

28th Iranian Conference on Organic Chemistry



1-3 March 2022 - Chemistry & Chemical Engineering Research Center of Iran



Lectures & Abstracts

Chemistry & Chemical Engineering Research Center of Iran Pajohesh Blvd,17th Km of Tehran-Karaj Highway, Tehran, Iran. Tel: +98 (21) 44787811

In the name of God, the Merciful, the Compassionate

The Synthesis in Organic Chemistry conference is a flagship event for the international organic chemistry community. The first meeting of this internationally renowned symposium was held in Tehran in 1369, organized by the Iranian Society of Chemistry and since then the meetings have alternated on a biennial basis between most famous Iranian university. The Synthesis in Organic Chemistry conference will cover all aspects of contemporary organic synthesis and provide a forum for the ever more exciting methodologies and strategies that continue to emerge. The conference will be of interest to all early-career and established scientists, post-graduate students and industrial researchers as well as anyone interested to be informed and discuss recent developments in the fields of organic Chemistry and Chemical Technology working in this field.

The 28th Iranian Conference on Organic Chemistry (ISOC2021) will be organized by the Association of Chemistry & Chemical Engineering Research Center of Iran (CCERCI) in collaboration with the Iranian Chemical Society. The 28th ISOC was initially planned for 2021 but it was postponed for March 2022 due to the COVID-19 pandemic.

The conference programme of the ISOC2021 will include plenary lectures, oral presentations and poster presentations and will include special workshops, presentation of awards and prizes, and attractive social events. Continuous Virtual Poster Session combined with the possibility of meeting at specially prepared virtual poster stands. The use of a conference application facilitates the exchange of information between participants. The great events feature five international keynote speakers and seven national keynote speakers giving 60-minute presentations with plenty of time for discussions and networking. The symposium is planned as a hybrid: both in-person and virtual participants are welcome.

On behalf of the Iranian Chemical Society and CCERCI, we want to thank you for attending the 28th Annual Conference on organic chemistry on March 1-3, 2022 at Chemistry and Chemical Engineering Research Center of Iran.

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28th Iranian Conference on Organic Chemistry

1-3 March 2022 Chemistry & Chemical Engineering Research Center of Iran

Conference Schedule



Day 1 (1 March 2022) Title Time Presenter 4:30 - 5:30* **Opening Ceremony** 8:00-9:00 $5:30 - 6:30^*$ Invited Lecture Stereoelectronic effects: A new approach to organic 9:00-10:00 Prof. Mohammad Ali Zolfigol chemistry $6:30 - 7:30^*$ **Invited Lecture** Organic Chemistry in the Context of Sustainability: 10:00-11:00 Prof. Asit K. Chakraborti A Few Concepts and Applications 7:30 - 8:30* Invited Lecture Designed Supramolecular for Molecular Recognition 11:00-12:00 Prof. Reza Zadmard $8:30 - 10:30^*$ Prayer and Lunch Break 12:00-14:00 10:30 - 11:30* Isocyanide-based multicomponent reactions in Invited Lecture 14:00-15:00 Prof. Ahmad Shaabani shaabani's research group 11:30 - 13:30* **Oral Lectures** 15:00-17:00 Theoretical Study on the Formation Mechanistic of 3-15:00-15:30 Associate Prof. phenyl-4-methyl-benzonitrile by using Suzuki-Miyaura and Mehdi Bayat Hiyama-Denmark Cross-Coupling Reactions Preparation of g-C3N4-based Nanocatalysts and Their 15:30-16:00 Associate Prof. Application in Condensation and Oxidation Reactions Hossein Ghafuri The Synthesis of An Organic Dyes Based on Thioindigo 16:00-16:30 Associate Prof. for Dye-Sensitized Solar Cells M. Hosseinnezhad One-Pot Three-Component Synthesis of 2-16:30-17:00 PhD Student Iminothiazolines in Catalyst-Free Procedure Elham Badali 13:30 - 14:30* **Invited** Lecture Design and synthesis of nanocatalysts and the 17:00-18:00 Prof. Ghodsi Mohammadi studies of their properties 14:30 - 16:30* Poster session 1 : From isoc28-00020244 To isoc28-01820315

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Greenwich Mean Time (GMT)





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Conference Schedule Day 2 (2 March 2022)		
Time	Presenter	Title
4:30 - 5:30*	Invited Lecture	From Medicinal Chemistry Routes to Scalable & Robust
8:00-9:00	Dr. Roozbeh Yousefi	Processes
5:30 – 7:30* 9:00-11:00	Oral Lectures	
9:00-9:30	Master of Science Amin Rahimzadeh	Raw Materials for The Production of Natural Cosmetics
9:30-10:00	PhD Student Faezeh Nemati	Synthesis of Novel Noscapine Analogues as Potential β- tubulin Inhibitors
10:00-10:30	Postdoctoral Researcher Mehran Ghasemi	Assembly of Indole Cores through a Palladium-Catalyzed Metathesis of Ar-X σ -Bonds
10:30-11:00	Associate Prof. Azadeh Ebrahimian Pirbazari	Efficient Degradation of Tetracycline Contaminant in artificial Wastewater Using Hybrid Photocatalysts Under Visible Light
7:30 – 8:30* 11:00-12:00	Invited Lecture Prof. Yanlong Gu	Acid-catalyzed tandem reactions for organic synthesis
8:30 - 10:30*		Draver and Lunch Drack
12:00-14:00		Prayer and Lunch Break
10:30 – 11:30*	Invited Lecture	2-Alkynylbenzaldoxim: A multipurpose building block for
14:00-15:00	Prof. Saeed Balalaie	the generation of N-heterocycles
11:30 – 13:30* 15:00-17:00	Oral Lectures	
15:00-15:30	PhD Student Roghayyeh Asgharzadeh	Biginelli Synthesis of Dihydropyrimidinone Dimers and Evaluation of Their in Vitro Anticancer Activity
15:30-16:00	Postdoctoral Researcher Malihe Pooresmaeil	Dialdehyde Carboxymethyl Cellulose as A Safe Crosslinker for Fabrication of Photoluminescent Gelatin Bionanogels
16:00-16:30	PhD Student Isa Shahroudbari	Investigation of Carbon Dioxide Conversion to valuable Hydrocarbons Over Promoted Iron Catalyst
16:30-17:00	PhD Student Homa Kohzadi	Synthesis and Characterization of NAS@Cu as a Novel Heterogeneous Nanocatalyst in the C-C and C-O Coupling Reactions
13:30 – 14:30* 17:00-18:00	Invited Lecture Prof. Issa Yavari	Old and new theories in chemistry
14:30 – 16:30* 18:00-20:00	Poster session 2 :	From isoc28-01830281 To isoc28-04400540

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28th Iranian Conference on Organic Chemistry

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Conference Schedule Day 3 (3 March 2022) Title Time Presenter 4:30 - 5:30* Mandelic Acid: A truly benign novel organocatalyst for **Invited** Lecture 8:00-9:00 Prof. Bubun Banerjee diverse organic transformations $5:30 - 7:30^*$ Oral Lectures 9:00-11:00 PhD Student 9:00-9:30 Spectral Characterisation and Computational Studies of Some New 3-(2-Arylhydrazineylidene) Fateme Ashouri Mirsadeghi Benzo[h]quinolin-2,4(1H,3H)-dione Dyes GAP Chemistry Principles for Access to 1,5-Diionic 9:30:10:00 PhD Student Highly Substituted Furans via Fast, Concise, and Reza Rezaivehraad Efficient One-pot Three-component Assembly 10:00-10:30 Assistant Prof. Chitosan Functionalized Polymer Supported Metal Nanoparticles: An Efficient Heterogeneous and Neda Seyedi Recyclable Nanocatalyst for Organic Reactions 7:30 - 8:30* Invited Lecture Benign-by-design nanomaterials for Sustainable 11:00-12:00 Prof. Rafael Luque Alvarez applications: present and future 8:30 - 10:30* Prayer and Lunch Break 12:00-14:00 10:30 - 11:30* Invited Lecture Synthesis of dithiazolopyridine derivatives and their 14:00-15:00 Prof. Hossein Reza Darabi ion sensor application 11:30 - 12:30* **Concluding Remarks** 15:00-16:00

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Invited Lectures



Prof. Mohammad Ali Zolfigol Minister of Science, Research and Technology Bu-Ali Sina University



Prof. Issa Yavari Tarbiat Modares University



Prof. Saeed Balalaie K.N.Toosi University of Technology



Prof. Ahmad Shaabani Shahid Beheshti University



Prof. Ghodsi Mohammadi Alzahra University



Prof. Hossein Reza Darabi



Prof. Reza Zadmard



Prof. Rafael Luque Alvarez Universidad de Córdoba- Spain



Prof. Yanlong Gu Huazhong University of Science and Technology- China



Prof. Asit K. Chakraborti Department of Medicinal Chemistry National Institute of Pharmaceutical Education and Research-India



Prof. Bubun Banerjee Department of Chemistry, Akal University-India



Dr. Roozbeh Yousefi Michigan State University-USA

Oral Lectures



Associate Prof. Mehdi Bayat Bu-Ali Sina University



PhD Student Elham Badali Kharazmi University



Postdoctoral Researcher Mehran Ghasemi University of Tehran



Postdoctoral Researcher Malihe Pooresmaeil University of Tabriz



PhD Student Fateme Ashouri Mirsadeghi Lahijan Branch, Islamic Azad University



Associate Prof. Hossein Ghafuri Iran University of Science and Technology



Master of Science Amin Rahimzadeh Payon Cosmetic Group



Associate Prof. Azadeh Ebrahimian Pirbazari University of Tehran



PhD Student Isa Shahroudbari University of Mazandaran



PhD Student Reza Rezaiyehraad Tarbiat Modares University



Associate Prof. M. Hosseinnezhad Institute for Color Science and Technology



PhD Student Faezeh Nemati Shahid Beheshti University



PhD Student Roghayyeh Asgharzadeh University of Mohaghegh Ardabili



PhD Student Homa Kohzadi Ilam University



Assistant Prof. Neda Seyedi University of Jiroft

Oral Lectures

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28th Iranian Conference on Organic Chemistry 1-3 March 2022

Chemistry & Chemical Engineering Research Center of Iran





Biography of presenting author

Isa Shahroudbari studied Chemistry at the Shahid beheshti University, Iran and graduated as MS in 1994. He received his B.S degree in 2015 at Payame Noor University, Ramsar branch, Mazandaran. He then joined the research group of Prof. Sarrafi at the Faculty of Chemistry, university of Mazandaran, Iran as Ph.D student in organic Chemistry in 2016. Email: isa.shahroudbari@stu.umz.ac.ir Contact Number: +98 911 391 6119

Investigation of Carbon Dioxide Conversion to valuable Hydrocarbons Over Promoted Iron Catalyst

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Abstract

Carbon dioxide is considered an inert gas because of its high thermodynamic stability. CO_2 is regarded as a potential carbon raw material, but also as an air pollutant. CO_2 is a cheap, nontoxic, and abundant C-1 feedstock, and its chemical utilization is a challenge and important topic. Many processes have been used to utilize CO_2 fully, including CO_2 reforming of CH_4 to produce synthesis gas, hydrogenation to produce methanol and hydrocarbons, and the synthesis of dimethyl carbonate, cyclic carbonate, and dimethyl ether.¹⁻³

Hydrogenation of CO₂ to valuable hydrocarbons is carried out over iron based catalysts. Fe-based catalysts have been used in the CO₂-Fischer-Tropsch Synthesis (FTS) process because they have catalytic activities in both Reverse Water-Gas Shift (RWGS) and FTS reactions.^{4,5}

The Fe-based catalysts are preferred for the production of olefin hydrocarbons, but the product distribution depends on the types and combinations of active metals, promoters, and support materials.⁶⁻⁸ In this study, iron based catalyst was prepared using Incipient wetness impregnation procedure. The catalyst was characterized by BET, XRD, H₂-TPR and TEM techniques. The evaluation of catalyst were carried out in a fixed bed reactor at the process conditions of temperature of 300 °C, pressure of 20 atm, H₂ to CO₂ ratio of 3 and GHSV of 3 nl.h⁻¹.g_{cat}⁻¹. The results of experiment showed that conversion of CO₂ was 26.8% with major products of C₁, C₂ to C₄, C₅+ and CO. Product selectivity were calculated using the data collected at 16 h time on stream. Products selectivity of the catalyst are indicated in Figure 1.



Figure 1: Products selectivity of the catalyst

Acknowledgements

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Biography of Presenting Author

Dr. Mozhgan Hosseinnezhad received her Doctor degree at Amirkabir University of Technology (Polytechnic Tehran, Iran) in 2014. After hers doctoral degree, she was appointed as an assistant professor at the Institute for Color Science and Technology in 2015. Hers current research interests include the design and synthesis of organic dyes and photosensitizers for dye-sensitized solar cells and optical devices Email: hosseinnezhad-mo@icrc.ac.ir Contact Number: 09123856689

The Synthesis of An Organic Dyes Based on Thioindigo for Dye-Sensitized Solar Cells

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^b Center of Excellence for Color Science and Technology, Institute for Color Science and Technology, Iran.

Abstract

The organic molecules with D $-\pi$ -A structures have attracted increasing attention since they can serve as electro active and photoactive materials in molecular electronics, such as biochemical fluorescent technology, efficient nonlinear optical (NLO) materials, electro generated chemiluminescence, organic light-emitting diodes (OLEDs), and solar cells.¹ Recently, more and more attention has been directed to the application of metal-free organic dyes in DSSCs.² In this work, a new metal free dye with thioindigo sensitizers is reported and its optical, electrochemical, photovoltaic properties and structural relationships are investigated in detail. The general procedure for preparing metal free organic dyes is given in Figure 1. The absorption spectrum of dye in THF has two distinct absorption bands at around 390 and 505 nm, respectively. The absorption peaks at around 390 nm correspond to the $\pi \rightarrow \pi^*$ electron transition of the conjugated molecule; and the absorption peaks at around 505 nm can be assigned to an intramolecular charge transfer.³ The λ_{max} of dye adsorbed on a TiO₂ film is 527 nm. Upon dye adsorption on to a TiO₂ surface, the wavelength of maximum absorption is bathochromically shifted by 22 as compared to the corresponding spectra in solution, implying that dye adsorbed on to TiO₂ surface contain partial J-type aggregates.⁴ The oxidation potential (Eox) of organic dye was measured in acetonitrile by cyclic voltammetry.² There are two distinct redox waves observed in the voltammogram. The first oxidative wave (I) was due to the oxidation of the internal standard of ferrocene, whereas the second wave (II) was due to the electrochemical oxidation of the dye. The oxidation peak potential (Eox) for organic dye can be calculated to be 0.67 vs Fc/Fc⁺ in acetonitrile. The $E_{0.0}$ of dye was calculated to be 2.25 V, therefore, the E_{ox}-E₀₋₀ level of dye is estimated to be -1.58 V vs Fc/Fc⁺ in acetonitrile. The DSSCs was prepared and compared to investigate the relationships between the sensitizing behavior of dye molecule and its structures. The solar-energy-to-electricity conversion efficiency (η), short circuit current (J_{sc}), the opencircuit photovoltage (V₀c) and the fill factor (FF) of the DSSCs are 3.07%, 7.39 mAcm-1, 0.62 V and 0.67, respectively.



Figure 1: Synthesis route of the dyes

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Biography of Presenting Author

Fatemeh Ashouri Mirsadeghi studied pure chemistry at the Guilan university and graduated as B. A in 2011. Then she studied organic chemistry at the Islamic Azad university Rasht branch. She received her M.A degree in 2015, after one year she started her PhD course supervised by Dr Enayatollah Moradi Rufchahi (Associate Professor) at the Islamic Azad university Lahijan branch in 2016. She is currently in her final year of PhD. She works on computational chemistry and synthesis of a new generation of dyes.

In addition to her academic work, she is also a professional self taught artist. She had many exhibitions in Iran. To learn more about her work, visit her Instagram.

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Spectral Characterisation and Computational Studies of Some New 3-(2-Arylhydrazineylidene) Benzo[*h*]quinolin-2,4(1*H*,3*H*)-dione Dyes

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Department of Chemistry, Faculty of Science, Lahijan Branch, Islamic Azad University, Lahijan, Iran.

Abstract

4-Hydroxyguinolin-2(1*H*)-one (2,4-dihydroxyquinoline) and N-butyl-4-hydroxyguinolin-2(1H)-one were respectively employed for the synthesis of C.I. Pigment Yellow 7 and C.I. Mordant Yellow 30. More recently, a wide range of substituted 4-hydroxyquinolin-2(1H)-ones have been synthesized and used as coupling components for the preparation of 3-aryl-azo disperse dyes in order to investigate their biological activities.¹⁻³ The visible absorption studies clearly indicated that the lactam moiety of quinoline-2(1H)-one section has strong electron withdrawing nature and the dyes bearing electron donating groups on diazo components show bathochromic shifts with respect to unsubstituted and electron-withdrawing substituents.⁴⁻⁷Herein, A series of substituted anilines with different electron releasing and electing accepting substituents have been diazotized and coupled with 4-hydroxybenzo[h]quinoline-2(1H)-one in basic ethanol solution at 0-5°C. The structures of these newly synthesized azo dyes were assigned by IR, ¹H NMR and Mass spectroscopic analyses. ¹H NMR spectroscopic studies implied that the dyes exist as keto-hydrazo-keto tautomeric form in solution state. The UV-vis absorption spectra of the dyes in solvents with different polarities showed no distinct change owing to their strong intramolecular hydrogen- bonding interactions. The results also showed that λ_{max} of hydroxyquinoline based azo dyes are mostly independent of the nature of the substituents bonded with phenyl rings of the diazo components. The effects of acid and base on the visible absorption spectra of the of the dyes in ethanol were also studied and showed that the spectral changes are clearly dependent upon the protonationdeprotonation of the dye molecules.



