171-172
2	3a	4	71	210-211
3	3b	4	60	264-265
4	3c	4.5	68	200-202
5	3d	4.5	64	194-196
6	3e	4.45	58	187-189
7	3f	4.5	56	215-218

[a] Total yield (isomer **3**+ isomer **4**)

Keywords: *Metalloprphyrin, Bisnaphtol, Oxidation.*

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Synthesis of Cu (II) Schiff base complex as a recyclable and highly efficient catalyst for one pot three component synthesis of tetrahydro-4H-chromenes

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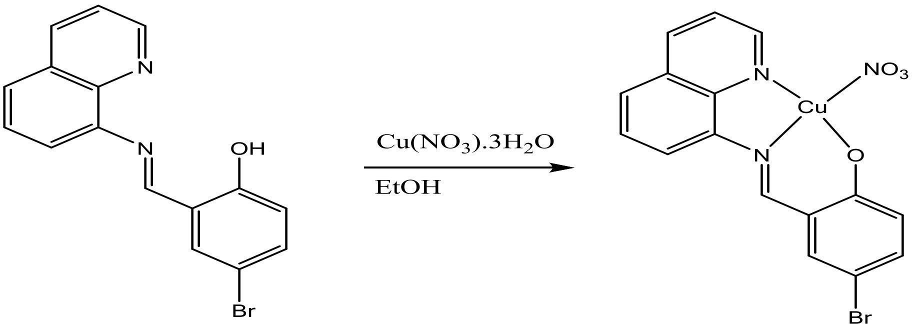
Schiff base ligands can bind to metal ions as chelating ligands and form metal complexes with interesting properties. These Schiff bases normally bind to metal ions via the azomethine nitrogen. [1] Schiff base complexes especially Copper (II) complexes have shown excellent catalytic activity in different reactions. [2]

A tridentate Schiff base ligand, 4-bromo-2-((quinolin-8-ylimino) methyl) phenol (HL), and its Cu (II) complex [Cu(L)(NO3)], have been synthesized and characterized by elemental analyses, FT-IR, molar conductivity, UV–Vis spectroscopy. The structure of catalyst has been accomplished by single crystal X-ray diffraction. The coordination geometry around the copper (II) ion in the mononuclear species is four coordinated square planar with one oxygen and two nitrogen atom from the tridentate ligand. The prepared compound was also screened for catalytic activities.

the catalytic activities of this complex have been investigated on the electrophilic reaction of malononitrile along with aldehydes, ethyl acetoacetate and dimedone in ethanol solution in order to tetrahydro-4H-chromenes, respectively. [3]



***Scheme1**. Synthesis of [Cu(L)(NO3)]*

***Keywords**: Cu (II) Schiff base complex, catalytic activity, tetrahydro-4H-chromenes*

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Photocatalytic degradation of direct blue 129 dye in the presence of nanostructured zinc chromite

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A large variety of spinel-type families has been extensively studied, as to which the correlation between the substitute ions and the physical properties of the final compound has been reported. These materials are very attractive in both scientific and technological importance. Since the transport properties of this type of spinel vary when it comes into contact with gaseous atmospheres, it has been utilized as the basis for sensing devices, particularly in the regard to humidity [1]. The ability to obtain single-phase $ZnCr_2O_4$ nanoparticles with controllable particle size and size distribution improves its adequacy in an extensive range of innovative technological application. In order to obtain single-phase $ZnCr_2O_4$ with the appropriate physical and chemical properties, its synthesis via different methods has become an important area of research and development [2].

$ZnCr_2O_4$ crystallizes in the cubic system and has a normal spinel structure. In this mixed oxide $ZnCr_2O_4$ nonmagnetic Zn^{2+} and magnetic Cr^{3+} ions have a strong preference for the tetrahedral A-sites and the octahedral B-sites, respectively. It is a geometrically frustrated antiferromagnet with a first order transition at 12.5 K from paramagnetic phase with cubic structure to antiferromagnetic phase with tetragonal structure. The nanocrystalline $ZnCr_2O_4$ spinel has many applications, e.g., as catalysts, sensors for toxic gases and semiconductors. $ZnCr_2O_4$ is also very attractive as air depollution catalytic material, for a variety of reactions like oxidation of hydrocarbons, oxidative dehydrogenation of hydrocarbons, synthesis of methanol, as gas sensing, humidity sensing and photocatalyst [3-5]. In this work, zinc chromite nanostructures have been synthesized through sol-gel method. The synthesized products were characterized by field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), fourier transform infrared (FT-IR) spectra and X-ray energy dispersive spectroscopy (EDS). The X-ray powder diffraction (XRD) confirmed the formation of cubic spinel phase $ZnCr_2O_4$. The photocatalytic activity of $ZnCr_2O_4$ nanoparticles was confirmed by degradation of direct blue 129 under visible light irradiation. The effects of process parameters like, catalyst dosage, initial dye concentration, and visible light irradiation on dye degradation have been investigated.

Keywords: *Zinc chromite, Photocatalyst, Visible light irradiation*

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Solvent free one-pot multi-component synthesis of 3,4-dihydropyrimidin-2(1*H*)-ones catalyzed by $ZnFe_2O_4$ magnetic nanoparticles as an environmentally friendly, cheap, and effective catalyst

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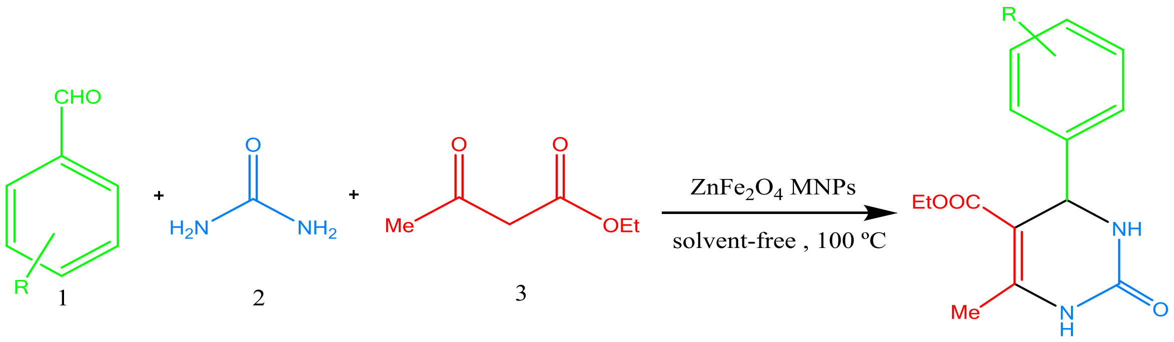
Recently, interest in the synthesis of 3,4-dihydropyrimidin-2-(1H)-ones (Biginelli compounds) and their derivatives has increased tremendously because of their diverse therapeutic and pharmacological properties such as antiviral, antibacterial, antitumour and antihypertensive activities. Some have been successfully used as calcium channel blockers, α-1a-antagonists and neuropeptide Y (NPY) antagonists. Several alkaloids which contain the dihydropyrimidine core unit have been isolated from marine sources. Most notable among these are the batzelladine alkaloids, which were found to be potent HIV gp-120-CD4 inhibitors. The Biginelli reaction is considered as an important multi-component reaction for generating compounds with diverse medicinal applications [1-3].

In the present work, a green and efficient method is described for the solvent free synthesis of 3,4-dihydropyrimidin-2(1H)-ones through one-pot three-component condensation of ethyl acetoacetate, an aryl aldehyde, and urea in the presence of $ZnFe_2O_4$ nanoparticles as high-performance magnetic catalyst (scheme 1). The present methodology offers several advantages such as high yields, relatively short reaction times, mild reaction condition, easy work up, and using a highly recyclable catalyst.



Scheme 1. *Synthesis of 3,4-dihydropyrimidin-2(1H)-ones by $ZnFe_2O_4$ MNPs*

Keywords: *Magnetic catalyst; Zinc Ferrite Nanoparticles; 3,4-dihydropyrimidin-2-(1H)-ones*

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A new and efficient method for aldol reaction using tetramethylguanidine-functionalized magnetic nanoparticles

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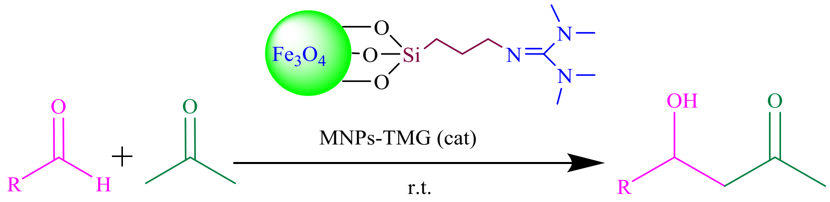
One of the most significant and well-known carbon-carbon bond forming synthetic reactions, functional in organic syntheses, is aldol reaction. These reactions provide high atom economies and produce β-hydroxycarbonyl structural unit [1,2]. Guanidine derivatives as strong organic super-bases have attracted much attention in synthetic organic chemistry. 1,1,3,3-tetramethylguanidine (TMG) as a typical and basic guanidine compound has been utilized in many different kinds of bases-catalyzed reactions [3,4].

In the present work tetramethylguanidine supported onto magnetic nanoparticles was prepared and characterized by different techniques including: TEM, SEM, XRD, TGA and FT-IR analyses. The prepared catalyst used as an efficient catalyst for the aldol reaction of acetone with various aldehydes to achieve *β*-hydroxy carbonyl compounds in excellent yields (Scheme 1). This procedure has several advantages, such as mild reaction conditions, short reaction time, excellent yields and easy purification of the products. Additionally, supporting this organosuperbase catalyst on magnetic nanoparticles offers a simple method for easy recovery and reuse of the catalyst using an external magnetic field.



Scheme 1. *MNPs-tetramethylguanidine catalyzed aldol reaction.*

Keywords: *Aldol reaction, Tetramethylguanidine, Magnetic nanoparticles.*

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Efficient photocatalytic coupling reactions on Au–Pd alloy nanoparticles under visible light irradiation

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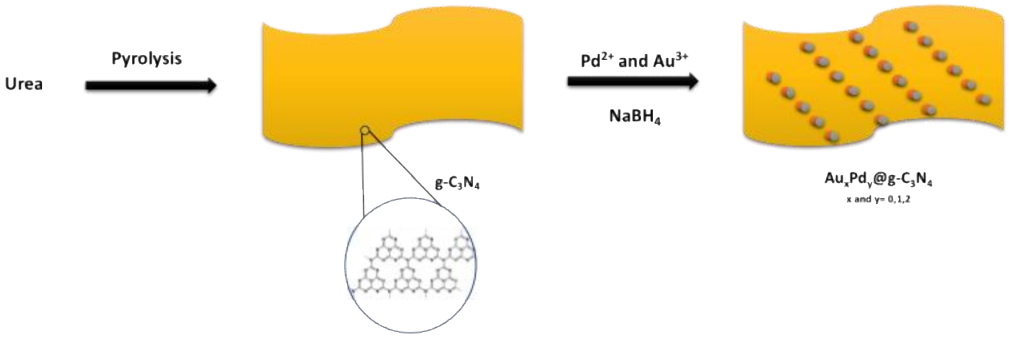
The highly efficient photocatalysts comprising supported nanoparticles (NPs) of gold and palladium alloys, which utilize visible light to catalyze the coupling reactions at ambient temperature was reported. The photocatalytic efficiencies strongly depend on the Au:Pd ratio of the alloy NPs.



Scheme 1. *Schematic illustration of the formation procedure of AuPd/N-C*

Keywords: *Photocatalyst, Coupling reaction, Alloy*

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Convenient Preparation of N-sulfonylimines Using Iron-Based Magnetic Nanomaterials

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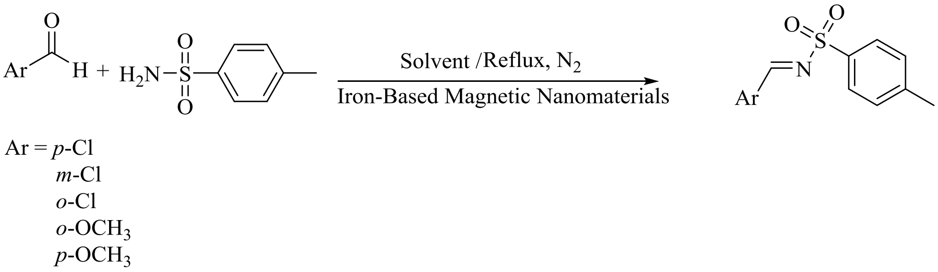
Activated aldimines are important intermediates in organic synthesis [1]. Their durability for long time and mild reactivity have led them to use in many organic reactions which can be pointed to reactions such as Diels–Alder reactions, radical reactions, nucleophilic additions and ene reactions also [2]. The facile way to prepare these compounds is the use of direct condensation of sulfonamide and various aldehydes, although the preparation of water is no favor. Several ways have been developed to accelerate this reaction by using different additives such as $AlCl_3$, ZrO_2/S_2O_8, $TiCl_4/Et_3N$, P_2O_5/SiO_2, montmorillonite K-10 and so on. However, harsh reaction conditions, sensitivity to water, low yields and high catalysts loading limited these reactions [3].