 $\begin{array}{l} X= \textbf{2a}= 4\text{-}\mathrm{OCH}_3, \ \textbf{2b}= 4\text{-}\mathrm{C}_2\mathrm{H}_5, \ \textbf{2c}\text{=-H}, \ \textbf{2d}\text{=}3\text{-}\mathrm{OCH}_3, \ \textbf{2e}\text{=}2\text{-}\mathrm{CF}_3, \ \textbf{2f}\text{=}3\text{-}\mathrm{CF}_3, \\ \textbf{2g}\text{=}3\text{-}\mathrm{CN}, \ \textbf{2h}\text{=}3\text{-}\mathrm{Cl} \quad \textbf{2i}\text{=}3\text{-}\mathrm{NO}_2, \ \textbf{2j}\text{=}2, 4\text{-}\mathrm{Cl}, \ \textbf{2k}\text{=}2\text{-}\mathrm{Br}, 4\text{-}\mathrm{CH}_3 \end{array}$

Scheme 1: Synthetic pathwayfor the preparation of the dyes 2a-k.

References

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Biography of Presenting Author

Elham Badali received her BSc in pure chemistry in 2013 from Kharazmi University, Tehran, Iran, and her MSc in organic chemistry from Shahid Beheshti University, Tehran, Iran, under supervision of Prof. Ahmad Shaabani, in 2017. Now, she is working as a PhD student under supervision of Dr Azizolah Habibi and Dr Azim Ziyaei Halimehjani at Kharazmi University, Tehran, Iran. Her research interests include synthesis of novel intermediate for organic transformation and providing efficient catalyst for organic transformations. Email: badaliela@yahoo.com Contact Number: +989354128791

One-Pot Three-Component Synthesis of 2-Iminothiazolines in Catalyst-Free Procedure

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Abstract

Two-imino-1, 3-thiazolines as a privileged heterocyclic compound shows various therapeutic properties in drug development. The thiazole-2-imine derivatives have gained significant biological attention due to their interesting pharmacological activities such as anti-inflammatory, analgesic, anti-bacterial, anti-fungal, anti-consultant and anti-viral.¹⁻² There are several methodologies for the synthesis of this type of compounds.³ In this research, the synthesis of 2-iminothiazolines was developed *via* one-pot three-component reaction of amines, isothiocyanates, and nitroepoxides in THF at 15 °C. The corresponding products were synthesized in high to excellent yields in optimized reaction condition. Moreover, cytotoxic activity of synthesized 2-iminothiazolines was elaborated in cultured C6 cells within 5 days through MTT assay and morphological observation. Anti-proliferative activity of the 5-(2,4-dichlorophenyl)-3-ethyl-4-methylthiazol-2(3*H*)-ylidene)aniline proved in higher concentrations with more than 3 folds growth inhabitance of cells compare with normal subcultured cells. Growth suppression of C6 cells indicates desirable impact of synthesized 5-(2,4-dichlorophenyl)-3-ethyl-4-methylthiazol-2(3*H*)-ylidene) aniline for cancer suppression in cancer treatment.



Scheme 1: Description for the synthesis of 2-iminothiazolines

References

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Chen, C. Y.; Barve, I.J.; Sun, C.M., *ACS Comb. Sci.* **2016**, 18, 10, 638–643.







Biography of Presenting Author Roghayyeh Asgharzadeh, PhD student in organic chemistry at the University of Mohaghegh Ardabili. Email: RoghayyehAsgharzdaeh@uma.ac.ir, Contact Number:09148392943

Biginelli Synthesis of Dihydropyrimidinone Dimers and Evaluation of Their in Vitro Anticancer Activity

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Abstract

There is a growing attracting interest against ethyl 4-substituted-6-methyl-3,4-dihydropyrimidine-2-one-5carboxylates (Biginelli DHPMs) in the synthetic chemistry community owing to their pharmaceutical potential and heterocyclic scaffold.¹ The multifunctionalized dihydropyrimidinones scaffold represents a class of heterocyclic compounds with significant pharmacological efficiency and are receiving considerable amount of interest. They exhibit a diverse pharmacological profile like calcium channel blockade, a1aadrenoreceptor antagonism, antibacterial, antifungal and other related properties.² Dimerization has the capacity to expand the biological spectrum, increase the activity, overcome the drug resistance, and improve pharmacological, pharmacokinetic, as well as physicochemical profiles, so dimerization represents a promising strategy to develop novel drugs. Furthermore, the metabolic pathways in healthy cells which are affected by monomers may be less affected by the dimers.³



Scheme 1. Synthesis of dimer of dihydroprimidinones.

With the attention to the importance of dimerization of pharmaceutical molecules and Biginelli products, in this project, we decided to synthesis dimers of dihydroprimidinone through the Biginelli reaction by dialdehyde and investigate in vitro anticancer activity of them.

References

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Biography of Presenting Author Homa Kohzadi was born in Ilam, Iran. She is a PhD student of organic chemistry at Ilam University, Iran. Her main research interest is organic synthesis and nanocatalysts.

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Synthesis and Characterization of NAS@Cu as a Novel Heterogeneous Nanocatalyst in the C-C and C-O Coupling Reactions

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Abstract

In recent years, nano-catalysts with carbon substrates, including carbon black, carbon nanofibers, graphene and nanotubes have been investigated as a useful and sustainable alternative catalyst substrate ¹⁻³. In this research, copper-grafted natural asphalt sulfonate (NAS@Cu) as a new and efficient catalyzing substrate was identified, synthesized and introduced, and its catalytic properties were investigated in the C-C and C-O coupling reactions (Scheme 1). This nanocatalyst is synthesized by sulfonating natural asphalt as a high-carbon, cost-effective and accessible substrate by high-concentration sulfuric acid. After being neutralized by NaOH, it is transformed into sodium natural asphalt sulfonate (NAS@Cu). Ultimately, the nanocatalyst was synthesized through a displacement reaction of sodium natural asphalt sulfonate with copper chloride.

NAS@Cu is a heterogeneous catalyst with advantages such as having a high specific surface area, being environmentally friendly and economically sound, and being simple to be purified and separated from the reaction mixture. Moreover, the nano-catalyst was recycled several times without any significant changes in its catalytic properties.



Scheme 1

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Synthesis of Novel Noscapine Analogues as Potential β-tubulin Inhibitors

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ABSTRACT

Cancer is one of the leading causes of death across the world. Nature is still the best source of new medicines, One of the most popular herbal drug source is *Papaver somniferum*, The dried Latex produced by the seed pods, the opium, contains a mixture of alkaloids such as morphine, noscapine, codeine, thebaine, papaverine, and narceine.^{1,2}Among opium alkaloids mentioned above, noscapine is the second abundant one and has the lowest toxicity among them. Furthermore, in contrast to morphine, noscapine is not addictive and narcotic. Noscapine is a phthalideisoquinoline alkaloid which was discovered in 1817 by Rabiquet.³

Twenty novel 1,2,3-triazole noscapine derivatives were synthesized starting from noscapine by consecutive *N*-demethylation, reduction of lactone ring, *N*-propargylation and Huisgen 1,3-dipolar cycloaddition reaction. In order to select the most promising molecules to subject to further biophysical and biological evaluation, a molecular docking analysis round was performed using noscapine as reference compound. The molecules featuring docking predicted binding affinity better than that of noscapine were then subjected to MTT assay against MCF7 cell line. The obtained results showed that all the selected triazole derivatives exhibited a remarkable lower cell viability compared with noscapine in the range of 20 μ M in 48h. In the attempt to correlate the biological activity with the ability to bind tubulin, the surface plasmon resonance (SPR) assay was employed. Compounds **8a**, **8h**, **9c**, **9f** and **9j** were able to bind tubulin with an affinity constant values in the nanomolar range and higher if compared to noscapine. Integrating computational predictions and experimental evaluation, two promising compounds (**8h** and **9c**) were identified, whose relevant cytotoxicity was supposed to be correlated with tubulin binding affinity. These findings shed more lights onto structural modifications of noscapine that will drive further development toward the identification of more potent cytotoxic agents targeting tubulin.



Reagents and conditions: a) H_2O_2 , ACN, r.t , 1 h, 98%. b) FeSO₄.7 H_2O , MeOH, -8 °C, 8h, 60%. c) HBr, Br₂/H₂O, r.t, 1h, 50%. d) BF₃.Et₂O, NaBH₄, THF, -5 °C, 24h, 80%. e) Propargyl bromide, K₂CO₃, ACN, reflux, 2h, 90%. f) R¹N₃, CuSO₄ 20%, NaAsc 40%, MeOH: CH₂Cl₂ (2:1), r.t, 5-20 min, 70-95%.

Scheme 1 : General pathway for the synthesis of target molecules.

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Theoretical Study on the Formation Mechanistic of 3-phenyl-4-methyl-benzonitrile by using Suzuki-Miyaura and Hiyama–Denmark Cross-Coupling Reactions

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Abstract

Palladium PEPPSI-type complexes with small NHC ligand were applied as catalyst precursors in crosscoupling reactions forming a wide range of non-symmetric biaryls with high yields.¹There are many examples of the application of PEPPSI complexes in the Suzuki–Miyaura reaction, in which their excellent catalytic activities and versatilities are clearly evidenced.² The general in catalytic cycle suzuki-miyaura cross-coupling reaction includes three main steps. Oxidative addition of C-X (X=F, Cl, Br etc.) bonds which occured in the Pd(0) center, sequential transmetalation which takes place to yield di-organometal intermediates, and finally reductive elimination affords the coupled product, regenerating the catalytically active species.³ At the Cam-B3LYP-D3 level of theory, the rivalry between Hiyama–Denmark and Suzuki–Miyaura Pd-catalyzed crosscoupling reaction mechanisms for the development of 3-phenyl-4-methyl-benzonitrile from two potential reactions is studied. Because of the nature of the experimental production of 2-phenyl-toluene synthesis from both Suzuki–Miyaura and Hiyama–Denmark cross-coupling reactions¹, the 3-phenyl-4-methyl-benzonitrile formation process was initially assessed computationally using two cross-coupling reactions. Computational findings that are consistent with experimental data show that Hiyama–Denmark cross-coupling is best suited thermodynamically and kinetically to the synthesis of 3-phenyl-4-methyl-benzonitrile in the presence of Pd(0)-NHC as a catalyst (See Scheme 1).



Scheme 1. Energetic profile of the potential reaction pathways for formation mechanism of 3-phenyl-4-methylbenzonitrile via Suzuki-Miyaura and Hiyama-Denmark cross-coupling reactions and their relative Gibbs energy (kcalmol⁻¹) at of Cam-B3LYP-D3/def2-TZVP//Cam-B3LYP-D3/def2-SVP level of theory in ethylene glycol as solvent.

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Assembly of Indole Cores through a Palladium-Catalyzed Metathesis of Ar–X $$\sigma$$ -Bonds

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Abstract

Phosphines play a crucial role in most transition-metal- catalyzed cross-coupling reactions in stabilizing the active metal center and fine-tuning the selectivity of the conversion.¹ The initially formed aryl palladium species, however, have been reported to frequently undergo an undesirable aryl/aryl interchange with the aryl substituents of triarylphosphine ligands via C-P bond scission, leading to undesired scrambled side products and deactivation of the catalyst.² Accordingly, early studies were focused on shutting down this side trail. However, by the accumulation of mechanistic data, new avenues for developing various catalytic reactions through the strategic utilization of the metathesis of Pd-C and P-C bonds have been recently opened.³ creating a suitable catalytic system to provide an appropriate platform for a productive ligand exchange would find great applications in organic synthesis. Inspired by recent advances in this area, we set out to identify reaction conditions to construct indole scaffolds with the benzoic ring built by the aryl section of simple triarylphosphines via the metathesis of Ar-X σ-bonds. Aryl's attachment to phosphorus can be activated via a controlled exchange between P-Ar and Pd-Ar, and it can participate in a cascade annulation reaction for the purpose of the construction of more complex molecules, which is unprecedented to the best of our knowledge and would be very attractive. This transformation exploits palladium catalyzed reversible oxidative addition/reductive elimination chemistry to offer the synthesis of a diverse array of highly functionalized indoles in high yields and opens a new window for the application of simple phosphines in the assembly of indole cores.

We describe the development of a new method for construction of highly substituted indole scaffolds through the strategic utilizing of the metathesis of Ar-X σ -bonds based on the dynamic nature of palladium-based oxidative addition/reductive elimination. A suitable and simple catalytic system has provided an appropriate platform for a productive ligand exchange and consecutive carbopalladation/C-H activation/amination of phosphine ligands with alkynes and aromatic/aliphatic amines for construction of structurally diverse indoles.



Scheme 1: synthesis of diverse indoles via the carbopalladation/C-H activation/amination cascade

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Efficient Degradation of Tetracycline Contaminant in artificial Wastewater Using Hybrid Photocatalysts Under Visible Light

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Abstract

Tetracycline (TC) antibiotics are the second most common antibiotics for treating a wide range of infections in humans and animals mainly due to their antimicrobial properties. Almost 70-90% of tetracycline antibiotics consumed by humans and animals are disposed without any structural change and can enter the ecosystem causing new environmental issue.¹ In recent years, there have been many concerns about the antibiotic contaminants and efficient strategies must be employed to reduce antibiotics pollution.^{2,3} In the present study, titanium dioxide nanosheets (TNs) and cadmium sulfide (CdS) nanoparticles were synthesized on graphene oxide. The synthesized samples were applied to the photocatalytic degradation of tetracycline (TC) antibiotic under visible light. We obtained 84% degradation of TC after 180 minutes under visible light. Active species trapping tests showed that active oxygen species had main role in the degradation process (Figure 1). The experimental results confirmed the hybrid photocatalysts are promising candida for treatment of industrial wastewater.



Figure 1: Degradation of TC with hybrid photocatalysts under visible light

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Dialdehyde Carboxymethyl Cellulose as A Safe Crosslinker for Fabrication of Photoluminescent Gelatin Bionanogels

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Abstract

Nanogels are three-dimensional, nanometric-sized hydrogels that combine the features of both nanoparticles and hydrogels.¹ Up to now, several types of polymers have been used for nanogels fabrication. Among them, gelatin is preferred and plays an outstanding role in the anticancer drug delivery process due to its special features.² There are different ways for the fabrication of gelatin-based nanogels but in recent decades the naturally-derived crosslinkers received increasing attention. In particular, DCMC with riched reactive aldehyde groups is a low-cost, water-soluble, renewable, and abundant polysaccharide-based crosslinker.³ By considering these in this work at first carbon dots (CDs) were green synthesized from low-cost and more available black pepper. Then the facile synthesized dialdehyde carboxymethyl cellulose (DCMC) was used as a safe chemical crosslinker for gelatin; a mixture of gelatin and CDs owing to its excellent chemical reactivity and biocompatibility (CDs/DCMC-Gel). The Schematic of crosslinking is shown in Figure 1. All used implemented physicochemical analytical methods, for instance, FT-IR, EDX, XRD, TEM, and UV-Vis confirmed the CDs/DCMC-Gel bionanogel fabrication route and the SEM analysis specified the spherical morphology with a diameter size of ~200 nm for it.



Figure 1. Schematic of the CDs/DCMC-Gel synthesis.

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GAP Chemistry Principles for Access to 1,5-Diionic Highly Substituted Furans *via* Fast, Concise, and Efficient One-pot Three-component Assembly

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Abstract

Finding the novel synthetic methods of furan-containing compounds has become challenging and interesting for chemists. This interest has resulted from the presence of these scaffolds in important natural products and biologically active compounds as key structural motifs. This subject is reflecting the importance of trying to find new and efficient methods to produce furan derivatives that allow facile access to substituted furans under mild conditions from commercially available precursors.¹⁻³

In recent years, our research group has been interested in the chemistry of 3-substituted chromones such as 3-formyl and 3-cyanochromones.^{4,5,7} These compounds can act as important synthetic intermediates since they possess three electrophilic positions and can be used as a dienophile. Furthermore, they can be served in a ring-opening reaction at the 2-position and its relevant secondary conversions.^{6,7}

Herein, we report an efficient synthetic approach for the preparation of novel highly substituted 1,5-diionic furan compounds (Scheme 1) using 3-cyanochromone substrates. Firstly, phosphonium salts were obtained *via* nucleophilic attack of Huisgen zwitterion to 3-cyanochromones. Finally, these intermediate salts underwent a proton migration, intramolecular cyclization, and ring-opening reaction converted to the target products. The synthesized furans could be easily purified without traditional purification techniques (chromatography and recrystallization). The proposed structures of **4a-g** were determined by the spectral data (IR, ¹H and ¹³C NMR, Mass). Finally, the structure of **4a** was confirmed by X-ray crystallography.



Scheme 1: Synthesis of novel fully substituted 1,5-diionic furans

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Preparation of g-C₃N₄-based Nanocatalysts and Their Application in Condensation and Oxidation Reactions

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Abstract

In this study, according to the structure and features of graphitic carbon nitride $(g-C_3N_4)$, the new heterogeneous catalysts and photocatalysts were synthesized based on $g-C_3N_4$. The $g-C_3N_4$ nanosheets were functionalized with thiamine hydrochloride (Vitamin B1)¹ and L-arginine² by using 1,3-dibromopropane as a covalent linker. As well as, $g-C_3N_4$ /FeWO₄ nanocomposite as a visible light-driven photocatalyst was prepared to improve the catalytic performance of the $g-C_3N_4$.³ Also, mesoporous $g-C_3N_4$ were modified with copper ions and used as an efficient catalyst with remarkable surface area.⁴ The structure of the synthesized heterogeneous catalysts were confirmed by various analyzes and they have been used in several condensation and oxidation reactions. The synthesized nanocatalysts have advantages such as ease of separation, shortening reaction time, and increasing product yields.