In other side, the use of nanoparticles due to the high surface-to-volume ratio, easy recycling and reusing is a good strategy for increasing the efficiency of chemical reactions.

Iron-based magnetic nanomaterials have been used as catalysts for a very wide range of catalytic processes and organic transformations such as coupling reactions, C-H activation, oxidation reactions, reduction reactions and synthesis of heterocyclic. Hence, magnetic nanocatalysts due to their pervasive applications on the field of catalysis are of high demand.

In this work, initially different nanoparticles were prepared, then the catalytic activity of obtained heterogeneous catalysts was investigated on the reaction between aromatic aldehydes and *p*-toluenesulfonamide. By optimization of the reaction conditions, various N-sulfonyl imines were afforded in high yields. After the completion of the reaction, heterogeneous catalyst was separated by a magnet form the reaction mixture and reused. The obtained products were characterized by melting point, Ft-IR ^{1}HNMR, ^{13}CNMR spectra.



Scheme 1. *Synthesis of activated aldimines by using iron-based magnetic nanomaterials.*

Keywords: *Aldimine, Iron-Based Magnetic Nanomaterials*

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Synthesis of new derivatives of pyranoquinolines by a one-pot, three-component reaction

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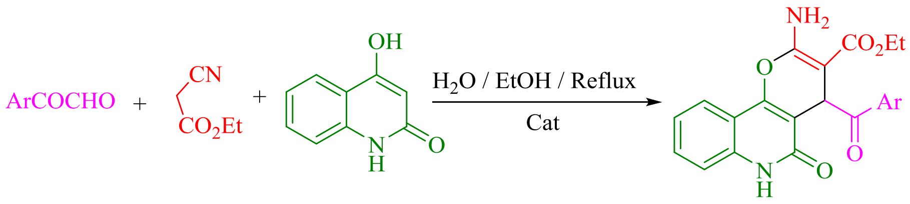
Recently, the use of one-pot, multicomponent reactions (MCRs) have received considerable interest in the synthesis of heterocyclic compounds with biological and pharmacological activities by a route with three or more components, which avoids the spread of poisonous intermediates [1].

Catalysts are the master key toward green chemistry goals [2], and by decreasing the activation energy, catalysts can make a chemical reaction happen in shorter time, more benign, and energy-efficient conditions. The biochemically significant processes are catalyzed. Research into catalysis is a major field in applied science and involves many areas of chemistry, notably organometallic chemistry and materials science.

The presence of pyranoquinoline moiety in many alkaloids have attracted serious attention. For instance, antitumor, antimicrobial, anti-inflammatory, antiallergic, antimalarial, inhibition of calcium signaling, and platelet aggregation are some of the unique properties, in behalf of this attraction [3, 4].

In continuation of our interest in the synthesis of new and various heterocyclic compounds [5, 6], an efficient protocol for the synthesis of pyranoquinolines **4** by multicomponent condensation of arylglyoxals **1**, ethyl cyanoacetate (**2**), 4-hydroxyquinolin-2(1*H*)-one (**3**) and catalyzed by TEACB in H_2O/EtOH under reflux conditions. Furthermore, effect of different catalysts on the reaction was conducted through different catalytic systems including sulfanilic acid, *p*-toluenesulfonic acid (*p*-TSA), *L*-proline, *L*-cysteine, three ethylamine (Et_3N), *etc*. The best results were obtained using TEACB as a catalyst (Scheme 1).



1 **2** **3** **4**

Ar = C_6H_5, 4-BrC_6H_4, 4-ClC_6H_4, 4-$O_2NC_6H_4$, 3-MeOC_6H_4

Scheme 1. *Synthesis of pyranoquinoline derivatives.*

Keywords: *Multicomponent reactions, Catalyst, Arylglyoxals, Pyranoquinolines.*

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An efficient synthesis of diarylmethylamine by copper catalysts

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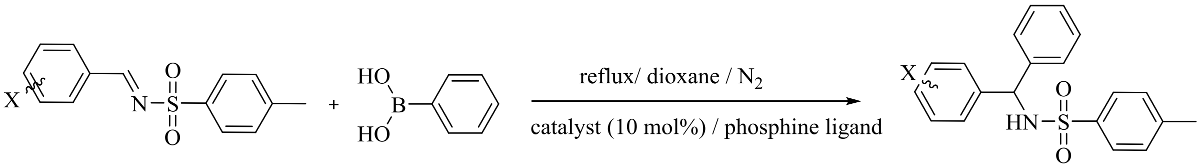
Amines are important building blocks of pharmaceutical and agrochemical compounds which are also used as ligand and base in organic reactions [1].This type of structure is of interest for preparing natural product, bioorganic and drugs that can mention as cetirizine (antihistaminic) to treat allergic, sertraline and tianeptine (anti-depression), letrozole (treat cancer) and many other medications [2,3]. Arylation of activated aldimines is a superior route for the synthesis of α-arylmethylamines. Due to the application of these compounds, the use of various transition metal catalysts, substrates and aryl donor groups have been developed to improve the catalytic activity, scope of substrates and other variables. However some of these methods were used toxic and expensive reagents [4].

Herein we have designed an arylation reaction on imines to synthesis of aryl amines. A wide range of aryl amines were afforded by addition of aryl boronic acid to different aldimines in presence of non-expensive copper metal and phosphine ligands. The desired products were produced in good yield and were characterized by IR, ^{1}HNMR and ^{13}CNMR.



Scheme 1. *Copper catalyzed arylation of activated aldimines.*

Keywords: *Arylation reaction, Copper catalyzed, Aldimine.*

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Preparation and characterization of Graphene Oxide/Nickel oxide nanocomposite and Investigation of Its Catalytic Effect on the Thermal Decomposition of Ammonium Perchlorate

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Graphene oxide (GO) modified transition metal oxide based composites were successfully synthesize. GO used as a modifier in the catalyst. The structural characteristics of GO/NiO nanoparticle were systematically studied by using various instrumental techniques including X-ray diffraction (XRD), Fourier transform infrared (FTIR), scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDX). The XRD and SEM results showed that the particle size was between 20 nm and 50 nm. The catalytic efficiency of the synthesized composite catalyst samples based thermal decomposition of AP was determined by differential scanning calorimetery (DSC) and thermogravimetric analysis (TGA) methods. The results show that GO/NiO nanocomposites exhibit high catalytic activity. The peak temperature of the high-temperature decomposition of AP decreased by 135 °C and at the same time the peak of the low-temperature decomposition disappeared. As a result, the GO/NiO nanocomposites could be a promising candidate material for an AP-based propellant.