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Raw Materials for The Production of Natural Cosmetics

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Abstract

In recent years, the cosmetic industry has grown up worldwide due to the high demand for consumer health and beauty-related goods in different fields such as oral-Care, body Care, Haircare, Skincare and Textile rinse. The turnover of this industry is estimated at around 50 billion Dollars in 2022. Also great effort has been accomplished via different academic and industrial institutes to provide formulation and producing Natural and Artificial raw material and finish products in cosmetics. Not only at this path mentioned, but organizations also face different problems in fields such as shortage of raw material, Quality of raw material and finish product, and side effects of products. For this aim in recent years, applying different natural ingredients in cosmetic products has become a trend in cosmetic products due to high adaptability with body cells without ant damaging to body, compatibility with the environment, and ease of access to reach.

This research has analyzed the different roles of natural ingredients in cosmetic products with a tendency to green chemistry. We suggest replacing new natural ingredients with harsh chemical ingredients in cosmetic products. Also, we present two of our unique formulations based on Organic and in-organic chemistry with different elements with novel performances by using near to 95 % of natural-based ingredients.

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Chitosan Functionalized Polymer Supported Metal Nanoparticles: An Efficient Heterogeneous and Recyclable Nanocatalyst for Organic Reactions

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Abstract

Herein, we extracted chitosan from shrimp shells waste by demineralization, deproteinization, and deacetylation processes. Afterward, different polymers was grafted to chitosan to employ as the support for Metal nanoparticles. Characterization of the nanocatalyst was done using Fourier transform infrared (FT-IR), X-ray powder diffraction (XRD), scanning electron microscopy (SEM), mapping, energy-dispersive X-ray spectroscopy (EDS), transmission electron microscopy (TEM), and thermogravimetric analysis (TGA). The prepared nanocatalyst exhibited excellent catalytic performance with a high turnover number (TON) and turnover frequency for ornanic reactions. The prepared catalysts could be readily recovered and reused without any noticeable change in structure and catalytic performance.

Acknowledgements

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Abstracts

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Graphene Oxide Catalyzed Synthesis of Thiazolidine Derivatives

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Abstract

Nowadays, demanding in synthesis of pharmaceutical compounds through affordable and environmentally friendly conditions leads to the development of multicomponent reactions (MCRs).¹ Widespread medicinal applications of thiazolidine derivatives as antimicrobial² and antidiabatic³ activity have prompted researchers to modify the synthesis of these compounds. Necessity of nontoxic and inexpensive conditions led to design simple catalysts. Graphene oxide (GO) as a carbon frame work with widespread conjugated system has good π - π interaction with organic compounds. This phenomenon leads to take active reaction sites nearly and progress the reaction. Furthermore, various oxygen functionalized groups like hydroxyl or epoxy on GO surfaces make it as effective acid catalyst to activate the reaction sites.⁴

In continuation of our investigation in heterogeneous catalyst,⁵ in this report we describe the synthesis of thiazolidine derivatives through three component reaction of amines, maleimide and isothiosyanates in tetrahydrofuran as solvent and in the presence of catalytic amount of GO as a heterogeneous catalyst. The obtained results indicated that the corresponding thiazolidine derivatives were obtained in high yield 85-90% after 2-4 hour.



Scheme 1. Synthesis of thiazolidine derivatives using GO catalyst

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Synthesis of Some New Bisamide-Solfunamide Derivatives

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Abstract

Bisamides have a wide range of pharmacological properties, as exemplified by their antitumor, antidiabetic and neuroprotective activities. In particular, chiral bisamides have been proposed as drugs for the treatment of many diseases for their activity as histone deacetylase inhibitors, serine protease inhibitors and neurological agents.¹

Sulfonamides were the first drugs with a selective effect on bacteria, and which could be used systemically against bacterial infections. The first successful experiments showing that mice intraperitoneally infected with Streptococcus pyogenes could be protected from peritonitis by the chemically synthesized Prontosil rubrum (4-sulfonamide-2',4'-diaminoazobenzene) were performed in 1932 by Gerhard Domagk.²

In this research we coupled bisamides and sulfonamides by ring opening azlactone derivatives by 4-Amino sulfonamide (Scheme 1). Based on good optimal features of bisamides and sulfonamides, we expect these derivatives to have good biological properties.



Scheme 1: Synthesis of bisamide-solfunamide derivatives

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Green Multicomponent Synthesis of Some Spirochromene Indole Derivatives via **Electro-Catalyzed Reaction**

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Abstract

Electrochemistry is an established approach in modern synthesis laboratories, and widespread application of electrochemistry in organic synthesis is considered as important and powerful tool. Electrochemical reaction-assisted synthetic organic chemistry is an increasingly popular field as indicated by numerous publications.1

Multicomponent reactions, which involve 1HIndole-2,3-dione (isatin) and occur as one-pot catalytic domino processes, are the most common and efficient methods of synthesis of spiro-fused heterocyclic compounds. The three-component reactions of isatin with malononitrile or cyanoacetic ester, and compounds with an enolic component or its synthetic equivalent in the structure were used to obtain a great number of carbo- and heterocyclic spirooxindoles, which are of interest for medical or combinatorial chemistry.²

Based on our interest in green synthesis by electro-catalyzed reaction, we developed a successful route as a green route in organic synthesis of Spirochromene indole derivatives, recently. In this reaction, we used isatines, malononitrile and, dimedone (Scheme 1).



Scheme 1: Synthesis of Spirochromene indole derivatives via electro-catalyzed reaction

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Selective Photocatalytic Oxidation of Benzyl Alcohol to Benzaldehyde by Molecular Oxygen on Ag/AgBr/TiO₂ Nanotubes Under Visible Light Irradiation

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Abstract

In recent decades, titanium dioxide semiconductor due to its properties such as the oxidation-reduction ability of adsorbed compounds on its surface, change of surface properties to hydrophilic state, cheapness, and chemical and physical stability as a high-potential photocatalyst has been introduced. However, this semiconductor needs to be modified due to the lack of absorbed visible light and low quantum efficiency, which uses methods such as doping, coupling, sensitization and other methods. The combination of titanium dioxide with the Ag/AgBr composite and the formation of the ternary Ag/AgBr/TiO₂ system increase the photocatalytic activity (due to the resonant property of the silver plasmon surface).¹⁻⁵

Carbonyl compounds (such as aldehydes and ketones) are valuable compounds in organic chemistry. Carbonyl compounds are used as precursors for vitamins and fragrances. Due to the limitations of alcohol oxidation, including high temperature and pressure, the production of hazardous waste due to the use of mineral catalysts (such as potassium bromate, potassium permanganate,...) as well as the use of chlorinated solvents has led chemists to focus on harmless green reactions with the help of air or molecular oxygen as oxidants in the presence of harmless and inexpensive catalysts.^{6,7} In this report, benzyl alcohol was selectively converted to benzaldehyde under mild conditions and without solvent in the presence of molecular oxygen and heterogeneous Ag/AgBr/TiO₂ nanotubes as photocatalyst in the presence of visible light (Scheme1).



Scheme 1: Strategy for photocatalytic radical oxidation.

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Ag/AgBr/TiO₂ Ternary Component as a Highly Efficient Photo-Induced Reusable Nano- Catalyst for the Thiocyanation of Heterocyclic Compounds

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Abstract

Nowadays among different kinds semiconductor solids, TiO₂ has appeared as the prominent candidate in green photocatalysis processes because of its excellent properties (low cost, nontoxic, operational simplicity, etc). But despite its many advantages, this semiconductor will have disadvantages, including non-absorption of visible light and low quantum efficiency. Today, there are different methods of modifying the optical properties TiO₂.One of the modification methods is the addition of nanocomposite systems such as silver halide to TiO₂ due to the surface plasmon resonance which impedes the recombination and enhances the photocatalytic activity. Ag/AgBr/TiO₂ ternary component nanotube exhibit much higher photocatalytic performance than pure TiO₂, AgBr, and Ag/AgBr under visible light. Generally, Ag/AgBr/TiO₂ is synthesized by cetyltrimethylammonium bromide (cation surfactant) adsorption and photoreduction technique.¹⁻⁴

In organic reactions, thiocyanates are very important because they can be an important intermediate in the synthesis of heterocyclic compounds that are precursors of pharmaceutical compounds, as well as the ability to be converted into different sulfur functional groups which lead to syntheses important compounds. There are many methods used for electrophilic thiocyanation, such as methods such as the use of thiocyanate salt in the presence of CAN or hyper valent iodine reagents or other oxidants, but all of these methods have certain defects such as using stoichiometric oxidants and etc.^{5,6}

In this report, after the synthesis and characterization of Ag/AgBr/TiO₂ ternary component as photocatalyst, we used it in the thiocyanation of heterocyclic compounds (Scheme 1).



THF (1mL), Air

Scheme 1: Visible-light-induced thiocyanation of indole using photocatalyst.

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MIL-53(AI)-N(CH₂PO₃H₂)₂ as a Mesoporous Catalyst for Synthesis of Novel (Nmethyl-pyrrol)-pyrazolo[3,4-b]pyridines via a Cooperative Vinyligous Anomeric **Based Oxidation**

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Abstract

Metal-organic frameworks (MOFs) have been employed at the various fields such as catalysts, electro catalysts, super capacitors, drug delivery, sensors, batteries, membranes, and absorbents due to the eyecatching features such as various synthesis methods, structural diversity, high surface area, and attractive architectures.¹ Besides, potential functionalization and post-modification of MOFs have exposed the art of chemists in different fields.² Lots of researches have been done to achieve a novel pyridine and other derivatives as drug candidates.³ Aryl and heterocyclic compounds substituted with β -ketonitriles have shown unique class of useful intermediates. Herein, we wish to report a green methodology for preparing of new MIL-53(AI)-N(CH₂PO₃H₂)₂ as an efficient mesoporous catalyst for synthesis of new (*N*-methylpyrrol)-pyrazolo[3,4-b]pyridines by condensation reaction of 3-methyl-1-phenyl-1H-pyrazol-5-amine, 3-(1methyl-1H-pyrrol-2-yl)-3-oxopropanenitrile and various aromatic aldehydes (mono, bis and tripodal) under green conditions (Scheme1).



Scheme1: Synthesis of new (N-methyl-pyrrol)-pyrazolo[3,4-b]pyridines using MIL-53(AI)-N(CH₂PO₃H₂)₂

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Nano-magnetic-iron Oxides@choline Acetate as a Heterogeneous Catalyst for the Synthesis of 1, 2, 3-Triazoles

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Abstract

Multi-component reactions (MCRs) are one of the substantial areas of green chemistry research which consist of several simultaneous bond-forming reactions in a one-pot manner.^{1,2} MCR synthesis of triazoles is one of the excellent examples The triazoles have been known for a century[3] and they get famous in the early 1980s.⁴ These days plenty of publications have been reported for organic synthesis regarding the progressive organo-catalysts, coordinated to inorganic solids, due to the economical aspect, and environmental dimension.^{5,6} Among inorganic solids, the magnetic nanoparticles iron oxide (Fe₃O₄ and γ - Fe₂O₃) have been used as a surface for heterogeneous catalysis synthesis.^{7,8} Lewis acidity capability, low toxicity, high surface area, simple preparation, their capacity for surface functionalization, and high recovery with an external magnetic field, cause these magnetite nanoparticles have been in focus.⁸⁻¹⁰ Herein, Fe₂O₃/MgO@Ch.OAc (choline acetate), Fe₂O₃/MgO@ Ch.OH (choline hydroxide), Fe₃O₄@Ch.OAc, and Fe₃O₄@Ch.OAt (choline acetate), benzyl azide, and nitro-methane in EtOH as a green solvent.



Scheme 1. Synthesis of 1,2,3 triazoles by three-component reaction

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Synthesis of New Antibacterial Drug Based on Ciprofloxacin

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Abstract

The menace of multi-drug resistance by bacterial pathogens that are responsible for infectious diseases in humans and animals cannot be over-emphasized. Many bacteria develop resistance to antibiotics by one or more combination of resistance mechanisms namely, efflux pump activation thereby reducing bacteria intracellular antibiotic concentration, synthesizing a protein that protects target site causing poor antibiotic affinity to the binding site, or mutations in DNA and topoisomerase gene coding that alters residues in the binding sites. The ability to use a combination of these resistance mechanisms among others creates a phenomenon known as antimicrobial drug resistance. The development of a new class of antibiotics to address bacterial resistance will require many resources, such as time-consuming effort and high cost associated with commercial risk. Hence, the researchers have adopted a strategic approach to enhance the antibacterial efficacy of existing antibiotics by conjugation or combination of existing antibiotics. A number of peptides have become known as antibacterial, cell-penetrating, or membrane-active agents. Antibiotics-Peptide Conjugates (APCs) are a combination of known antibiotics with a peptide connected through a linker.

Thus, joining antibacterial peptides with Ciprofloxacin may be good idea to get benefit of the both compounds' properties and therefore gives better antibacterial agents. The aim of this study was to synthesize Ciprofloxacin- antibacterial peptide conjugates and to investigate the antibacterial activity of the resultant compounds.



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Efficient Synthesis of Cu(II) Modified Mesoporouse Catalyst and its Application in Multicomponent Organic Reactions

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Abstract

In recent years, Mesoprous materials have been attracted the most attention due to special properties such as high surface area, large pore volume, uniform pore size, and high thermal stability couldemployed.^{1,2} The hexagonal MCM-41 is one of the most common mesoporous materials with pore size 2–50 nm.³ Herein we reported an efficient method for sythesis of 2-amino-4-H-pyran and 2,4,5-trisubstituted

Imidazole derivatives in the presence Cu(II)-acetohydrazide supported on MCM-41 as a recyclable nanocatalyst (Scheme 1).

In conclusion, the advantages of this protocol are the use of commercially available, cheap, the simple methodology, practicability, easy of product isolation, short reaction times and high products yields. More importance, the catalysts can be easily recovered using simple filtration and reused for several time without significant loss of their catalytic activity.



X= Cl, Br, CH₃, OCH₃, 3,4OCH₃, 3OH, 4OH, 2NO₂, 3NO₂, H

Scheme 1: sythesis of 2-amino-4-H-pyran and 2,4,5-trisubstituted Imidazole derivatives in the presence Cu (II)-acetohydrazide supported on MCM-41.

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Immobilization of Ni(II) into Functionalized MCM-41 and it's Application in Synthesis of Multicomponent Organic Reactions

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Abstract

The solid materials that have pores in their structure are named porous materials that their porosity is the most important notion about these materials.

According to the IUPAC classification, the three main groups of nanoporous materials are microporous materials (pore size <2 nm), mesoporous materials (pore size 2-50 nm) and coarse pores (pore size > 50 nm).¹ Because of mesoporous silica materials have unique feature such as high specific surface area, plasticity, permeability to fluids¹, high thermal stability and large specific pore volume² this material have many applications in various fields as separators.³

In this work, a new mesoporous catalyst based on MCM-41 was successfully synthesized. The catalyst functionalized MCM-41 (MCM-41@Pr-PTSC-Ni(II)) was identified using FT-IR, TGA, XRD, EDX, AAS, BET and SEM techniques. This mesoporous catalyst was used as an efficient, heterogeneous, recyclable and environment friendly catalyst in the synthesis of tetrahydrobenzo[b]pyran and 1,4-dihydropyrano[2,3-c]pyrazole. (Figure 1).



X= CI, Br, CH₃, OCH₃, 3,4OCH₃, 3OH, 4OH, 2NO₂, 3NO₂, H

Figure 1: synthesis of tetrahydrobenzo[b]pyran and 1, 4-dihydropyrano [2, 3-c] pyrazole

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A Systematic Review on Recent Metabolomics-based Malarial Studies: Importance, Analytical Techniques, and Applications

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Abstract

Malaria is still a serious health and economic problem worldwide. According to the WHO report, there were approximately 219 million cases of malaria in 2019.¹ The complexity of the malaria parasite's life cycle and drug resistance requires research more about malaria with the help of new research strategies. Metabolomics as an efficient approach can perform the process of simultaneous identification of all small molecule metabolites (<1500 Da) in biosamples. Metabolomics using NMR, LC-MS and GC-MS followed by chemometrics can significantly contribute to new malaria studies (Figure 1).²

Sample Collection		
Sample Preparation		
Sample Analysis: MS or NMR		
Data Acquisition		
Data Analysis and Interpretation: Multivariate Analysis, e.g. PCA		

Figure 1: Key stages of a metabolomics study.

In the present study, the latest findings of malaria research utilizing metabolomics were examined in terms of research scopes as well as the analytical techniques used. Articles were searched using the keywords "Malaria" and "Metabolomics" on the PubMed website. Keywords were searched in the title and abstract of the articles. Also, the analytical techniques used in the articles were reviewed using the available valid sources.³ Valid English-language original and review articles in which metabolomics-based malaria research has been included in the results. Relevant charts were drawn using Microsoft Office Excel software. The obtained articles were related to the years 2009-2021. The number of articles on *Plasmodium* biology, drug discovery, and hostparasite interaction was 31, 22 and 19, respectively. In addition, the type of analytical platform used in 21 key metabolic studies was identified. The number of MS, NMR and MS / NMR techniques used were 17, 3, and 1, respectively. The results of the study showed that due to recent advances in the field of systems biology, the MS / NMR-based metabolomics technique is able to provide a powerful tool on Plasmodium biology, malaria drug discovery, host-parasite interaction and changes in disease conditions in patients. Also, more use of MS technique can be given to its high specificity and high sensitivity compared to other conventional methods. Therefore, it seems that the wider use of metabolomics in various fields of new malaria research can significantly help information on basic malaria biology, as well as overcoming the drug resistance of the parasite and development of effective antimalarial drugs. Of course, it is necessary to pay attention to the current limitations in the use of metabolomics in malaria studies.