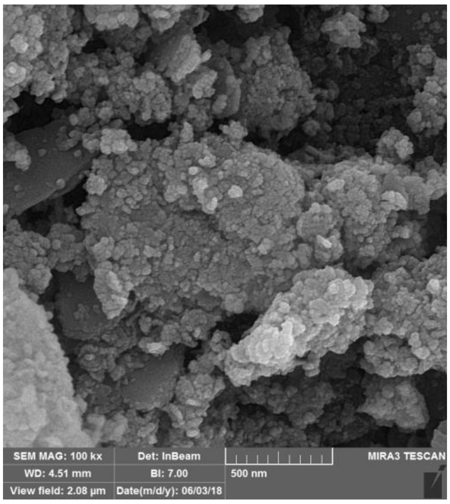

fig 1. *SEM image of GO/NiO nanoparticle*

Keywords: *Ammonium perchlorate, Graphene oxide, catalyst, propellant.*

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Green synthesis of $NiFe_2O_4$ nanoparticles using *H.rawanium* and their use as a green catalyst for the synthesis of pyrimidinone derivatives

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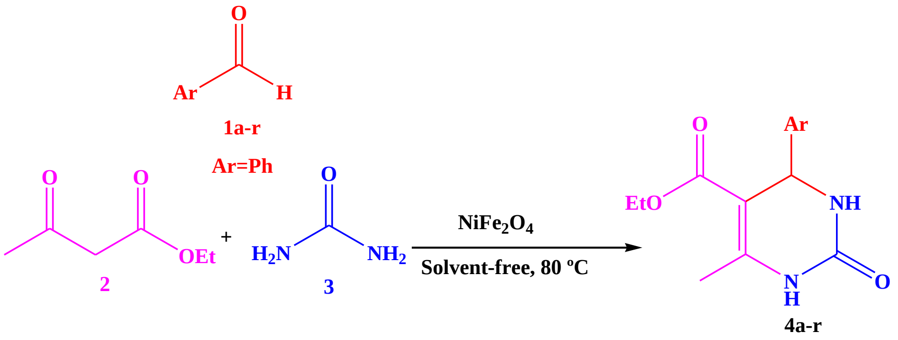
Here we represent green and efficient synthesis of $NiFe_2O_4$ nanoparticles (NPs) by *Heracleum rawanium* fruit extract as non-toxic reducing agent and stabilizer without adding any surfactant. The extraction of fruit of this plant with water is described by maceration. The natural products found in plants have an important role in synthesis of nanoparticles [1,2]. FT-IR spectroscopy, X-ray diffraction (XRD) pattern and field emission scanning electron microscopy (FESEM) have been used in the characterization of the nanoparticles thus prepared. The results showing that MNPs synthesized by *H.rawanium* extract have high purity and the average particle size is 33 nm. In addition, Nickel ferrite nanoparticles as an efficient catalyst were used for the synthesis of pyrimidinone derivatives via multi-component reactions under solvent-free conditions at 80 °C. This method have several advantages such as short reaction time, excellent products yields (86-94), simple work and use of recoverable catalyst.



***Scheme 1.** Synthesis of pyrimidinone derivatives*

Keywords: *Nickel ferrite, Pyrimidinone, Solvent-Free*

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N, N'-dicyclohexylcarbodiimide functionalized Fe_3O_4 magnetic nanoparticles: an efficient heterogeneous organocatalyst for esterification reaction

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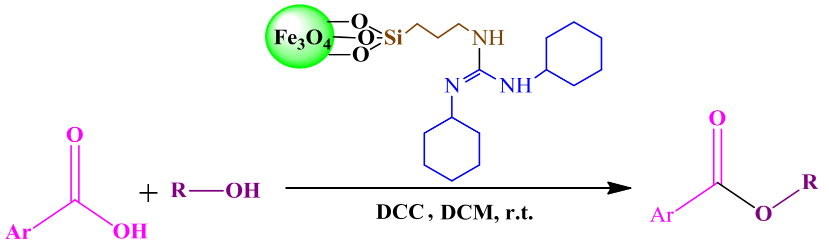
Esters are one of the most important and plentiful functional groups in chemistry, and can be found in pharmaceuticals, natural products, polymers fine and bulk chemicals [1,2]. It is well known that the utilize of heterogeneous catalysts instead of homogeneous catalysts has many advantages in organic synthesis. In heterogeneous reaction, tedious methods like filtration and centrifugation are used to recover catalysts and end in loss of solid catalyst in the separation process [3].

Considering importance of esterification reaction in organic chemistry, in the present work we have developed new methodology for this reaction in the presence of N, N'-dicyclohexylcarbodiimide (DCC) as a coupling reagent and DCC-functionalized Fe_3O_4 magnetic nanoparticles (MNPs-DCC) as an efficient heterogeneous organocatalyst (Scheme 1). This procedure has several benefits, such as short reaction time, mild reaction conditions, easy purification of the products and excellent yields. Additionally, supporting this organosuperbase catalyst on magnetic nanoparticles offers a simple method for easy reuse and recovery of the catalyst using an external magnetic field.



Scheme 1. *MNPs-DCC catalyzed esterification reaction.*

Keywords: *Esterification, Magnetic Nanoparticles, N, N'-dicyclohexylcarbodiimide.*

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https://doi.org/10.1007/s12633-017-9757-0

Synthesis of $Ni_{0.5}Co_{0.5}FeAlO_4$ nanospinel and evaluation of its photocatalytic activity

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The general formula of spinel compounds is AB_2O_4, in which the A-site is mostly occupied by divalent metal and the B-site is occupied by trivalent one. Over the past decades, oxides with spinel structures have received much research attention due to their physicochemical properties [1,2].

The present study concentrates on synthesis of $NiCoFeAlO_4$ nanoparticles by the means of sol-gel technique using tragacanth gel. The synthesized nanoparticles were then characterized by Fourier transform infrared spectroscopy (FTIR), X-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM), and vibrating sample magnetometer (VSM).