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The Survey of Phytochemical Properties of *Citrus aurantifolia* Pomaces: As Sources of Natural Medicinal Products

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Abstract

The massive pomace of *Citrus aurantofolia* exhibits a challenging losses exposure difficulty for the processing industries. The resent study was aimed to evaluate the composition and quality of pomace and understand its bioactive compounds to introduce it to different industries such as pharmaceutical, food, medicinal, agricultural etcetera for optimum use. Volatile compounds (VCs) were extracted by hydrodistillation (HD) and Static headspace (SHS) methods.¹ Four different extracts were analyzed for polyphenol compounds identified by HPLC-DAD, total flavonoid content (TFC), total phenolic content (TPC) and antioxidant activity.^{2,3} Limonene (71.7%), β -pinene (8.5%), γ -terpinene (7.3%), myrcene (1.8%) and α -pinene (1.7%), were the main compounds of essential oil (EO) of *C. aurantifolia* pomace by HD extraction. The dominant VCs of *C. aurantifolia* were limonene (49.3%) followed by β -pinene (21.7%), γ -terpinene (9%), α -pinene (6.8%) and sabinene (4.9%), respectively by static headspace analysis. *Trans*-ferulic acid was major polyphenol compound in all studied extracts of *C. aurantifolia* marcs. Methanolic extracts from *C. aurantifolia* pomaces represented higher antioxidant activity, TPC and TFC than other investigated extracts. Our results demonstrated highly positive correlation coefficient between DPPH assay, TPC and TFC of *C. aurantifolia* extracts (P<0.01; R²=0.92, 0.89). Also, Pearson's correlation coefficients (R²) was 0.98 between TPC and TFC in this plant (P<0.01).

This studied marc can be introduced to different industries as a source of bioactive and medicinal natural compounds because of its valuable phytochemical characterization.



Figure 1: Description of some phytochemical assay on C. Aurantifolia pomaces

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Phytofabrication and Characterization of Copper Nanoparticles Utilizing Punica Granatum Leaves Extract and its Antibacterial Activity

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Abstract

This article was done to evaluate an eco-friendly and simple copper nanoparticles (CuNPs) CuNPs biosynthesis by extracts of Punica granatum leaves as the decreasing agent of CuNPs. The formation of CuNPs was characterized by UV-Vis spectrum, Fourier Transform Infrared Spectroscopy (FT-IR), and Scanning Electron Microscopic (SEM) analysis. Based on the results obtained from UV-Vis spectra, a potent resonance oriented can be seen on the silver nanoparticles (CuNPs) surface at 280 nm. According to the FT-IR, the extract of the Punica granatum leaves played the decreasing agent role. The nanoparticles sized around19.82-38.15 nm are inferred by analysis of scanning electron microscopic (SEM).¹ The structural characterization was carried out using XRD consistent with (111), (200), (311), and (400) reflections of the face-centered cubic (fcc) phase of the CuNPs. Since XRD corresponds to the reflections b (111), (200), (311), and (400) of the face-centered cubic (FCC) phase of CuNPs, it has also been used to perform structural properties. One of the most effective ways to control the growth of human pathogens, namely Salmonella, is biologically synthesized CuNPs.² Keywords: Punica granatum leaves, SEM, XRD, FTIR, UV-Vis, Salmonella.

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Synthesis of Copper Oxide Nanoparticles Using Aqueous Plant Extract and its Antibacterial Activity

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Abstract

Nanotechnology is a fascinating research area as a result of producing nanoparticles with different shapes, sizes, chemical composition, dispersity, and their several applications for the human being. Manipulation, creation, and using metallic nanoparticles is greatly important considering reduction of dimensions. Therefore, unique thermal, electronic, and optical characteristics are obtained. The biosynthesis approaches of nanoparticles are prioritized compared to physical and chemical processes as a result of the lower time costs and energy. Green synthesis of nanoparticles is an eco-friendly technique using natural solvents.¹ The current work includes the eco-friendly, and green synthesis of CuNPs utilizing Cu(NO3)2.H2O solution and Peel of Pomegranate extract. Various bio-components exist in the Pomegranate Peel extract works as a reducing agent for this synthesis. The diminant surface plasmon resonance (SPR) peak achieved at 350 nm in UV-Visible spectra confirmed the formed CuNPs. Based on SEM analysis, the spherical uniformly and morphology sized particles (36.99-55.17 nm) were obtained. The green synthesis of copper nanoparticles mediated by the Pomegranate Peel extract was clearly illustrated by FTIR spectrum. The structural characterization was performed utilizing XRD in line with reflections of the face-centered cubic (fcc) phase of the CuNPs (111, 200, 220, and 400). It was found that biologically synthesized copper nanoparticles effectively controlled the progression of human pathogens, namly Salmonella.²

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Yasemi In the summer of 2019 joined Dr. Ashouri research group at the laboratory of Organic Chemistry, University of Kurdistan, as a MS student. And began her research work with working on the synthesis of chiral amines.

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Asymmetric Addition of Phenyl Group to Aromatic Aldimines in The Presence of Nanomagnetic Pd/Fe₃O₄ and Chiral Phosphine Ligands

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Abstract

Chiral amines play an important role in biological activities, pharmaceutical, agricultural and natural products. They are very important intermediates in the synthesis of some drugs and chemicals and act as important ligands in the synthesis of chiral compounds also. One method concerning the preparation of chiral amines is the increase of aryl group to imine using organometal catalysts.¹

Among various catalytic systems, Pd/Fe₃O₄ magnetic nanocatalysts possess the properties of both homogeneous and heterogeneous ones and in addition have several advantages, such as fewer metal residues in the products, a recyclable/reusable catalytic system.² The Pd/Fe₃O₄ catalytic system increases selectivity and reactivity of reaction and easily separated from the mixture with an external magnetic field.^{3,4} In this study, the preparation of chiral secondary Amines **3** through the arylation of protected imines **1** and organic boron compounds **2** in the presence of nanomagnetic catalysts Pd/Fe₃O₄ and chiral phosphine ligands was examined.⁵ The use of Pd/Fe₃O₄ nanomagnetic catalyst with the possibility of recovery and reuse of the nanomagnetic catalyst coordinated with phosphine ligands is one of the highlights of this reaction (Scheme1).

The structure of chiral products is characterized by melting point, IR, ¹H NMR, and ¹³C NMR spectroscopies. The enantiomeric excess (ee) of chiral products is also detected by the polarimeter. The structure and morphology of prepared nanocatalyst Pd/Fe₃O₄ were characterized by EDAX, SEM, FT-IR, TEM, and TGA-DTA.



Scheme 1: Synthesis of amine by *N*-arylation of of imines.

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The First Report of the Synthesis of Hercynite Sulfuric Acid and its Application in the Synthesis of Polyhydroquinolines and 2,3-Dihydroquinazolin-4(1H)-ones

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Abstract

During recent decades, there has been developed a great interest in using heterogeneous (solid) acid catalysts instead of those homogeneous ones, due to their possible recovery and recycling solids, which results in reducing the environmental impact.^{1,2} Some applications of solid acids in organic synthesis have been reviewed by Niknam et al. in 2020.³

In this work, we have developed the Hercynite MNPs as a novel heterogeneous support for the immobilization of sulfuric acid to generate a novel magnetic solid acid catalyst. According to the best of our knowledge, this is the first report on the immobilization of the Sulfuric acid (SO₃H) groups by Zolfigol's method on the surface of hercynite as nanomagnetic catalytic support to get a novel solid acid catalyst.

While exploring its catalytic activity, we found it suitable in the multicomponent Hantzsch synthesis of a wide range polyhydroquinoline derivatives under solvent-free conditions and the cyclocondensation of aromatic aldehydes with anthranilamide for the synthesis of 2,3-Dihydroquinazolin-4(1H)-ones in ethanol under reflux conditions (Scheme 1). Besides, it is worth mentioning that the reactions were highly productive. The role of Sulfuric acid was inevitable as the bare hercynite catalyst failed to make significant impact on the reaction. After the reaction, the catalyst was easily retrieved by magnet and reused for five times with consistent catalytic reactivity. There was also no leaching of Sulfuric acid species in the reaction medium, justifying its true-heterogeneity.



EtOH, reflux

Scheme 1: Hercynite sulfuric acid catalyzed the synthesis of Polyhydroquinolines and 2,3-Dihydroquinazolin-4(1H)-ones.

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Silica Sulfuric Acid Bonded Hercynite MNPs: Synthesis, Characterization and Catalytic Applications in the Rapid Production of bis(pyrazolyl)methanes

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Abstract

The art of synthesis targets molecules via domino reactions including sequentially named reactions have attracted great interest. In this regard, Knoevenagel condensation–Michael addition is one of the most popular sequencies which was utilized to synthesize a wide variety of functionalized organic molecules.¹ *N*-containing heterocycles e.g. bis(pyrazolyl)methanes are a series of the most important compounds which could be prepared by this sequencie.² When the catalysts are present, these compounds with the functionalized aromatic rings, which have fascinated much interest because of their diverse pharmacological and therapeutic properties, can be generated from this reactions.^{1–3}

In this work, the Silica sulfuric acid bonded Hercynite MNPs was designed and synthesized by Zolfigol's method as a novel magnetic solid acid catalyst. Then it was introduced as a new and efficient magnetically recoverable nanocatalyst for the synthesize bis(pyrazolyl)methanes in good to excellent yields via the following protocols: (i) the one-pot pseudo five-component reaction of phenylhydrazine (2 equivalents), ethyl acetoacetate (2 equivalents) and arylaldehydes (1 equivalent), and (ii) the one-pot pseudo three-component reaction of 3-methyl-1-phenyl-1H-pyrazol-5(4H)-one (2 equivalents) with arylaldehydes (1 equivalent). In addition, the magnetic and heterogeneous nature allows easy separation of the catalyst from the reaction mixtures by magnetic decantation and the catalyst could be reused at least 5 catalytic cycles for both of the mentioned reactions without obvious drop of initial activity.



Scheme 1: Silica sulfuric acid bonded Hercynite MNPs catalyzed the synthesis of bis(pyrazolyl)methane derivatives via the one-pot pseudo five-component and one-pot pseudo three-component methods.

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Synthesis of a New Chitosan-*p-tert*-butylcalix[4]arene Polymer as Adsorbent for Toxic Hg²⁺ Metal Ion

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Abstract

In this study, we have synthesized a novel chitosan-*p-tert*-butylcalix[4]arene polymer (CCP) as a highlyefficient adsorbent for Hg²⁺ removal from water. In fact, a lower-rim diamine derivative of *p-tert*butylcalix[4]arene has been cross-linked with chitosan chain by Carbonyl Diimidazole (CDI) as the linker. The structure and properties of the new polymer were characterized by spectrophotometer Fourier Transform Infra-Red, X-Ray Diffraction and Scanning Electron Microscope. Moreover, the adsorption capacity of CCP was studied towards some heavy metal cations such as Hg²⁺, Cd²⁺, Ni²⁺, Co²⁺ and Cr²⁺ in aqueous medium. Particularly, the results showed a considerable ability of CCP to remove Hg²⁺. Therefore, CCP can be introduced as a promising adsorbent for the elimination of Hg²⁺ from wastewaters.



Scheme 1. Synthesis rout of chitosan-*p-tert*-butylcalix[4]arene (CCP).

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Synthesis of a New Polymer-Appended Calix[4]arene for DNA Recognition

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Abstract

In this study, we have synthesized a novel polymer-appended calix[4]arene for DNA recognition. In fact, an upper-rim diamine derivative of calix[4]arene has been synthesized and immobilized onto 2-chlorotrityl chloride (CTC) resin. The structure of the calix[4]arene derivative was characterized by ¹HNMR and ¹³CNMR. The content of chemically bound calix[4]arene derivative in CTC resin was determined by elemental analysis with nitrogen detection. Moreover, the binding affinity to calf thymus DNA (ct-DNA) was investigated using UV/visible spectrophotometry.



Scheme 1. Synthesis rout of CTC-appended calix[4]arene.

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Synthesis of Alendronate as a Bone Seeking Pharmaceutical Agent in Nuclear Medicine

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Abstract

The bisphosphonates (BP's) are a class of drugs that have received considerable attention as efficient osteoporosis drugs to prevent the loss of bone density and excessive bone destruction.¹ The specificity of bisphosphonate-based drugs comes from geminal bis (phosphonates) that work together to coordinate calcium ions. Bisphosphonate molecules preferentially bind to calcium ions. The largest store of calcium in the human body is in bones, so bisphosphonates accumulate to a high concentration only in bones. The most popular first-line bisphosphonate drugs are alendronate and risedronate. Alendronate (4-amino-1-hydroxybutylidene)bisphosphonic acid), sold under the brand name Fosamax, was first describe in 1978 and approved for medical use in United State in 1995 ^{2,4} and was used first by Merck in 1996 as a therapeutic agent.⁵ This compound illustrate high efficiency and long duration period.

Several processes to synthesize mono-phosphonates through C-P bond formation have been established. Our group has a long standing interest in development of new C-P bond formation reactions, C-C bond formation using phosphorus reagents, and synthesis of phosphorus compounds. In this study, alendronate was prepared by using γ -aminobutiric acid, phosphorous acid, and methanesulfonic acid then PCl₃ was added. The product was collected by filtration, washed with cold water and 95% ethanol, and dried. The target product was characterized with Nuclear Magnetic Resonance (NMR) and Infra red (IR) spectroscopy (figure 1). This compound can be used as a precursor to preparation of radiopharmaceutical for diagnostic and therapeutic purpose for bone disorders in nuclear medicine.



Figure 1: Schematic view of synthesis of alendronate

Acknowledgements

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Preparation of Iron-Based Catalyst for Carbon Monoxide Hydrogenation

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Abstract

Due to high concern about global warming, rise of CO₂ level in the atmosphere, depletion of oil reserves and increased cost of petroleum, sustainable and environmentally friendly alternatives are preferred to be used.¹ Fischer-Tropsch synthesis (FTS) is an important technology for producing super-clean transportation fuels.² Conversion of syngas into liquid fuel through catalytic polymerization results in a large range of products such as paraffins, olefins, alcohols and aldehydes and assumes to be an excellent route for the production of green petroleum-based products.³ Several metal catalysts can be used for the FTS among which Iron catalysts seems to be economically achievable on an industrial scale due to lower cost, lower selectivity to methane, less sensitivity to poisoning and greater selectivity for the production of alkenes, oxygenates and branched hydrocarbons.⁴ In this study the iron-based catalyst over γ -alumina support was prepared by a wet-impregnation method.⁵ Catalyst characterization was performed by ICP, XRD, BET, FESEM, TEM(Figure1) and H₂-TPR(Figure2).The Fischer-Tropsch (FT) synthesis reaction of the catalyst was also performed in a fixed bed reactor under condition including of pressure of 20 atm, H₂ to CO ratio of 1, temperature of 300° C and GHSV of 2 nL.h⁻¹.gcat⁻¹. CO conversion and product selectivity were calculated via results of gas chromatography (GC).



Figure 1. TEM image of histogram plot of particle size

distribution for the catalyst



Figure 2. H₂-TPR profile of the catalyst

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Poly(N-2-aminoethylacrylamide)-Cu(I) Grafted on Fe₃O₄@SiO₂: An Efficient Catalyst for N- and O-arylation Reactions

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Abstract

In recent decades, the development and use of heterogeneous silica-based catalysts have been considered. Among different supports for immobilization of catalyst, Fe₃O₄@SiO₂ core-shell have attracted much attention.^{1, 2} A high density of single reaction sites will be available for chemical transformations via the functionalization of these composites. High thermal stability, and easy surface functionalization are some other advantages of these supports. Perhaps, easy magnetic recovery mode is the most attractive feature from the economic and the environmental viewpoints.

The present work describes the synthesis and characterization of poly(N-2-aminoethylacrylamide) grafted on magnetite via surface-initiated atom transfer radical polymerization of acrylamide on Fe₃O₄@SiO₂ coreshell and a subsequent trans-amidation with ethylenediamine.³ The supported polymeric ligand was the complexed with Cu(I) to afford a magnetic supported catalyst, Scheme 1.



We observed that the catalyst can effectively catalyze N-arylation and O-arylation of anilines and phenols

by various aryl halides, known as the Ullmann reaction ⁴, under mild reaction conditions, Scheme 2.



Scheme 2. The Ullmann coupling reaction

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Catalyst-free and Diastereoselective Synthesis of Coumarin-Pyrrolizidine Based Compounds *via* 1,3-Dipolar Cycloaddition Reaction

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Abstract

Multi-component reactions are remarkable tools that are important as a central strategy for achieving environmental adaptation and sustainable advancements in modern chemistry. Herein, we report a green and efficient method for diastereoselective synthesis of pyrrolizidine-coumarins from 1,3-dipolar cyclization using different combinations of L-proline ninhydrin and coumarin. The synthesis of these derivatives is done under noncatalytic conditions.

Preparation of products with high yields, Diastereomeric Selectivity, time efficiency, non-catalytic environment, and non-toxic solvent in the synthesis of pyrrolizidine-coumarin derivatives are the bright sides of this eco-friendly method.

Due to the biological properties of this family of substances as anticancer compounds, anticancer tests on them are underway.



$X = CH_2$ or

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Copper Supported MCM-functionalized 1,2,3-Triazol-4-ylmethanamine: a Nano-Heterogeneous Catalyst Activate for the Click Reaction

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Abstract

Copper-catalyzed reactions of benzyl halides with phenylacetylene are very important routes to constructing triazole units in organic synthesis. Triazoles structures have a crucial role in natural products and pharmaceutical compounds.¹

Recently the heterogenization of homogeneous catalysts and their investigation in the synthesis of the fine chemical has become a major attention of research. On the other hand, triazoles compounds can employ as an efficient ligand for chelating with copper. Therefore, herein we wish to synthesize a heterogeneous copper catalyst grafted on MCM-functionalized 1,2,3-Triazol-4-ylmethanamine and demonstrate its catalytic activity in Click Reactions.²



Scheme 1. Schematic diagram of catalyst preparation



Scheme 2. Conditions for the click reaction.

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Investigation of Structural, Electronic, and Reactivity Properties of the S-Ibuprofen Drug by Quantum Mechanical Calculations

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Abstract

Ibuprofen (2 R, S) with the chemical name 1- [4- (2-methyl propyl) phenyl] is the first member of propionic acid derivatives, the most common NSAID¹ and a non-selective inhibitor of cyclooxygenase (COX).² Many NSAIDs are chiral and marketed as racemic mixtures.³ Experimental research has shown that the Sibuprofen enantiomer is approximately 160 fold more involved in inhibiting prostaglandin synthesis than its R enantiomer, and its anti-inflammatory activity has been attributed almost entirely to the Senantiomer.⁴ In this study, quantum chemical calculations were performed for S-ibuprofen as a stable form of this drug using the density functional theory (DFT) method with the Gaussian09 program at the hybrid functional B3LYP level of theory with 6-31G* basic set (Figure 1). The optimized molecular structures and some electronic properties such as energy of the highest occupied molecular orbital (EHOMO), energy of the lowest unoccupied molecular orbital (ELUMO), energy gap, charge density for all atoms, hardness (η), dipole moment (μ), polarizability (α), electronegativity(χ), global electrophilicity index (ω) and the fraction of the transferred electron (ΔN) were calculated and discussed.⁵ Electron populations, the role of electron transfers, Lewis-occupied orbital donors, and Lewis-Acceptor unoccupied orbital were also calculated for S-ibuprofen using natural bonding orbital analysis (NBO). The results of B3LYP / 6-31G * calculations showed that the energy gap and the dipole moment of S-ibuprofen are (Eg = 6.12 eV) and (μ =1.57), respectively. By comparing the reactivity indices of ibuprofen, results are obtained that determine a low value of chemical potential (μ) and hardness (η) and high value of ω . The value of μ , η and ω showed (-3.30, 3.06, 1.78) for S-ibuprophen.



Figure 1: Optimal structure of S-ibuprofen enantiomer

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Preparation, Characterization, Density and Thermal Conductivity of Graphene-Al2O3 / Ethylene Glycol-Water Hybrid Nanofluid at Low Temperatures: An Experimental Study

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Abstract

Nanofluid research at sub-zero temperatures is limited and their application in the cooling industry has not been progressed. Accordingly, experiments were conducted to investigate the effect of temperature and concentration of nanoparticles on the density and thermal conductivity of Graphene-Al₂O₃/Ethylene Glycol-Water hybrid nanofluid at low and sub-zero temperatures. Nanoparticles were characterized by Brunauer-Emmett-Teller (BET), Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM) and X-ray diffraction (XRD) methods. Hybrid nanofluids were prepared at room temperature by adding nanoparticles with different volume fractions (0.05-2.5%) to base fluid containing a combination of water and ethylene glycol (W:EG/50:50 vol%) and oleic acid and sodium dodecyl sulfonate as surfactants. The density and thermal conductivity of the hybrid nanofluids were experimentally assessed for temperatures between 253 and 303K. Density measurements revealed that the mixing model predictions agreed properly with the experimental outcomes. Results revealed that the thermal conductivity of hybrid nanofluids was dependent on temperatures and nanoparticle concentrations, especially at sub-zero temperatures It was discovered that the greatest improvement of thermal conductivity of hybrid nanofluid is 44% that achieved at nanoparticle volume fraction of 2.5% at temperature of 303.15 K. The obtained results are promising in view of use of Graphene-Al2O3/Ethylene Glycol-Water hybrid nanofluid in cooling applications.

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Design and Synthesis of New 2-Alkylthio-3-arylquinazolinone Derivatives with Potential Anti-cancer Effects

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Abstract

Cancer is known as the second leading cause of mortality in many countries. Due to the side effects and the lack of effectiveness of anti-cancer drugs, finding new compounds is of interest to scientists. Heterocyclic compounds play an important role in medicinal chemistry, and many drugs contain heterocyclic rings. Quinazoline and thioqinazolinones are important heterocycles with different biological effects such as antifungal, anti-inflammatory, anti-HIV, and anti-cancer.¹ In this research a novel series of quinazolinone derivatives were synthesized as anti-cancer compounds.

Thioquinazolinone nucleus was synthesized by refluxing the mixture of anthranilic acid and phenyl isothiocyanate in ethanol in the presence of triethylamine. The obtained compound was added to appropriate alkyl halides in methanol and stirred at room temperature.² The S-alkylated thioquinazolinones were filtered and purified. The structure of the synthesized compounds was characterized by FT-IR,¹HNMR and LC/MS.

In this study some new thioquinazolinone derivatives were synthesized as anticancer agents. The structure of synthesized compounds was confirmed by different spectroscopic techniques and the anticancer activity of them is under investigation.



R = Propyl, Ethyl, Butyl

Scheme 1: The synthetic route of designed compounds.

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An Efficient Catalyst-free Synthesis of Novel Spiro[indoline-3,5'-pyrido[2,3-d:6,5d']dipyrimidinones] *via* the Reaction of 6-Aminouracils and Isatins

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Abstract:

Due to the widespread biological and medicinal properties of N-containing heterocyclic compounds¹ specially isatin² and pyridopyrimidine³ derivatives have received much attention in recent years and considerable efforts have been made to develop their synthetic methods in organic chemistry.

As a part of our ongoing program on the synthesis of novel heterocycles⁴, here in, we report our recent achievements in the synthesis of a variety of novel spirooxindole derivatives using 6-aminouracils and isatin derivatives in acetic acid. The reactions were run in glacial acetic acid at 80 °C and completed within 6 hours without using of catalyst (Scheme 1). In addition to the simplicity of procedure, our method has appropriate reaction time, simple work-up, and excellent isolated yields.



Scheme 1: Synthesis of spiro[indoline-3,5'-pyrido[2,3-*d*:6,5-*d*']dipyrimidinones] of 6-aminouracils and isatins

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Arylation of Aromatic Aldehydes in the Presence of

Copper-Phosphine Catalysts

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Abstract

Diarylmethanols are very important compounds in the synthesis of drugs, flavors, chemicals, and materials which used in the agricultural industry. Secondary alcohols also play the role of intermediary compounds in organic reactions.¹ In the organic syntheses, there are numerous ways for the preparation of secondary alcohols that among them, reduction of ketones or addition of organic-metallic reagents to carbonyl-containing compounds are the most important reactions of C-C bond formation.² The use of boron reagents as a source of aryl through the exchange of the aryl groups between boron reagents and metal is one of the most commonly used methods for the arylation of aldehydes.³

In this research, we have investigated the addition of phenylboronic acid to aldehydes in the presence of an available, active, and selective homogeneous catalytic system with copper salts and phosphorus ligands (Scheme 1).

The structure of the prepared products was characterized by melting point and spectral analysis techniques as IR, ¹HNMR, ¹³CNMR.



Scheme 1: Arylation of aromatic aldehydes via copper-phosphine catalysts

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Synthesis of New Dihydropyrido-Dipyrimidines Contain Chitosan

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Abstract

Chitosan is a semi-synthetic commercial amino polysaccharide derived by deacetylation of the naturally occurring biopolymer chitin. Chitin is the most abundant of the renewable polysaccharides in the marine environment and one of the most abundant on Earth after cellulose. Pyrimidine derivatives are valuable organic compounds that have been studied extensively and have many application in the synthesis of organic compounds. In this study, chitosan was first used as a large molecule of biopolymer containing glucosamine in multicompound reaction to synthesizes pyrimidine derivatives.

The three-compound reaction of chitosan, Benzaldehyde and Barbituric acid in the presence of acetic acid resulted in the formation of various pyrimidine compounds in the aqueous solvent.

Due to the biological properties of pyrimidine compounds as anti-cancer and anti-viral compounds, antivirus tests of these compounds are under way.



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Poly (N-vinyl imidazole)/ Graphene Oxide Nanocomposite Hydrogels as an Efficient Metal Ion Adsorbent from Aqueous Systems

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Abstract

Polymeric hydrogels containing selective functional groups are extensively used in different fields such as medicine, pharmacy, agriculture, food industry and removal of azo dye, heavy metal ions and other organic pollutants.^{1,2} Among these, pH sensitive polymeric hydrogels are considered as highly effective adsorbents for wastewater treatments. Recently, imidazole/Imidazolium-based nanocomposite hydrogels with large swelling capacities in aqueous media have been received much attention as adsorbent for removal of heavy metal ions.³ In this work, a series of novel pH-sensitive nanocomposite hydrogels (PVI/GO) based on Nvinyl imidazole (VI) were synthesized using an imidazolium-based dicationic ionic liquid as a crosslinker in the presence of different amounts of graphene oxide (GO) (0.25-3.0 wt%) and AIBN initiator in aqueous solution. FT-IR, DSC, XRD and SEM equipped with energy dispersive X-ray spectroscopy analysis were used to characterize the structure and analyse the surface morphology of the adsorbent before and after metal ions adsorption. The adsorption behavior of Ni(II), Cd(II), Cu(II), Co(II) and Cr(VI) on PVI/GO adsorbent was investigated in batch experiments. It was found that adsorption was dependent on pH, ions concentrations, adsorbent dosage, and contact time. Removal efficiencies for Ni(II), Cd(II), Cu(II), Co(II) and Cr(VI) ions were found to be 85%, 81.4%, 96.52%, 96.11% and 90.17% at pH=7.0, optimal ions concentration of 500 mg/L and in contact times of 45, 40, 25, 25 and 180 min, respectively. The results suggest that the developed nanocomposite hydrogel containing 3.0 wt% GO has a very good potential for the adsorption removal of studied metal ions from aqueous solution.



Figure 1. Effect of contact time of adsorbent (0.5 g/L) on removal of Ni(II), Cd(II), Cu(II) and Co(II) (500 mg/L) at pH = 7.0.

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Biography of Presenting Author

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One-Pot Three-Component Synthesis of 5-(6-amino-2,4-dioxo-1,2,3,4tetrahydropyrimidin-5-yl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-diones Derivatives

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Abstract:

Heterocyclic compounds represent an important class of naturally occurring substances and their characteristic is the highly pronounced biological properties.¹ Among them, pyrimidine derivatives play an important role in several biological and pharmacologically active substances such as antimicrobial and antitumor agents.²⁻³ In continuous of our study on the finding green procedures to the efficient synthesis of novel N- and O-containing heterocyclic compounds, in this work, we try to report a new, facile, and efficient pathway toward the synthesis of 5-(6-amino-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-diones **4** *via* one-pot three-component cyclo-condensation-oxidation reaction of isatin **1**, 6-aminouracils **2** and 1,3-dimethylbarbituric acid **3**. All reactions were performed in glacial acetic acid as solvent at 110 °C followed by the addition of Pb(OAc)₄ to the reaction mixtures. The reactions were completed in less than 15 h and product **4** obtained in good to excellent yields. High yields, easy work-up, practical simplicity, and no extraction and chromatographic purification steps are of the most advantages of this method to synthesis of pyrimido[4,5-*b*]quinoline derivatives.



Scheme 1: Reaction pathway for the synthesis of 5-(6-amino-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5yl)pyrimido[4,5-*b*]quinoline-2,4(1*H*,3*H*)-diones **4**

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Heterobimetallic Rh^{III}-Au^I Complex as a Catalyst for Tandem Reaction: A Density Functional Theory (DFT) Mechanistic Study

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Abstract

Heterobimetallic complexes offer the potential for cooperative catalysis, where the combination of two different metal ions into a single molecule produces synergistic catalytic activity.¹ They have played a significant role in the development of catalyst research area and emerged as a hot topic in tandem reactions.² Tandem reactions can provide high-value organic products *via* multiple chemical transformations proceeding in a one-pot reaction.³ A significant benefit of such transformations is the atom economy of the strategy. Research toward improved activity and selectivity of tandem systems dramatically reduces waste, costs, energy consumption, and time.³

We herein describe the preparation of Rh^{III} complex with a bisphosphine ligand. This compound acted as an intermediate to the production of Rh^{III}-Au^I heterobimetallic complex (Scheme 1). The Rh^{III}-Au^I complex is characterized by various spectroscopic techniques and tested in the transfer hydrogenation/dehalogenation tandem process. Also, density functional theory (DFT) calculations were carried out to study the complete catalytic cycle for this transformation.



Scheme 1. Synthetic route for the preparation of heterobimetallic Rh^{III}-Au^I complex.

Acknowledgments

This work was supported by the Institute for Advanced Studies in Basic Sciences (IASBS) Research Council.

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Comparison of Chemical Compositioin of Essential Oils and Evaluation of Antioxidant and Antimicrobial Activity of Methanolic Extracts of *Ferula lutensis Rech. Fil* and *Ferula szowitsiana DC.*

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Abstract

Chaerophyllum genus plants belong to the Asteraceae family which play the role of beneficial therapeutics in modern and traditional medicine. In this study, chemical compounds of essential oils, antioxidant and antimicrobial activity of extracts of medicinal plants including Ferula lutensis Rech. Fil and Ferula szowitsiana DC. were investigated along with the amount of phenolic compounds. Clevenger apparatus and Maceration method were used for distillation and extraction of these plants. Identifying chemical compounds of these essential oils were conducted using gas chromatograph/mass spectrometry (GC/MS) instruments. Respectively, 28 and 12 chemical compounds were found in essence of F. Szowitsiana and F. lutensis. Main ingredients of F. lutensis essence were Teridecanioc acid (18.44%), 1,3-Dioxolane-4methanol, 2-ethyl (15.17 %) and 2,3,4,4- Tetra methyl pentane-1,3- diol (15.76%). main ingredients of F.szowitsiana essence were carotol (12.70 %), 1,3- dioaxane (92.9%), alpha- cadinol (8.11%), 1-Pentylamine (7.55%), y-Eudesmol (6.11%) and Germacrene D-4-ol (5.95%). Antioxidant activity of extracts of these plants was measured by calculating percentage of inhibition of DPPH free radical and determining IC₅₀ and FRAP method. Phenolic compounds' content of all extracts was measured using folin-ciocalteu reagent (FCR) and gallic acid standard curve. The highest phenolic content of different extracts of these plants were observed in F.lutensis extracts. In addition, among two exteracts studied, F. Lutensis extracts had the lowest IC₅₀; therefore, it showed the highest antioxidant activity. Antimicrobial effect of plants under study was evaluated using disk diffusion, Agar wells and microbroth dilution. In both methods, F. lutensis extracts represented the highest antimicrobial activity against microorganisms under study. Of bacteria studied, the most susceptible and resistant strains against extracrs studied were Bacillus cereus and, Escherichia coli respectively.

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A Theoretical Investigation on the Physicochemical Properties of the Functionalized Ionic Liquids Based on Pyridinium

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Abstract

The ionic liquids (ILs) as biocompatible liquid organic salts composed of cations and anions are widely used in many fields, including synthesis, catalysis and electrochemistry. The most attractive property of ILs is their high design ability. Therefore, various task-specific ILs can be produced by the combination of various functional groups and proper of anions and cations.¹⁻³ By tuning sterically and electronically characteristics the cationic part of ILs, a photoresponsive room temperature ionic liquids could be developed. Vast studies had examined photoresponsive properties of these types of ionic liquids.^{4,5} The aim of the present research is to determine the influence of different substituents electron-donating or electron-withdrawing group at the phenyldiazenyl moiety of cation part on their physical, chemical and optical properties using the quantum chemical calculations at M06-2X/AUG–cc–pVDZ level of theory.

We chose ILs based on methyl pyridinium tetrafluoroborate, where the cation is functionalized with a phenyldiazenyl moiety linked to 4 position of the cationic head group and substitution of different electrondonating or electron-withdrawing group on para position of the phenyldiazenyl moiety ([(p-X-PDA)MPy][BF₄]). The substituents selected for this study cover almost the whole set of classical substituents (X: NH₂, OH, OCH₃, C₂H₅, CH₃, H, F, CHO, CN and NO₂) (see Figure 1). In the work, interaction energy between these cations and tetrafluoroborate anion, geometrical parameters and topological properties and electrochemical stability of mentioned ILs based on their electrochemical window values were explored. In addition, we characterize nature of intermolecular interactions in the ILs by NBO, QTAIM and NCI index to provide a deeper understanding of the effect of different substitution on the interaction between cations and anion and the subsequent impact on their physicochemical properties. Also, the optical properties such as excitation energies (E), wavelengths (λ), oscillator strengths (f) and the absorption spectra of the ionic liquids were calculated using TD-M06-2X/cc-pVDZ level of theory. The results demonstrate that the strength of interaction between the cations and tetrafluoroborate anion increases with increase in the electron-accepting power of the substituents. Also, the TD-DFT calculations in gas and solvent phases show that the absorption peak of [(p-X-PDA)MPy][BF4], X: NH2, OH, OCH3, C2H5, CH3, H, F, CHO, CN and NO2 ILs is in the range of 401.3-309.5 nm. From the comparison of λ_{max} , it can be estimated that the absorption peak of ILs having electron donating substituents to be more than those of electron accepting ones.



Figure 1: The optimized structure of [(p-X-PDA)MPy][BF₄], X: NH₂, OH, OCH₃, C₂H₅, CH₃, H, F, CHO, CN and NO₂ ILs at M06-2X/AUG–cc–pVDZ.