The photocatalytic activity of $NiCoFeAlO_4$ MNPs has been determined for basic red 5 (BR5) dye degradation in the presence of visible light. The photocatalytic efficiency has been carried out at various initial dye concentration, photocatalyst dosage, and irradiation time. The results depicted that $NiCoFeAlO_4$ MNPs can degrade of BR5.

This method is cost-effective, simple, less time consuming, eco-friendly, and can consequently be utilized for scale-up production.

Keywords: *Sol-gel method, Basic red 5, Nanospinel.*

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Palladium nanoparticle decorated on magnetic pomegranate peel-derived porous carbon nanocomposite as an excellent catalyst for cross-coupling reactions

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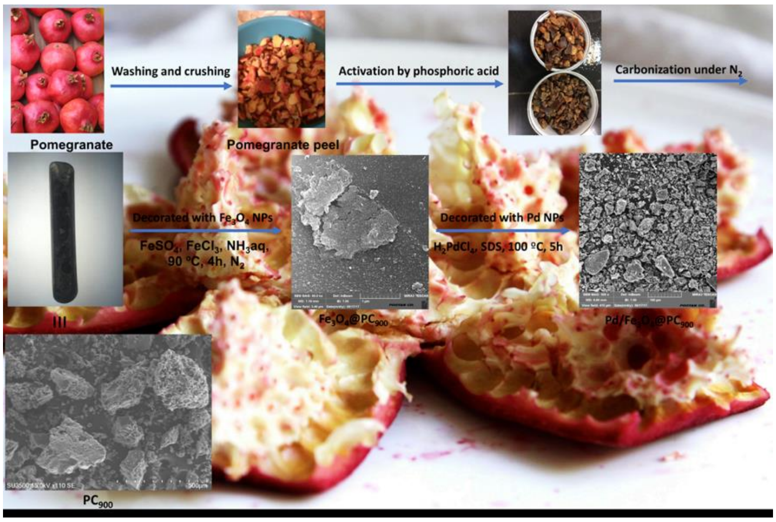
The porous carbon (PC) material was prepared from the carbonization of pomegranate peel waste. Subsequently, the magnetically separable Fe_3O_4@PC was synthesized from the Fe_3O_4 nanoparticles decorated on PC by the co-precipitation method of iron ions. Finally, Fe_3O_4@PC was successfully decorated with palladium nanoparticles in a simple route by reducing H_2PdCl_4 in the presence of sodium dodecyl sulfate, which is used as both a surfactant and reducing agent. Additionally, the effect of temperature on carbonization process was studied. The Pd/Fe_3O_4@PC nanocomposite was used as an efficient and heterogeneous catalyst for the Suzuki-Miyaura and Sonogashira cross-coupling reactions in an environmentally friendly medium.



Scheme 1. *Schematic illustration of the formation procedure of Pd/Fe_3O_4@PC*

Keywords: *Carbon, Coupling reactions, Biowaste, Magnetic.*

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Synthesis of 3,4-dihydropyrimidinones (thiones), 1,8-dioxo-octahydroacridines and 1,8-dioxo-octahydroxanthenes as heterocyclic compounds using Ti-MOF nanocatalyst

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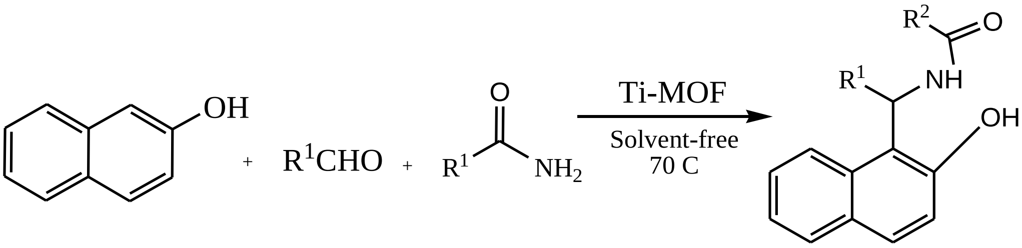
In this Study, Ti-MOF (Metal organic framework) has been used as a novel, an excellent, stable, recyclable, highly porous hybrid material with large surface area and highly efficient catalyst for one-pot synthesis of some heterocyclic compounds such as dihydropyrimidinones and dihydropyrimidinthiones as Biginelli compounds, octahydroquinazolinone, pyrimido[4,5-d] pyrimidine and tetrahydropyrimidine derivatives as biginelli-like products, 1-amidoalkyl-2-naphtol, 1-aminoalkyl-2-naphtol, acridines, tetrahydrobenzoxanthene-11-one, dioctahydroxanthene and dibenzoxanthene derivatives under solvent-free conditions. The Ti-MOF catalyst was characterized by FT-IR, X-ray diffraction (XRD), Scanning electron microscopy (SEM), energy dispersive X-ray analyzer (EDAX). The structure of the synthetic products identified by spectroscopic methods and the physical properties such FTIR , melting point and ^{1}H-NMR. The main advantage of these reactions compared to the previous reported results involves shorter reaction time, lower amount of catalyst, simple procedure, lower temperature, easy workup, reusability of the catalyst and the products are obtained in high yield.



***Scheme 1.**: The concerned reaction for the synthesis of 1-amidoalkyl-2-naphtol using Ti-MOF*

Keywords: *heterocyclic compounds, nanocatalyst, Ti-MOF.*

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Photocatalytic degradation of Congo red dye using La(OH)$_3$ nanoparticles under visible light irradiation

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Lanthanides are an attractive class of elements and have unique optical, catalytic, and magnetic properties because of their unique electron configuration (4f electrons). Lanthanide hydroxides Ln(OH)$_3$ are of great importance because they represent a straightforward approach toward oxides or sulfides through dehydration or sulfuration. Hydroxyl groups may also act as active sites for surface grafting through condensation reactions of organic and/or biological reagents [1]. Lanthanum, the lightest element in the lanthanide series, has been widely studied in its oxide, hydroxide, phosphate, or oxychloride form and has been extensively applied in optoelectronic devices, phosphors, solid electrolyte, catalysis, sorbent, and a gas sensor [2,3]. Especially, lanthanum hydroxide (La(OH)$_3$) is one of the novel rare earth compounds, and has been used in many field, such as ceramic, superconductive materials, hydrogen storage materials, electrode materials, etc, especially in catalyst and sorbent materials. The study of one-dimensional La(OH)$_3$ has also been of growing interest owing to the promising applications in lanthanum hydroxide nanowires modified carbon paste electrode (LNW/CPE), catalyst, sorbent materials, sensors, multiplex materials, and the procedure for the collection of As(III) [4,5].