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Investigation of Photovoltaic Properties of Dye-Sensitized Solar Cells Based on Indigo Dyes in the Presence of an Anti-Aggregation Agent

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Abstract

Nanostructure dye sensitized solar cells (DSSCs) based on indigo dyes exhibit medium to great power conversion efficiency.¹ Such organic dye molecules are easily undergone for aggregation. Aggregation in dye molecules lead to reduce electron transfer process in dye-sensitized solar cell. Therefore, antiaggregation agents are commonly added to organic solution in DSSCs.² In this work, Spectrophotometric evaluations of the indigo dye on a TiO₂ substrate in the presence and absence of an anti-aggregation agent were carried out in order to assess changes in the status of the dyes. Therefore, an antiaggregation agent such as chenodeoxy cholic acid (CDCA) is used with organic dyes. The λ_{max} of dye adsorbed on a TiO₂ film in the absence of CDCA and in the presence of CDCA are 595 nm and 580 nm, respectively. Upon dye adsorption on to a TiO2 surface in the absence of CDCA, the wavelength of maximum absorption is bathochromically shifted by 46.5 as compared to the corresponding spectra in solution, implying that dye adsorbed on to TiO₂ surface contain partial J-type aggregates³ but the wavelength of maximum absorption is bathochromically shifted by 31.5 in the presence of CDCA as compared to the corresponding spectra in solution. Therefore, the officious aggregations were reduced in the presence of an anti-aggregation agent. The oxidation potential (Eox) of organic dye was measured in acetonitrile by cyclic voltammetry³. There are two distinct redox waves observed in the voltammogram. The first oxidative wave (I) was due to the oxidation of the internal standard of ferrocene, whereas the second wave (II) was due to the electrochemical oxidation of the dye. The oxidation peak potential (Eox) for synthesized dye can therefore be calculated to be 0.57 vs Fc/Fc⁺ in acetonitrile. The E₀₋₀ of dye was calculated to be 1.88 V, therefore, the Eox-E0-0 level of dye is estimated to be -1.31 V vs Fc/Fc+ in acetonitrile. Finally, dye sensitized solar cells were fabricated in order to determine the photovoltaic properties and influence anti-aggregation agents on their performance. The photovoltaic properties of DSSCs were presented in Table 1. Increased conformational flexibility, diffusion values of dye and reduced aggregation of dye are directly correlated with faster electron transfer from excited state of dye to TiO₂ semiconductor in DSSCs.

Photovoltaic characteristics	In the absence of CDCA	In the presence of CDCA
Short-circuit current (J _{sc}) (mA/cm ²)	7.47	8.75
Open-circuit voltage (V _{oc}) (V)	0.64	0.64
Fill factor (FF)	0.65	0.66
Efficiency (%)	3.11	3.7

Table 1: Photovoltaic properties of DSSCs

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A Dendritic Cu(I) Complex Based on the Triazine Ring Supported on Magnetic SBA-15 for Catalyzing Ullmann Coupling Reactions

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Abstract

The transition metal-catalyzed C–X (X = N, O) cross-coupling reactions play an important role in the preparation of numerous important products in biological, pharmaceutical and material sciences. Both the Ullmann reactions (copper catalyzed *N*-arylation of amines and O-arylation of phenols, Scheme 1. ¹



Scheme 1. The Ullmann coupling reaction

During the recent years, immobilization of catalysts onto inorganic substrates has attracted the attention of many chemical researchers. Among these materials, composition of mesoporous silica such as SBA-15 and MCM-41 with magnetite nanoparticles have found special place.^{2, 3} Anchored catalysts onto these highly dispersible, nontoxic, biocompatible nanoparticles also have the advantage of quick and straightforward magnetic separation from reaction mixtures.⁴

In this work, a dendritic Cu(I) complex based on the triazine ring has been supported on magnetic SBA-15, Scheme 2.



Scheme 2. Synthesis of dendritic-Cu(I) complex on Fe₃O₄@SBA-15.

It was observed that the prepared catalyst could effectively catalyze the Ullmann reactions. The recycling experiments showed that the catalyst could separate magnetically and re-used several times.

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Biography of Presenting

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Theoretical Study of 2 and 3-Diaminopyridine Proton Transitions with Salicylic Acid Based on Density Functional Theory (DFT)

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Abstract

Proton transfer compounds can be introduced as the chemistry of supermolecule combinations. Today, supermolecular chemistry is known as a broad and exhastive field so that, in 2005, the word supermolecular chemistry was used 2532 times in the title or summary of scientific texts. The supermolecule composition was first used in a new way by Jean-Marie Lehn in 1978. Supermolecule chemistry can be elucidated as beyond a molecule, whereby a supermolecule is a compound formed by the juxtaposition of two or more molecules or ions with a non-covalent bond. Supermolecular Chemistry is based on non-covalent interactions, such as hydrogen non-covalent interactions, metal coordination, hydrophobic forces, π - π interactions, and electrostatic forces.¹ In these interactions, atoms and, in fact, the molecules are attracted to each other without the exchange of electrons. Although these bonds are weak on their own, their combination can put molecules together in a huge crystal lattice. Spontaneous aggregation of molecules to create stable structures, which are created by noncovalent interactions, is called self-assembly.² Proton transfer compounds are the product of proton transfer between two donor and receptor proton species when a proton is transferred from one type to a primary center. This phenomenon is called proton transfer with miscellaneous names, such as Proton Transfer Compounds³, Charge Transfer Complex,³ and Hydrogen Bond Complex. Proton transfer compounds are formed by the transfer of one or more protons between two donor and acceptor groups which, in the following, can form complexes as ligands with metal nuclei. In this study, proton transfer from the reaction of 2,3-diamino-pyridine with salicylic acid was selected for calculations of Density Functional Theory at the level of B3LYP / 6311 + G (d, p). Optimization, frequency, electron transfer calculations in visible-ultraviolet spectroscopy, boundary orbital energy and NBO for 2 and 3-diamino-pyridine-3-nitro benzoic acid ligand were performed by using NWCHEM software. Comparison

of the vibration peaks of the prepared proton transfer ligand and the proton donor and acceptor species shows the formation of intermolecular hydrogen bonds in the ligand. The calculated peaks of visible-ultraviolet spectroscopy of this ligand is related to ILCT transmissions in both donor and acceptor species with n (p) / $\pi \rightarrow \pi^*$ characteristics. Hydrogen bonds O – H \cdots N and N – H \cdots O stabilize the above-mentioned proton transfer composition in the amount of -393.30 kcal.mol-1 figure1.



Figure 1: Transfer electrons of 2 and 3-Diaminopyridine to Salicylic Acid

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Investigation of Iron Promoted Catalyst in Fischer-Tropsch Synthesis

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Abstract

Fischer-Tropsch synthesis (FTS) is a highly attractive route for producing ultra-clean fuels from natural gas, coal, and biomass without undesirable components such as sulfur, nitrogen, and aromatic compounds. Therefore, coal and natural gas can be utilized as the feedstock of the chemical industry and the transportation fuels market.¹ Furthermore, the conversion of natural gas to hydrocarbons is currently one of the most promising topics in the energy industry due to the economic utilization of remote natural gas to environmentally clean fuels, specialty chemicals, and waxes.² Catalyst is the main object of FTS technology, usually composed of active metal, support, and promoter. Iron is common active metal in the FT synthesis catalysts. Due to its lower price and better properties, such as higher activity for Water Gas Shift (WGS) reaction and light olefins selection at high temperature and low H_2/CO ratio.³⁻⁶

In this study, the iron-based catalyst on γ -Al₂O₃ support was prepared by the impregnation method. The sample was dried at 120°C for 24 h and calcined at 400°C for 3h. The catalyst was characterized using XRD, H₂-TPR, and BET techniques. The performance of the catalyst was studied in a fixed bed reactor at the following conditions: the pressure of 20 atm, H₂ to CO ratio of 1, Gas Hourly Space Velocity of 2 l.h⁻¹.gcat⁻¹, and temperatures of 285°C. Results of Gas chromatography calculated the catalyst activity and product selectivity.



Figure 1: CO conversion and yield of the catalyst Figure 2: SEM of the catalyst

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Theoretical Study of the Effect of Organic Solvents on the Structure and Stability of Small Water Clusters

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Abstract

Most of chemical and biological processes take place in the water.¹ The unusual features of liquid water can be understood by considering the bulk water as an assembly formed from a huge number of different water clusters (**WC**s).²⁻⁵ We have reported the effect of some non-polar organic solvents with different dielectric constant on the small water clusters including 2 to 9 water molecules using DFT method at M06/6-31+G^{**} level of theory (Figure 1). Our investigation has revealed that the octamer water cluster with high binding energy is the most stable small water cluster that can be existed in the non-polar solvents (Figure 2).



Figure 1. The optimized structure of the more/most stable small water clusters, (H₂O)_n, n= 2-9; using M06/6-31+G^{**} level of theory at room temperature in the gas phase



Figure 2. The binding energy of water clusters, E_b , in the gas phase and non-polar solvents, using M06/6-31+G^{**} level of theory at room temperature

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Synthesis and Characterization of a Florescent Schiff Base Probe for Selective Detection of Zn(II) Ion

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Abstract

The designe and synthesis of newly molecular sensor, which is eco friendly, non-harmful and highly sensitive and selective towards metals ions, are always essential for practical research in various fields of science.¹⁻³ Accordingly, here a new Schiff base ligand derived of 1-phenyl-1,2-propandion-2-oxime and 1,2-diaminocyclohexane (Figure 1) has been synthesized and characterized by FT-IR and ¹H NMR spectroscopic methods. In neutral conditions (pH ~ 7.4), Schiff base ligand can interaction with Zn(II) ion. The prepared Schiff base ligand show large fluorescence enhancement after addition of Zn(II) which is recognized by calorimetry. The stability constant and the detection limit of the Schiff base ligand-Zn(II) complex were found to be 4.84×10^5 M⁻¹ concluded through the titration method. *I*n conclusion this receptor could be employed for the estimation of Zn(II) qualitative as well as quantitative.



Figure 1: Path for the synthesis of florescent Schiff base probe

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Biological Activity of Two Novel ligands by Spectroscopic and Molecular Docking Methods

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Abstract

Schiff base ligands represent a major group of organic compounds which have a wide variety of biological properties, such as antibacterial, antifungal, antimalarial, anti-proliferative, anti-inflammatory, antiviral and antipyretic activities.¹⁻⁴ Schiff base ligands have the imine group (-R=CN-) and are synthesized by the condensation between primary amine and active carbonyl (RCOR') compounds [5]. In this study ,new Schiff base ligands (I) 1-(3-iminopropyl)piperazine-1,2-diacetylmonoxime)bis-propylimimne-¹,^rand (II) 1-phenyl-1,2-propandion-2-oxime) (Fig. 1) were synthesized and completely discussed with spectroscopic and theoretical methods. The ligands were studied *in vitro* by 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging method. Our findings showed that ligands have moderate antioxidant properties with this trend: II > I. Biophysical techniques were adopted to study the binding of these ligands with Human serum albuline (HSA). Fluorescence results showed that the combination of HSA with both ligands undergoes static quenching mechanism (Kb = 4.3×10^4 M⁻¹ for I and 6.7×10^6 M⁻¹ for II at 310 K). The interaction process was spontaneous, exothermic and van der Waals and hydrogen bonds forces played major roles. UV-Vis, 3D, and synchronous fluorescence measurements indicated the changes in the microenvironment residues in the presence of Schiff base compounds. According to the molecular modeling analysis, both ligands develop bonds to the remnants that exist in the subdomain IIA of HSA.



Figure 1: The molecular structure of Schiff base ligands

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Reduction of Imines & C-X Phosphonation by Diethyl Phosphite

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Abstract

Amine functional groups are ubiquitous in natural products and drug molecules. The reduction of imines represents one of the most important methods for accessing amines, owing to the ease of preparation of imines from readily available ketones and aldehydes. Use of catalysis for the reduction of imines affords opportunities to control selectivity, especially in the reduction of substrates containing multiple reactive functional groups. Platinum-group metal-complex catalyzed hydrogenations of imines are well-established methods, however the expense and scarcity of precious metals provides impetus for the development of alternative methods.

Phosphonates are an important group of compounds in pharmaceutical, biological and Medical Chemistry fields because these functional groups are commonly found in biological systems.as well as Phosphoruscontaining heteroaromatic molecules are an important class of compounds that find useful applications in synthetic transformations, medicinal chemistry, and photoelectric materials, and as useful ligands for transition metal catalysis.

so we used Diethyl phosphite as the first example for reduction and phosphonation in this paper.

This reaction of chloroanil and aniline in the presence of diethyl phosphite, led to the formation of new phosphorous dirivatives.



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Synthesis of Aminated Polymers of Alginate for Preparation of Glucose Sensitive Hydrogel

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Abstract

This study deals with the production of novel pH responsive beads for delivery of bioactive substances that can be controlled by external stimuli. For this purpose, ethylenediamine grafted onto Sigma Sodium alginate (SA) with high viscosity, through amide bond linkages in the presence of 1-ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) and N-Hydroxysuccinimide (NHS). The hydrogel copolymer matrices were compare with sodium alginate (SA) beads. The graft copolymers were characterized by physical and spectral properties such as Differential Scanning Calorimetry (DSC), Thermo Gravimetric Analysis (TGA), Fourier transform infrared spectroscopy (FTIR), ¹³C and ¹H magnetic resonance (NMR), X-Ray Diffraction (XRD) and Environmental Scanning Electron Microscope(ESEM). Effects of variables such as graft yield, temperature, pH, glutaraldehyde(GA) and Trisodium phosphate (TPP) on the strength of hydrogels investigated and discussed at two different pH values (4.4 and 6.8) and temperature range (2-70°^C). It was observed that strength of the beads when the grafting of diamine ratio and extent of cross linking with GA and TPP were increase. The results also showed that the grafted beads were positive pH responsive.



Scheme 1: synthesis of linear diaminated alginate using EDC and NHS as coupling agent

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A Comparison of Physico-Chemical Properties of Persian Gulf Alginate Derivatives with Commercial Sodium Alginate

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Abstract

Sodium alginate (SA) is a non-toxic, biocompatible, and biodegradable polysaccharide with several unique physicochemical properties for which has used as delivery vehicles for drugs and is an excellent carrier in various drug delivery systems. In this study, SA was extracted from brown seaweed, *Sargassum Bovaneum* with a yield of 24.38% compared with two commercial samples. The analysis of physicochemical properties of extracted alginate determined its purity. The structural confirmations of SA were studied through FTIR, ¹³C,¹HNMR, CHNS analysis and XRD. Thermal behaviour of these samples were investigated by thermogravimetry (TG) and differential scanning calorimetry (DSC). Under nitrogen the compounds exhibited three successive thermal decomposition steps: dehydration, decomposition of the polymeric matrix and finally, burning of carbonaceous residue. The stability order of this series of compounds was: Alg H(High viscosity) << AlgEX(Extracted alg) < Alg L(low viscosity). The viscosity and content of sulfate were also measured. Viscosity varied much more widely than other physical properties and was the best criterion of state of polymerization. Fucoidin was detected as impurity in extracted alginate.



Scheme 1: Structure of alginic acid: chain conformation, M: mannuronic acid residue and G: guluronic acid residue.

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Liquefaction Strategy for Extraction of Cellulose from Agricultural Wastes

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Abstract

As one of the world's most abundant natural and renewable materials, cellulose is low in cost and extensive in source.¹ Development and utilization of lignocellulosic biomass resources represent a long-term solution for alleviating the depletion of non-renewable fossil fuels. As a main agricultural waste in tropical and subtropical regions, banana stem (BSs) is an abundant, renewable and low-cost resource.² This work aimed to extract cellulose from BSs via liquefaction method for fabrication of cellulose nanofibers. The BSs was initially subjected to an atmospheric liquefaction process to remove waxes, pectin, hemicellulose and partly lignin. Bleaching treatment was further conducted to eliminate residual lignin and polycondensate in the liquefied residues. Liquefied residue content as well as its constituent varied with respect to liquefaction time and temperature. According to the results, 90 min and 150 °C are optimal reaction time and temperature for liquefaction. The producing bleached liquefied residue (BLR) were characterized by Fourier transform infrared (FTIR) spectroscopy and X-ray diffraction (XRD) technique (Figure 1). Moreover, the molecular weight of the BLR was determined by viscometry method. The diffraction pattern manifested a typical cellulose I crystalline structure. The relative crystallinity index and the average thickness of cellulose crystallites was 26.8% and 23.1 nm, respectively. In addition, the molecular weight of the extracted cellulose from BSs is about 3×10^5 g/mol. Accordingly, the liquefaction method can be a good strategy in the synthesis of pure and high molecular-weight cellulose.



Figure 1: The XRD pattern of BLR.

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Cellulose-Based Scaffolds with Enhanced Structural Properties for Hard Tissue Engineering

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Abstract

Electrospun fibers have high structural similarity to the extracellular matrix (ECM) of natural bone.¹ Many researchers have tried to fabricate cellulose fibers using electrospinning method, however the fabricated electrospun fibers usually suffer from low mechanical and structural properties.² Combination of biodegradable polymers and bioactive inorganic materials may take advantages of the mechanical properties, biocompatibility and cell affinities of the individual components. Here, nanofibrous scaffolds from banana cellulose and hydroxyapatite (HAp) were electrospun for application in bone tissue engineering. The key factors associated with the electrospinning process, including the intrinsic properties of cellulose solutions, flow rate, the rotating speed of collector and the applied voltage, were systematically investigated, and nanofibrous scaffolds were finally fabricated based on optimal electrospinning conditions (Scheme 1). The cellulose/HAp scaffolds were then characterized by scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDXA), contact angle measurement, universal testing machine and thermal analysis. SEM and EDX-mapping clearly indicated a uniform distribution of nanoparticle within the matrix. Contact angle measurements showed that increasing the percentage of HAp increases the hydrophilicity of the scaffolds. Finally, the results of mechanical and thermal analyses showed that increasing the percentage of filler has a great effect on mechanical strength, tensile modulus and thermal properties.



Scheme 1 : Schematic of fabrication of electrospun cellulose/HAp fibers.

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Synthesis of Diethyl-2-Iminocoumarin-3-Phosphonates from N-Tosyl Salicylimines

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Abstract:

Organophosphorus compounds (OPCs) are chemical compounds containing at least one carbonphosphorus bonds. OPCs have been widely used in various industry such as: agriculture, medicinal and plastics, flame retardants for fabrics.¹ 3-Substituted-2-iminocoumarins are known not only due to their versatile biological activity, such as anti-inflammatory, antimicrobial, antifungal and antitumor, but also as luminescent indicators and laser dyes.² As far as we know diethyl-2-iminocoumarin-3-phosphonates have never been synthesized using N-tosylsalicylimine. According to the literature several attempts have been made to synthesize q-cyano-vinyl phosphonates, such as: the reaction of *N*-tosylsulfonyl imines with diethyl cyanomethyl phosphonate in the presence of potassium *tert* butoxide in tetrahydrofuran³ or by using Et₃N in DMSO⁴ and Takeshi Oriyama et al. reported this reaction by using MS 4A in DMSO.⁵

Herein we report for the first time the synthesis of diethyl-2-iminocoumarin-3-Phosphonates **3** from the reaction between N-tosyl salicyl imines **1** and diethyl cyanomethylphosphonate **2** in presence of tetra methylguanidine and molecular sieve in tetrahydrofuran as solvent at room temperature. (scheme1).



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Synthesis and Characterization of Acidic Nano-Diatomite Catalyst and its Application in the Synthesis of 1.4-dihydropyridine Derivatives via Hantzsch Reaction.

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Abstract

A homogenous acid catalyst such as HCl, H₂SO₄ or HNO₃ covers abroad range of application such as electrophilic addition esterification, ester hydrolysis aromatic electrophilic substitution or rearrangement reaction. Despite their usefulness, these acids are highly corrosive, many of them release gasses and suppression product from the acid is often difficult that pose safety the health hazards. In addition, most of them are impossible to reuse. Due to the importance of acid catalysts, a significant effort was made to solve these problems. Supported catalyst on the different careers such as diatomite, silica, and bentonite was investigated.

Diatomite, is a material of sedimentary origin. The structure of diatomite is quite complex and contains numerous ifne microscopic pores, cavities, and channels, and therefore has a large specific surface area high absorption capacity, and low density. Other intrinsic properties are low thermal conductivity, relatively high melting-point, chemical inertness, and small grain size. Additionally, its relatively low price and high abundance mean that diatomite can be used extensively as insulating materials, conventional catalyst support, membranes, and biocatalytic proteins and cells.^{1, 2}

When the dimensions of the diatomite become nano, the number of operating units increased. So, in a catalytic process, the more effective contact surface between the catalyst and the raw material increases and the rate of the reaction increase.³

In this work, we have prepared a novel acidic nano-diatomite as catalyst via a three-steps method from diatomite soil. After characterization of this catalyst by XRD, FT-IR, and TGA it was used in the synthesis of 1,4-dihydropyridine under solvent-free Hantzsch reaction (Scheme 1). The catalyst showed high catalytic activity for synthesis 1,4-dihydropyridine after five-time reusing of the catalyst.



Scheme 1: Synthesis of 1,4-dihydropyridine derivatives

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Multi Component Reaction for Synthesis of Pyrrolidinesderivatives

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Abstract

The 1,3-dipolar cycloaddition is a chemical reaction between a 1,3-dipole and a dipolarophile to form a fivemembered ring system. The synthesis of pyrrolidine-based heterocycles has been considered in recent decades due to the formation of an important group of substance with high biological activity. These compounds are at the center of the structure of countless alkaloids and drugs and serve as a beautiful synthetic target in organic synthesis.

In this regard, I will report the synthesis of new pyrrolizidines by substituting new heterocyclic compounds and examining the pathways of selective region and streo-selective.

In this research, we seek to investigate a green and non-toxic method for the synthesis of these compound and for this purpose we have designed a reaction between the raw materials of Isatin, Proline and cinnamic acid.Then, using a chiral catalyst, we synthesized this family of compound in a stereo-selective manner.



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Domino Synthesis of 5-Amino-4,6-Dicyano-Terphenyl Derivatives Over SiO₂ Nanoparticles Under Solvent-Free Conditions

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Abstract

Biaryls are recognized as an important class of compounds in organic synthesis because of their versatility in both ligand chemistry and materials chemistry. Biaryls are also found in various types of natural products that show unique biological activity.¹⁻²

The synthesis of these compounds have attracted attention of chemists. Though several methods for their synthesis have been reported ³⁻⁵, many of these procedures are not fully satisfactory with regard to operational simplicity, cost of the reagent, and isolated yield; moreover, the majority of those synthetic methods were carried out in nocuous organic solvent.

In this report, an efficient one-pot green procedure for the synthesis of 5-amino-4,6-dicyano-terphenyls has been reported via three-component condensation of acetophenone, malononitrile and aldehydes under solvent-free conditions at room temperature using Nano SiO_2 (50 nm) (scheme 1). This methodology has valuable advantages such as convenient one-pot operation, short reaction times, environmentally friendly conditions, ease of catalyst recovery.



Scheme 1: Solvent-free synthesis of 5-amino-4,6-dicyano-terphenyls over Nano SiO₂

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Multi-Compounent Synthesis of 2-Amino-Dihydropyranopyran-3-Carbonitriles Derivatives Over SiO₂ Nanoparticles in Water

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Abstract

Silica nanoparticles (SiO₂ NPs) have provided great opportunities for a wide range of applications in organic synthesis and chemical manufacturing processes.¹⁻² Nowadays, multi-component reactions (MCRs) have been provided highly elegant and practical approach for the synthesis of diverse structure of heterocyclic compounds.³⁻⁴ MCRs are the processes that trigger the conversion of several starting materials in one-pot to a functionalized product with high diversity, complexity, and impressive selectivity. The combination of two important scaffolds such as kojic acid and pyran may lead to new alternative drug candidates with enhanced pharmacological properties.⁵ Consequently, there is also great efforts to provide practical and efficient methods for the preparation of fused-kojic acid heterocycles. To continuation of our interest to develop green and economical methods for the synthesis of biological active compounds, now we wish to report a three component synthesis of 2-amino-dihydropyrano[3,2-b]pyran-3-carbonitriles using nano SiO₂ (50 nm) as a recyclable and heterogeneous catalyst at room temperature in aqueous media (Scheme 1).



Scheme 1: Synthesis of 2-amino-dihydropyrano[3,2-b]pyran-3-carbonitriles over Nano SiO₂ (50nm) in water

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Synthesis of Fumarate Salt of Sorafenib and Preparation of its Nanoliposomal Polyethylene Glycolated Drug Carrier

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Department of Chemistry, Faculty of Science, University of Guilan, Rasht, Iran **Abstract**

Pharmaceutical nanotechnology plays a pivotal role in the field of biomedical and bioengineering, and is the greatest tool to overcome the obstacles that chemotherapeutic agents create in the body.¹ Drug delivery systems are the subunits of pharmaceutical nanotechnology. Among various kinds of nanocarriers, nanoliposomes have absorbed particular attention because of their biocompatibility, biodegradability, non-toxicity, and ease of preparation.² Moreover, nanoliposomes can carry both hydrophilic and lipophilic drugs due to their amphipathic property. However, they have some limitations such as having a short half-life and elimination from the blood by the macrophages. Surface modification of nanoliposomes with polyethylene glycol (PEG) have been developed to overcome these barriers.³ On the other hand, synthesis of pharmaceutical salts is of special importance to increase the dissolution of drugs in water and also to increase its bioavailability.⁴ In this study, our purpose is the synthesis of fumarate salt of anticancer drug of sorafenib (SOR) and prepare its nanoliposomal polyethylene glycolated drug carrier to increase the delivery, reduce the toxicity and side effects of this drug. For this aim, SOR was changed to its free base form and fumaric acid was added to it via methylethyl ketone solvent. After that, sorafenib fumarate was encapsulated through a reverse-phase evaporation method in PEGylated liposomal nanoparticles, see fig. 1 (a), and the drug-loaded in these nanoliposomes was evaluated in terms of zeta potential, particle size, size distribution, and encapsulation efficiency. The morphology of nanoparticles was shown by TEM, see fig. 1 (b).



Fig 1. (a) Schematic structure of a nanoliposomal polyethylene glycolated of SOR fumarate. (b) TEM image

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Synthesis of 3-(4-fluorobenzyl)-2-thioxo-1,3-thiazinan-4-one in solvent free condition and evaluation of its antibacterial properties

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Abstract

The use of organic solvents is one of the most important challenges in the synthesis of organic compounds. However, organic solvents have some advantages but they are facing some drawbacks as well. Using organic solvents during reaction process may result in some environmental problems. An effective method to overcome this challenge is to do reactions under solvent-free conditions.¹ Besides this, the reaction time and energy consumption could be decreased through solvent-free conditions. Dithiocarbamates are analogues of carbamates which are in the focal point of scientists.² In this project, our purpose is the synthesis of 3-(4-fluorobenzyl)-2-thioxo-1,3-thiazinan-4-one using the reaction of primary amines and carbon disulfide in the presence of acrylamide in solvent-free conditions and evaluation of its antibacterial properties, see scheme. 1. The structure of final product was confirmed via FT-IR, ¹HNMR, and ¹CNMR spectroscopy.





Scheme 1. Synthesis procedure of 3-(4-fluorobenzyl)-2-thioxo-1,3-thiazinan-4-one

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DFT Study on the Interaction of 6-Thiouguanine Drug with Beta-Cyclodextrin Nanocarrier

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Abstract

Recently, more attention has been paid to the preparation of nanoparticles as drug carriers due to controlled drug release from pharmaceutical nanocarriers, nanoparticles smaller than cells, biocompatibility and increasing the therapeutic efficiency of drugs can be considered as a very effective drug delivery system.¹⁻³ In this study, a theoretical study on the interaction of the anticancer drug 6thioguanine with beta-cyclodextrin (β -CD) was investigated using density functional theory (DFT) calculations are performed to determine the effect of nanocarrier interaction on drug stability. The impacts of the estereoelectronic effect associated with donor-acceptor electron delocalizations and dipole-dipole interactions on the structural and electronic properties and reactivity of β -CD in interaction with 6-Thioguanine anticancer drug was studied based on the DFT calculation by using the B3LYP/6-31G* level of theory in gas and water phase. Thermodynamic functional analysis indicate that the relative energies (ΔE), free Gibbs energies (ΔG) and enthalpies (ΔH) are negative for the complex of (6-Thioguanine drug/ β -CD) but the calculated entropies (Δ S) are Positive, suggesting thermodynamic favorability for covalent attachment of drug on β -CD surface. These results confirm the structural stability of the (6-Thioguanine drug/ β -CD) complex. According to the natural bond orbital (NBO) results, 6-Thioguanine and β -CD molecules play as electron donor and acceptors at the (6-Thioguanine drug/ β -CD) complex. Also, the charge transfer is occurred between the bonding, antibonding or nonbonding orbitals in (6-Thioguanine drug/ β -CD) complex. Based on the results, beta-cyclodextrin can be used as a drug delivery system for the transportation of 6-Thioguanine as anticancer drug within the biological systems.

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Investigation of Electronic and Reactivity Properties of the Structure of S-Oxazepam by NBO Calculation

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Abstract

The structural, electronic, stability and reactivity properties of S-oxazepam have been analyzed using the density functional theory [DFT] method with the Gaussian09 program at the hybrid functional B3LYP level of theory with 6-31G* basic set.¹ Oxazepam is used to treat anxiety and also acute alcohol withdrawal. This medication belongs to a class of drugs called benzodiazepines, which act on the brain and nerves to produce a calming and anti-seizure effect.^{2,3} In this study, the structure of the S-oxazepam was first drawn using the Chemoffice08 and optimized using the Gaussian09 program. Delocalization of charge density between the bonding or lone pair and antibonding orbitals calculated by NBO[natural bond orbital] analysis and the total electronic energy, dipole moments, orbital energies, orbital occupancy, donoracceptor molecular orbital energies, structural parameters, charge density, molecular orbital energy bond gaps, Mulliken atomic charges were calculated. The HOMO – LUMO energy gap is related to the molecular chemical stability and it has been used to prove the bioactivity from intramolecular charge transfer.^{4,5} The results of theoretical calculations at the level of B3LYP / 6-31G * showed that [E_{HOMO} = -6.6441(Electronvolt)], [ELUMO = -1.7984(eV)], [Energy gap = 4.85(eV)] and [Dipole moments = 4.1473(Debye)] are for S-oxazepam. By comparing the reactivity indices of S-oxazepam, results are obtained that determine the value of Electron chemical potential [µ= -4.2187 (eV)]and Chemical hardness $[\eta = 2.4208 \text{ (eV)}]$ and Electrophilicity value of $[\omega = 3.6747 \text{ (eV)}]$. According to the results of NBO analysis, the highest rate of electronic transfers is related to the transfer of LP(1) N 4 → BD* (2) O 3- C 13 with resonance energy of 58.23 (Kcal/mol) and an orbital overlap of 0.117 atomic units (a.u) and bandgap energy of 0.29 atomic units (a.u).

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Synthesis of Novel Noscapine- Inspired Tetrahydroisoquinoline Derivatives

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Abstract

Cotarnine, a natural tetrahydroisoquinoline (THIQ) alkaloid, is an oxidative degradation product of noscapine which have remarkable biological activity like noscapine, its parent compound.¹ There are different pharmaceutical active compounds with cotarnine core that exhibit considerable biological activities.²

In this work, a novel series of *N*-substituted THIQ derivatives have been designed and synthesized as antitumor agents.

To furnish this work, cotarnine was synthesized by oxidative degradation of noscapine with HNO₃. Cotarnine then converted to hydrocotarnine followed by *N*-demethylation reaction in which norhydrocotarnine was prepared. Introduction of amino acids into norhydrocotarnine resulted in 11 new derivatives.



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Study of Iron Catalyst Performance in CO Hydrogenation Reaction

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Abstract

Fischer-Tropsch synthesis (FTS) was discovered in 1913 in collaboration with Franz Fischer and Hans Tropsch in Germany. This process is a set of chemical reactions in which mixture of carbon monoxide and hydrogen produce a set of hydrocarbons such as fuels.¹⁻³ During the FTS, the reactive molecules CO and H₂ are separated and forming CH_x species which this species bonding together to form alkanes, alkenes, alcohols, and other oxygenated hydrocarbons through chain growth.^{4,5}

In this paper iron based catalyst prepared by wet impregnation method. We investigated product selectivity and catalyst activity in CO hydrogenation reaction. The catalyst was conducted in a fixed-bed reactor and tested in pressure of 16 atm, temperature of 290, H₂ to CO ratio of 1, GHSV of 2 l.h⁻¹.g cat⁻¹ and the results showed that CO conversion and C₅⁺ hydrocarbons 64.59 and 44.03 respetivety. The catalyst was characterized using XRD, BET, SEM and H₂-TPR techniques.



Figure 1: XRD of catalyst

Figure 2: CO Conversion in diferent time on stream

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Palladium Nanoparticles Supported on Nitrogen-doped Porous Carbon: An Efficient and Heterogeneous Catalyst for Sonogashira Coupling Reaction

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Abstract

Heterogeneous catalysis plays an important role in industrial chemical production. They are preferred due to their robustness and lower operational cost, in particular through easier recovery separation from the products allowing chemical processes to be streamlined. The palladium catalyzed cross-coupling reactions are a valuable reaction with applications in the organic synthesis to have emerged recently. These reactions carry out a coupling of the aryl, vinyl or alkyl halide substrates with different organometallic nucleophiles that can be catalyzed by Pd-based catalysts are C-C coupling reactions.¹ Among, Sonogashira reaction potentially can be applied for the synthesis of a wide range of synthetic compounds. Classic methodologies for coupling reactions contained use of homogeneous Pd catalysts along with co-catalysts and ligands. Moreover, disclosing new catalysts, which didn't require use of co-catalyst and ligand and could promote the reactions in non-toxic solvents, has attracted intensive attention. In the following our study and research group²⁻³, herein, we describe the synthesis of 2,3-dialkynyl derivatives by using Pdcatalyzed Sonogashira coupling reaction. This palladated nitrogen-doped porous carbon was synthesized through multi-step procedure according to the previously reported method.⁴ The catalytic activity of the palladated nitrogen-doped porous carbon as a heterogeneous catalyst, Pd/MT/C, was investigated for ligand and copper-free Sonogashira coupling reaction under mild reaction conditions (80-90%), Scheme 1. Furthermore, the catalytic recyclability of Pd/MT/C was examined. The catalyst could be successfully removed from the reaction mixture by simple filtration and also recycled for several consecutive reaction times with slight loss of the catalytic activity.



Scheme 1. Sonogashira coupling reaction catalyzed by Pd/MT/C.

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Nano TiO₂ an Efficient Photocatalyst for the Synthesis of Xanthone Derivatives

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Abstract

Chemists have long been fascinated by the use of photochemistry to synthesize various molecules. However, synthetic photochemistry was for a long time a specialised region with limited applications, mastered by only a few chemists. In recent years, this situation has changed dramatically and many photochemical methods have been developed, greatly expanding the synthetic scope of modern chemists. This strategy relies on the use of new photocatalysts that harvest the energy of visible light to activate readily available substrates and to produce reactive radicals under very mild reaction conditions.¹

The synthesis of xanthones derivatives with Pharmacological properties and therapeutic possibilities such as antimicrobial, anticarcinogenic, antioxidant, Alzheimer's disease, or antidiabetic nature is currently of great interest.²

Visible light activation of TiO_2 electrons in the valence/HOMO in the photo-catalytic reaction system, while the light absorption results in electron holes into the conduction/LUMO to oxidize organic molecules. In recent years, titanium dioxide photocatalysis used for the selective photo oxidation of aromatic alcohols or phenols.³

We have demonstrated a simple method for the photochemical synthesis of xanthones derivatives using Nano TiO_2 as reusable, eco-friendly, inexpensive, and efficient photocatalyst under the mild conditions. The procedure for the preparation of Nano TiO_2 was simple, environmentally benign, and cost-effective.⁴



Scheme 1: The photochemical synthesis of xanthones.