In the present study, La(OH)$_3$ nanoparticles were prepared by the sol-gel method. The synthesized Lanthanum hydroxide nanoparticles were characterized by powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy, scanning electron microscopy and energy dispersive X-ray analysis (EDX). The X-ray powder diffraction (XRD) analysis revealed the formation of hexagonal phase La(OH)$_3$ with average crystallite size of 29 nm. The present photocatalyst displays notable catalytic activity for the removal of Congo red dye in water under visible light irradiation. It was established that the catalyst could remove *ca.* 90% of the Congo red dye. The effects of initial dye concentration, photocatalyst dose, and visible light irradiation on dye degradation were evaluated.

Keywords: *Lanthanum hydroxide nanoparticles, Visible light irradiation, Photocatalysis.*

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Magnesium oxide nanoparticles as a recyclable catalyst for the green multicomponent synthesis of benzochromene derivatives

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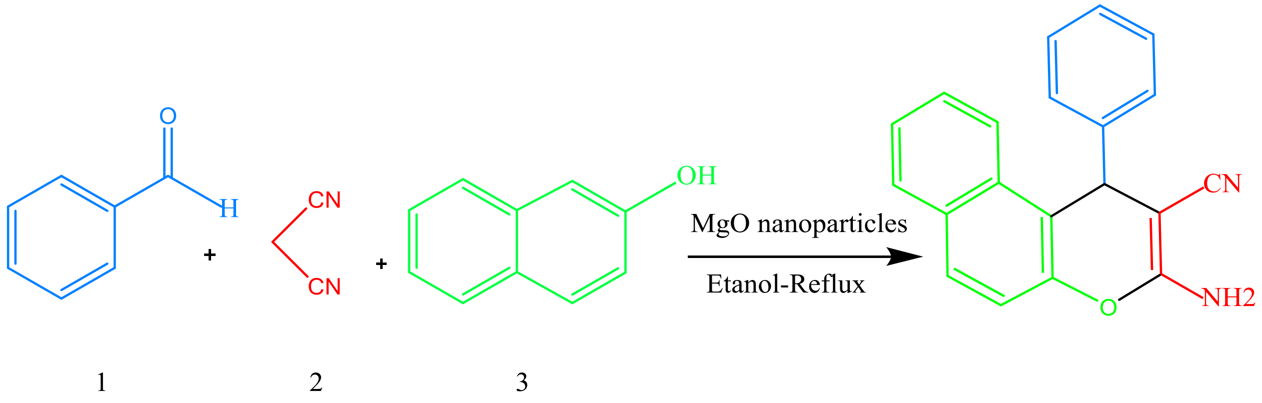
Chromenes are a common structural motif in variety of natural and non-natural products. Their derivatives have been known to exhibit a wide range of biological and pharmacological activities such as antioxidant, anticancer, antimicrobial, hypotensive and local anesthetic. In addition, they can be used as cognitive enhancers, for the treatment of neurodegenerative diseases, including Alzheimer's disease and schizophrenia disorder [1,2].

Heterogeneous catalysis has been in use since the start of organic chemistry. The activity and selectivity of these catalysts are enhanced by the surface of a support. Hence, the effective surface area of the reagent is increased significantly. The catalyst can be reused when recycled, although after some time it gets deactivated depending on its half-life. The main advantages of heterogeneous catalysts are the relative ease of catalyst separation from the product, recyclability, non-corrosiveness and tolerance of extreme operating conditions which makes them environmentally friendly [3,4].

In this work, a facile and efficient one-pot method has been developed for the synthesis of benzochromenes using MgO NPs as a heterogeneous catalyst by the condensation of aldehydes, β-naphthol and malononitrile in ethanol as solvent (Scheme 1). The reaction, with this catalyst was carried out under mild reaction conditions with very good to excellent yields.



***Scheme 1.** Synthesis of benzochromene derivatives by MgO NPs as catalyst*

Keywords: *Magnesium Oxide nanoparticles; Benzochromene derivatives; Heterogeneous catalyst*

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Synthesis of substituted polyhydroquinolines using zinc chromite nanoparticles as a heterogeneous catalyst *via* the Hantzsch reaction

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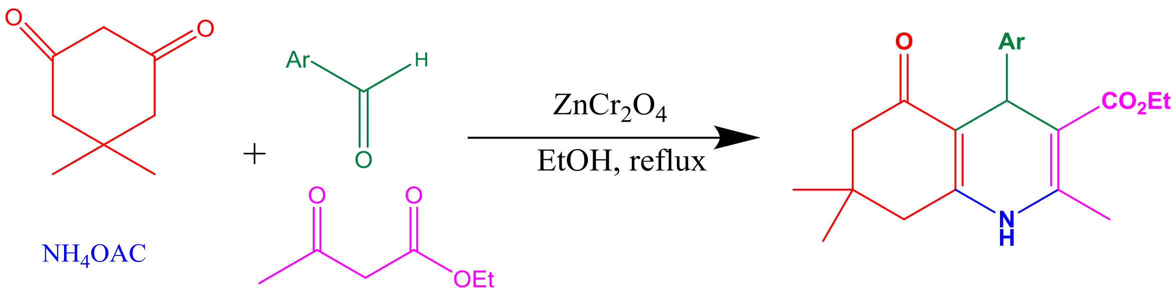
Polyhydroquinolines are one of the most important groups of nitrogen heterocycles that have attracted considerable interest because of various important pharmacological and therapeutic properties. Some pharmacological activities of polyhydroquinolines are calcium channel blockers, vasodilator, bronchodilator, antiatherosclerotic, antitumor, geroprotective, hepatoprotective, and antidiabetic agents [1,2]. Furthermore, some polyhydroquinolines exhibit other medicinal applications which include platelet antiaggregatory activity, neuroprotectant, and cerebral antischemic activity in the treatment of Alzheimer's disease. Hantzsch synthesis of polyhydroquinolines is one of the most significant multi-component reactions due to its key role in the production of these pharmacologically useful compounds. This method generally involves one-pot condensation of aldehydes with β-dicarbonyls and amine sources under acidic conditions [3,4].

Zinc chromite nanoparticles were used as a reusable and robust heterogeneous catalyst for one-pot four component synthesis of polyhydroquinoline derivatives *via* the esteemed Hantzsch reaction using aryl aldehydes, ethyl acetoacetate, dimedone and ammonium acetate under mild reaction conditions in short reaction times and good to excellent yields in ethanol medium (scheme 1). Moreover, the catalyst was also recovered and reused at least four times without significant decrease in its activity.



***Scheme 1.** The one-pot four-component preparation of substituted polyhydroquinolines*

Keywords: *Heterogeneous catalyst, Hantzsch reaction, Substituted polyhydroquinolines*

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Antibacterial effect of Aluminum zirconium oxide nanocomposite against clinical pathogens

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Nano-materials are the more efficient, since they are able to attach more copies of microbial molecules and cells [1]. Nanoscale materials have been investigated for antimicrobial activity as growth inhibitors [2], killing agents [3] or antibiotic carriers [4]. The objective of this study was to evaluate the antibacterial potential of Aluminum zirconium oxide nanocomposite ($Al_2Zr_3O_9$) against a clinical isolates of *Pseudomonas aeruginos*. *Pseudomonas aeruginosa* has become an important cause of gram-negative infection, especially in patients with compromised host defense mechanisms. It is the most common pathogen isolated from patients who have been hospitalized longer than 1 week, and it is a frequent cause of nosocomial infections. Pseudomonal infections are complicated and can be life-threatening.

In this study the antibacterial activities of nanocomposite ($Al_2Zr_3O_9$) was investigated against a clinical isolates of *Pseudomonas aeruginosa* using agar well diffusion method. Briefly, 6mm-diameter wells were made on the surface of solid medium using a sterile cork borer. Aluminum zirconium oxide nanocomposite was dissolved in Dimethyl sulfoxide (DMSO) and a solution with 1mg/ml concentration was prepared. Nanocomposite solution and DMSO (Dimethyl sulfoxide was used as negative control) separately placed in 6mm diameter-wells and incubated at 37 ± 2◦C for 24h**.** Final results were evaluated by measuring the average diameter of inhibition zone around each well. The results show that zoon inhibition of Aluminum zirconium oxide nanocomposite was 12mm (Fig1**).** These results confirm the potential of Aluminum zirconium oxide nanocomposite as new antimicrobial materials.

Keywords: Nanocomposite, Aluminum zirconium oxide, Antimicrobial, Antibacterial, Clinical pathogens

Fig 1. *Inhibition zone of Aluminum zirconium oxide nanocomposite against Pseudomonas aeruginosa in 1mg/ml concentration*

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Magnetically Nanoparticles of Copper Ferrite@antimony: An Efficient Catalyst for Synthesis of Biscoumarins from 4-Hydroxycoumarin and Aromatic Aldehydes

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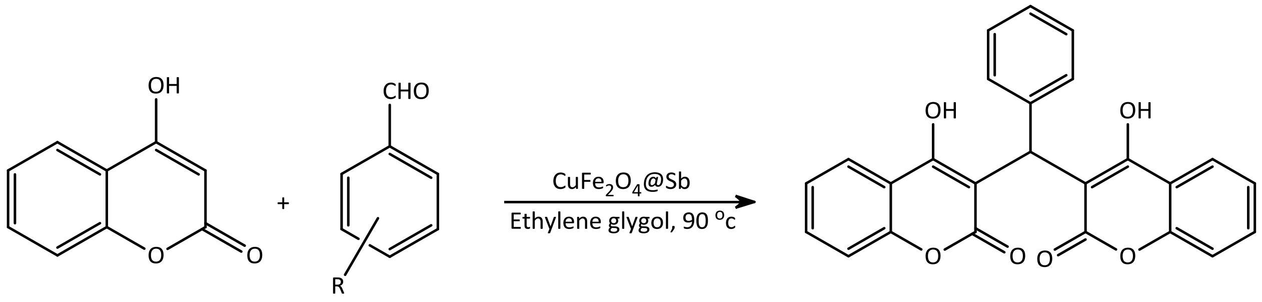
Coumarins are biologicaly active compounds with antifungal, antineoplastic, antibacterial, spasmolytic or cytotoxic activity. 4-Hydroxycoumarin and its derivatives such as dicoumarol are known as anticoagulants [1-2]. Bis (4-hydroxycoumarin-3-yl) methanes are obtained by the condensation of two molecules of 4-hydroxycoumarin with one reusable catalyst [3]. These subjects prompted us to prepare $CuFe_2O_4$/Sb as an efficient nanocatalyst toward synthesis of biscoumarins with 4-hydroxycoumarin and aromatic aldehydes in ethylene glycol (Scheme 1). High activity and easy separation makes, $CuFe_2O_4$/Sb as an ideal catalyst for this transformation. The procedure has the advantages of mild reaction conditions, high yields of products, short reaction time, and simple experimental technique, making it a useful and attractive process.



***Scheme 1.** Synthesis of biscoumarins with $CuFe_2O_4$/Sb*

***Keywords:** $CuFe_2O_4$, Sb, 4-hydroxycoumarin, biscoumarin*

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Magnetic Niacin sulfonated: A highly efficient and green catalyst for synthesis of α-aminonitriles under solvent-free conditions

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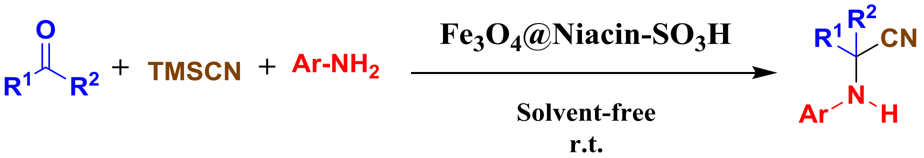
Vitamins are valuable natural small bimolecules which have been used as organocatalysts [1]. Some vitamins like Niacin can directly be used in supporting a metal owing to carboxyl functions in its structures and plays important roles for bind to surface magnetic nanoparticles [2,3]. Also, nitrogen atom in its structure can be easily sulfonated. Therefore, in continuation of our study on the use of organocatalysts in organic reactions and the immobilization of natural compounds on solid supports for the synthesis of a heterogeneous organocatalyst and extension of environmentally friendly methods, we design a strategy for the preparation of reusable magnetic organocatalyst *via* grafting Niacin on magnetic nanoparticles and employed it as an environmentally friendly and recyclable catalyst for one-pot synthesis of three-component *via* Strecker reaction, incorporating aldehydes/ketones, amines and trimethylsilyl cyanides (TMSCN), under solvent-free conditions. Operational simplicity, product purity, natural resources and reusability of the catalyst are considered as evident features of this protocol which will hopefully develop to an inexpensive, efficient, and clean strategy for the synthesis of α-aminonitriles.



Scheme 1. *Synthesis of α-aminonitriles over Fe_3O_4@Niacin-SO_3H*

Keywords: *Niacin, α-aminonitrile, Strecker reaction.*

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Synthesis of silver particle supported on polysiloxane: Characterization and catalytic application in reduction of para nitrophenol

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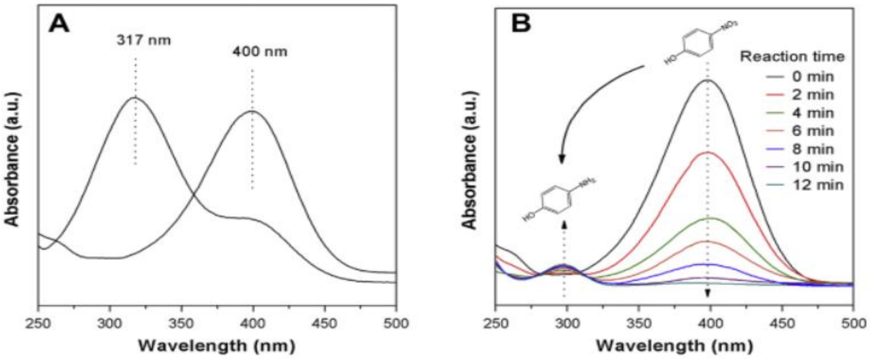
Noble metallic nanoparticles (Au, Ag, Pt, etc.) have attracted extensive attention due to their optical and electronic properties and potential utility in catalysis. Among these noble metallic nanoparticles, Ag is particularly attractive because of its much lower cost. In particular, its application in catalysis is most important since it often combines the characteristics of high reactivity and selectivity. There are many reactions catalyzed by Ag, such as oxidative conversion of methanol into formaldehyde, 4 selective butadiene epoxidation5 and oxidation of D-glucose. Especially, the 4-nitrophenol (4-NP) reduction by borohydride in the presence of Ag catalysts has been accepted as an alternative effective and eco-friendly route to produce 4- aminophenol (4-AP) in industry [1].

Catalytic reduction of 4-nitrophenol: In order to study the catalytic activity of the as synthesized particles 25 mL of 4-NP (0.12 mmol/L) aqueous solution were stirred with freshly prepared $NaBH_4$ solution (25 ml, 60 mmol/L). Then 5 mg, 10 mg, 15 mg of micron-SiO_2 nano-Ag particles were added into the flask, respectively. As the reaction proceeded, the color of the solution changed gradually from yellow to colorless at room temperature. UV–vis absorption spectra were recorded with a time interval of 45 min, 10 min, 7 min, respectively, to monitor the change of the reaction mixture at room temperature. In comparison with free Ag NPs the Ag-SiO_2 NCs exhibited a better catalytic activity for the reduction of 4-nitrophenol at room temperature. The final products were thoroughly characterized by Fourier Transform Infrared spectroscopy (FT-IR), X-ray powder diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM) along with Energy Dispersive X-ray (EDX) Spectroscopy, thermo gravimetric and differential thermal analysis (TG/DTA) and X-ray photoelectron spectroscopy (XPS) [2].



Scheme 1. *UV-vis spectra of (A) 4-NP before and after adding NaBH4 solution and (B) the reduction of 4-NP in aqueous solution recorded every 2 min using micron-SiO2nano-Ag as a catalyst* [2]

Keywords: *4-Nitrophenol, Catalytic activity, micron-SiO_2 nano-Ag particles*

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One-pot multi-component synthesis of octahydroquinazolinone derivatives *via* Biginelli condensation using $ZnCr_2O_4$ nanoparticles as an efficient catalyst

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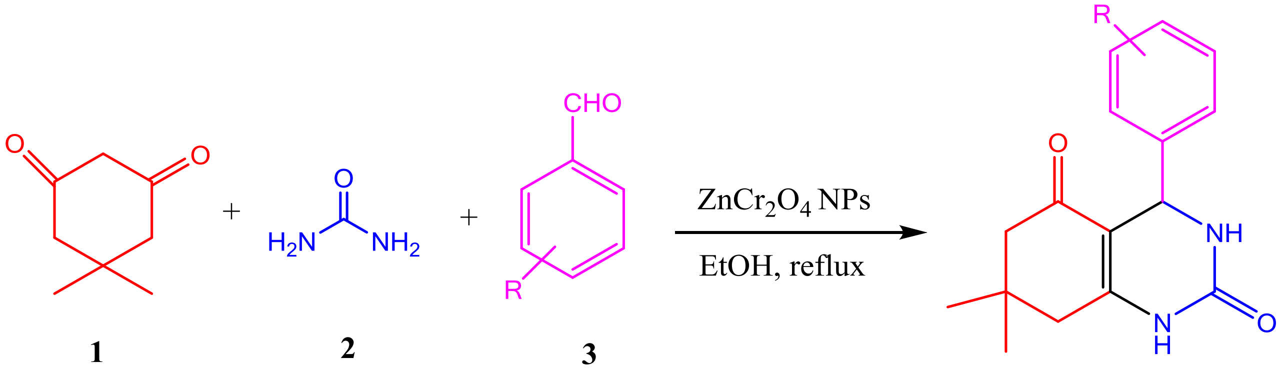
In recent years, the Biginelli reaction has been employed for the synthesis of octahydroquinazolinones, which used cyclic β-diketones instead of open-chain dicarbonyl compounds using concentrated H_2SO_4 and HCl as the catalyst. These octahydroquinazolinone derivatives have attracted considerable attention owing to their diverse pharmacological properties [1,2]. The quinazolinone moiety is found, as alterative in a wide variety of biologically active compounds which can be used as hypnotic/sedative drugs for treatment of cancer. Furthermore, quinazolinone derivatives are of interest because they exhibit a broad spectrum of biological properties, such as analgesic, antiinflammatory, antimicrobial and anti-tubercular, anti-HIV, antimalarial and antihistamine [3,4]. $ZnCr_2O_4$ nanoparticle has been shown to be an inexpensive, efficient and mild catalyst for the one-pot synthesis of octahydroquinazolinone derivatives using dimedone, urea and appropriate aromatic aldehydes in ethanol as a solvent under reflux condition (scheme 1). This methodology is of interest due to the use of ethanol as a solvent without use of any organic solvent and toxic metals as catalyst, thus minimizing the cost, the operational hazards, and environmental pollution. Also this modified route provides much higher yields and simple work-up procedure of products.



Scheme 1. *$ZnCr_2O_4$-catalyzed synthesis of octahydroquinazolinone derivatives*

Keywords: *$ZnCr_2O_4$ nanoparticles, Biginelli reaction, Octahydroquinazolinone derivatives*

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