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Nano TiO₂ an Efficient Photocatalyst for the Synthesis of Thiochromane Derivatives

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Abstract

Scientists have long been fascinated by the use of photochemistry for synthesise of organic molecules. Only a few chemists mastered synthetic photochemistry for a long time. In recent years, this point has changed completely and many photochemical methods have been developed and greatly grew the synthetic scope of modern chemists.¹

Thiochromane derivatives are not common in natural compounds, but they show important pharmacological properties and therapeutic possibilities such as anticancer, Alpha-2 adrenergic antagonistic and estrogen receptor downregulation activities.² Thus, the synthesis of thiochromane derivatives is currently of great interest.

 TiO_2 is almost the only material which is suitable for photocatalytic applications in the photocatalytic reaction systems especially in industrial scale. Among many candidates at present and also probably in the future. TiO_2 has shown the best efficient photoactivity activity, high stability, and low cost.³ In recent years, titanium dioxide photocatalysis have been applied for the selective photo oxidation of benzyl alcohol or phenols.^{4,5} This article was a descriptive synthesis of thiochromane derivatives under the mild conditions, with photochemical synthesis using Nano TiO_2 as efficient photocatalysts, a reusable, eco-friendly, and inexpensive. The procedure for the preperation of Nano TiO_2 is simple, non-toxic, specialized instruments, green, environment friendly,and cost-effective.⁶



Scheme 1: The photochemical synthesis of xanthones.

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Reinforcement of Low-density Polyethylene Films Using a Novel Carbon-based Nanocomposite

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Abstract

Low-density polyethylene (LDPE) is one of the most conventional polymers in the production of plastic compounds. The various properties of LDPE include low cost, high compression capability, recyclability, moisture absorption resistance, good chemical resistance, and easy production.¹ Polyethylene films are customarily produced from LDPE in a variety of ways, such as calendaring, extrusion, blowing, and casting. LDPE films have good electrical, mechanical, thermal, and optical properties, and they are usually reinforced by various additives.² Improving these properties is one of the most important issues in the plastic industry. Advances in nanotechnology and synthesis methods led to the production of nanocomposites which adding them to LDPE films, improved properties of LDPE films.³

In the presented paper, we synthesized a novel polymeric nanocomposite based on graphene, silica, and styrene. The low weight ratios including 0.5-2 (wt %) of this nanocomposite added to the LDPE films by solvent/vaporization solvent method (SVS). FT-IR, FE-SEM, and EDX analyzes were used to characterization novel cost-effective nanocomposite. After preparing the reinforced LDPE films by different weight ratios of the synthesized nanocomposite, tensile, contact angle, and AFM analysis were used. The values of thickness, force, extension, stress, and elongation-at-break for fabricated films were explored, which the best results related to the film containing 2 (wt %) nanocomposite. The AFM analysis of LDPE films showed that adding nanocomposite to pristine LDPE increases the roughness, which also confirmed that the reinforced LDPE was more hydrophobicity. In summary, the tensile properties at elongation, hydrophobicity, and roughness of the reinforced LDPE film by 2 % nanocomposite have increased about 63.2, 40.91, and 71.19 %, respectively. Although, our research has some novelty and advantages compared with the other studies including the synthesis of the new nanocomposite, low cost and short term synthesis than other nanocomposites, production of reinforced LDPE film using a simple and cost-effective system, and using low ratios of synthesized nanocomposite to reinforced LDPE.



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Investigation of Physical Properties of Bagasse-Based Papers and Their Application to Remove Environmental Pollutions

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Abstract

In this research, we employed a series of papers based on bagasse from Pishro Kaghaz Negar Pars company to exploration of their physical properties and anti-pollution performance. The pulp papers of these samples were fabricated using the basic Kraft and eco-friendly method.¹ In this case study, the physical properties of papers were examined in terms of Grammage, Tensile index, Breaking Length, Burst Index, Brightness, and Tear Index. The results indicate the papers with 170, 185, and 220 (g/m²) have grammages in the range of 163-175, 176-186, and 191-210 g/m², respectively. For papers with grammage of 170 (g/m²), the tensile index, breaking length, burst index, brightness, and tear index were 54-57 (Nm/g), 5.2-5.8 (km), 1.8-1.9 (kPa.m²/g), 73.3-78.3 (% ISO), and 5.2-7 (mN.m²/g), 76.9-83.4 (% ISO), and 5-6.8 (mN.m²/g); also this results for papers with grammage of 220 (g/m²) included: 54-57 (Nm/g), 5.5-5.8 (km), 1.8-1.9 (kPa.m²/g), 73.3-78.3 (% ISO), and 5.2-6.5 (mN.m²/g).

These papers were used for the filtration of lead ions in distilled water. In order to determine the filtration performance, a piece of papers as a filter with the size of $4 \times 4 \text{ cm}^2$ was placed on a glass funnel; then the Pb²⁺ solution with 20 ppm concentration was poured on the filter and slowly passed through it.² All papers showed a high ability to filter the lead metal ions. The lowest efficiency of filter obtained 85.13 % for a paper with a grammage of 163 (g/m²) and the highest efficiency was 96.15 % for a paper with a grammage of 210 (g/m²). Besides, the microbiological properties of three paper samples with grammages of 169, 185, and 207 g/m² were explored according to Standard No. 14000, Iran National Standard Organization. The total number of microorganisms was calculated between 10² and 5.5×10²; the amount of Enterobacteriaceae was less than 10; observation of negative Escherichia Coli and Bacillus Cereus was less than 10², and value of Mold less than 10² was obtained.

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N-Heterocyclic Carbenes (NHCs) as the Catalyst in the Three-component Reaction of Dimedon, Aryl aldehydes, and Malononitrile

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Abstract

Heterocyclic compounds with benzopyran skeleton are an important class of "drug-like" compounds due to their interesting chemical structures and potential medicinal activities, including anti-inflammatory, anticoagulant, anti-cancer, antibacterial, antifungal, antioxidant and diuretics. These compounds have been studied to treatment of schizophrenia, Down syndrome, Alzheimer's disease, Huntington's disease, and Parkinson's disease.^{1,2} Benzimidazolium salts are a quaternary ammonium salt that has been considered by many researchers due to its wide applications in various fields such as catalyst and medicinal chemistry.^{3,4} These salts are the basis of important products called N-heterocyclic carbenes (NHCs), which are widely used as ligands and catalysts due to their strong sigmatic and weak acceptance.⁵ In this work, 1,3-dibenzyl-1*H*-benzo[*d*]imidazol-3-ium chloride is synthesized, characterized, and converted to N-heterocyclic carbene (NHC). This NHC was used as a catalyst in the reaction of aryl aldehydes, dimedone, and malononitrile to synthesis of tetrahydrobenzo[*b*]pyrans (Scheme 1). The use of other NHCs in the synthesis of tetrahydrobenzo[*b*]pyrans is also under investigation.



Scheme 1: Synthesis of tetrahydrobenzo[*b*]pyrans (4a-z) in the presence of NHC.

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Synthesis of Tetrahydro-1*H*-xanthens Using N-Heterocyclic Carbene Catalyst

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Abstract

Heterocycle compounds such as chromans and chromenes are important kinds of benzopyran derivatives to be found in many natural.¹ Especially, Compounds containing a xanthene are important biologically active heterocyclic compounds, which have antiviral, antimicrobial, antiinflammatory, anticonvulsant, and antimalarial activities.² Benzimidazole derivatives have various pharmacological activities such as antitumour, anti-ulcer, antibacterial, and antifungal properties. One of the important uses of these compounds is to make benzimidazolium salts.³

N-heterocyclic carbons are special compounds derived from benzimidazolium salts which show promising antimicrobial activity and has caused them to be widely used as suitable catalysts and ligands.⁴ In this work, 1,3-dibenzyl-1*H*-benzo[*d*]imidazol-3-ium chloride is synthesized and converted to NHC by Calcium carbonate then use this catalyst for reaction of salicylaldehyde derivatives and dimedone or Cyclohexane-1,3-dione to synthesis of Tetrahydro-1H-xanthens (Scheme 1).



Scheme 1: Synthesis of Tetrahydro-1*H*-xanthens (4a-z) in the presence of NHC.

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A Novel and Efficient Synthesis of Oxime Derivatives

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Abstract

Synthesis of novel biologically active heterocyclic compounds are undertaken with the ultimate hope of development of drugs.¹Quinoxalines are an important class of nitrogen-containing heterocyclic compounds which have shown wide variety of applications in pharmacology, so, they have received special interest by synthetic chemists for many years. These invaluable heterocycles have shown different pharmacological activities.²

The general synthetic pathway for the preparation of novel quinoxalines derivatives is shown in (Fig 1). We studied the O-alkylation of structurally diverse oximes with carbon electrophiles and employed the O-oxime ether bond to synthesize some novel compounds with bioactive various potential.³ In this synthesis, the oximation of aromatic ketones followed by an O-alkylation reaction with epichlorohydrin produce the corresponding *O*-oxime ether adducts. The *N*-alkylation of 1,2-phynelen diamine with *O*-oxime ether adducts led to synthesis of new analogues of quinoxaline compounds. In this context and in line with the global interest in design and synthesis of new *N*-heterocyclic compounds hereby, we disclose the synthesis of Quinoxalines compounds as antibacterial agent.



Scheme 1. Synthesis of quinoxaline derivatives

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Synthesis of two Copper (II) Schiff Base Complexes with Biological and Catalyst Property

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Abstract

In recent years, the development of efficient new catalysts for several organic reactions like click reaction have received considerable attention.^{1,2} we report a new catalyst system based on Cu(II) and ascorbic acid as reducing agent for regioselective 1,3-dipolar Huisgen cycloaddition reaction to access diverse 1,2,3-triazole cores. 1,2,3-Triazole moieties are attractive compounds in medicinal chemistry because of their wide range of applications including use as HIV protease inhibitors, as well as anticancer, anti-tuberculosis, antifungal and antibacterial agents.^{3,4} The present study describes the synthesis and characterization of some Schiff base ligands and their Cu(II) complexes. The two catalysts in this research were tasted against two pathogenic bacteria in order to assess their antibacterial properties. The results showed that the complexes possess higher antibacterial activity as free Schiff base ligands. Both complexes are effective catalysts for the cyclization reactions. As can be seen in schem1, the 1,2,3-Triazole compounds prepared via click reaction in the present of two catalyst. The percentage product of reactions show [CuL₂] complex being more active then [CuL1] complex.



Scheme 1: Synthesis of two Copper (II) Schiff Base Complexes with Catalyst Property

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Synthesis of 4H-pyran Derivatives Using Ferrous Silicate Sulfursalicylic Acid Nanoparticles (Fe3O4@SiO2@5-SA)

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Abstract

An efficient and straightforward method for constructing of biologically active 4H-pyran derivatives by the michel addition cycloaddition reaction of Dimedone, malononitrile and benzaldehyde in the presence of ferrous silicate sulfursalicylic acid nanoparticles (Fe3O4@SiO2@5-SA) has developed. Using a magnetically recoverable acidic ionic catalyst allows eco-friendly and facile conversion and simplifies experimental setup and work-up procedure that enables the direct synthesis of 4H-pyran derivatives under mild conditions. The designed catalytic system provides a broader scope under short reaction times in good to excellent yields. Fe3O4@SiO2@5-SA could be simply recovered by magnetic separation using an external magnet, maintaining stable activity up to five cycles without appreciable loss of activity.



Scheme 1: Synthesis of some novel 4H-pyran derivatives Using Ferrous Silicate Sulfursalicylic Acid Nanoparticles

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Synthesis of 4-hydroxy chromene-2-one Derivatives Using Ferrous Silicate Camphorsulfonic Acid Nanoparticles (Fe3O4@SiO2@GMSI-CMA)

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Abstract

ferrous silicate camphorsulfonic acid nanoparticles (Fe3O4@SiO2@GMSI-CMA) synthesized and proved to be a green and recyclable catalyst for Synthesis of 4-hydroxy chromene-2-one derivatives products under mild reaction conditions. It is manageable to large-scale preparation with simple instruments and gives the desired compounds in short reaction times with good-to-excellent yields (73–95%) under mild conditions. Magnetic separation protocol has used to achieve a simple separation and reuse of catalysts from unpuried reaction mixtures using external magnets without loss of catalytic operation after five cycles.



Scheme 1: Synthesis of 3,3'-(phenylmethylene)bis(4-hydroxy-2H-chromen-2-one) derivatives Using Ferrous Silicate Camphorsulfonic Acid Nanoparticles

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The Application of MOF-199 Organic-Metal Framework in the Highly Efficient Synthesis of 2'-aminospiro[indeno[1,2-*b*]quinoxaline-11,4'-[4'H] pyran]-3'carbonitrile

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Abstract

The compounds of spiro indenoqinoxaline are produced from a cyclic structure of indene and quinoxaline. Quinoxaline derivatives are biologically active heterocycles that are known as antifungal, antidepressant, antitumor, antioxidant, anticancer, and antitubercular agents.¹ In addition, indene derivatives have attracted much interest due to their anti-inflammatory, analgesic, and antibacterial properties.² Combining these two rings into one compound could create a new class of biologically active compounds with prominent pharmacological effects.

One of the methods that can successfully synthesize 2'-aminospiro[indeno[1,2-*b*]quinoxaline-11,4'-[4'H]pyran]-3'- carbonitrile derivatives is a multicomponent reaction. Multicomponent reactions (MCRs) are useful tools for one pot synthesis of multifunctional polycyclic compounds.³

In this study, we wish to report the application of separable metal–organic framework (MOF-199) catalyst, in the four component synthesis of 2'-aminospiro[indeno[1,2-*b*]quinoxaline-11,4'-[4'H]pyran]-3'–carbonitrile. MOF-199 is a metal–organic framework that composed of copper (ii) and 1,3,5-benzenetricarboxylic acid as ligand (BTC-Cu).⁴



Scheme1. The synthesis of spiro indene derivatives using metal-organic framework (MOF-199).

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Catalyst-Free Three-Component Approach to Synthesis of Spirooxindole Scaffolds Using Ketene Aminals

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Abstract

An important challenge to discover biological molecules is the design of an economical and highly efficient synthetic reaction to provide structural variety products with valuable biological properties. The spirooxindole scaffold is one of the most extraordinary spirocycles and central structural frameworks found in various natural compounds and bioactive structures. The existence of a chiral spiro center in a biologically active compound leads to structural rigidity and complexity which is a significant target for synthetic organic chemists.¹ Isatin and its derivatives have noteworthy biological activities and are broadly used in spirooxindole-based organic compounds synthesis.² In addition, ketene aminals (KAs) have been used as usefull and versatile enamine analogues with unique structural properties in synthesizing different kinds of fused five- and six-membered heterocycles drug-like molecules.³

Due to the essential demand for the production of small molecules containing bioactive heterocycles with potential biological activities for drug designing, here we developed a new method based on a three-component reaction of the (*E*-)-*N*-methyl-1-(methylthio)-2-nitroethenamine **1**, isatin **2** and new enolizable C-H activated compound **3** under mild and catalyst-free conditions leads to new functionalized chiral spirooxindole **4** in moderate to good yields (Scheme 1).



Scheme 1: Synthetic approach for the formation of spirooxindole scaffolds 4.

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Three-Component Synthesis of Novel Propargylamines Involving theophylline as Potential Therapeutic Agents

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Abstract

Xanthine alkaloids including caffeine, theophylline, and theobromine are the key structural motif present in the structure of numerous drugs and biologically active compounds. Theophylline (1,3-dimethyl xanthine) is a natural compound which is found in the tea and cocoa beans. Theophylline was first extracted from tea and synthesized chemically in 1895. It was initially used as a diuretic. In 1922, it was discovered that theophylline has the property of dilating the airways and since then it has been used in the clinical treatment of asthma.¹

Propargylamines are an important synthetic intermediates which are used for the synthesis of various types of chemical and biological active compounds such as polymers, heterocycles, therapeutics, natural compounds, and β -lactams.^{2,3} The most common route to access propargylamines is the three-component reactions (3CRs) between aldehyde, amine and terminal alkyne.⁴

Given the significance of xanthine alkaloids and propargylamines in organic and medicinal chemistry, we wish to report the synthesis of propargylamine derivatives containing theophylline via 3CRs between aldehyde, amine, and N-propargyl theophylline catalyzed by silica-tethered cuprous acetophenone thiosemicarbazone (STCATSC) (Scheme 1). After the optimization of the reaction conditions including the solvent, temperature, and catalyst amount,10 compounds were successfully synthesized and their biological activities are currently under investigation.



Scheme 1: Synthesis of propargylamine derivatives using STCATSC

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One-pot Synthesis of 4,4'-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s Catalyzed by [TMEDSA][HSO₄]₂, as a Highly Efficient Bronsted Acidic Ionic Liquid Catalyst

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Abstract

Heterocycles, especially nitrogen-containing ones, are among the fundamental components of many drugs and biological compounds For instance, pyrazole containing heterocycles {e.g. 4,4'-(arylmethylene)-bis(3methyl-1-phenyl-1H-pyrazol-5-ol)s} represent a numerous biological and medicinal properties, such as antinociceptive, antiviral, analgesic, antitumor and antifungal activities.¹

One of the conventional chemical approach to 4,4'-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5ol)s involves one-pot tandem Knoevenagel-Michael reaction of arylaldehydes with 2 equiv of 3-methyl-1phenyl-1H-pyrazol-5(4H)-one performed under a variety of reaction conditions.² However, most of the methods have one or more limitations such as moderate yields, long reaction times, application of hazardous solvents, use of toxic organic solvents and harsh reaction conditions.³

"Solvent-free conditions" in organic synthesis compared to "classical solution conditions" has often advantages such as decreasing or avoiding production of waste/by-products, higher selectivity, easier work-up and purification of product and environmentally benign nature.⁴ In this research, the synthesis of 4,4'-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol) derivatives in solvent-free conditions was performed in the presence of [TMEDSA][HSO4]2 (Scheme 1). The results show that this ionic liquid is as an excellent catalyst for the condensation of 3-methyl-1-phenyl-1H-pyrazol-5(4H)-one with aromatic aldehydes. This method has the advantages of high yield, simple operation and short reaction time.



Scheme 1. Synthesis of 4,4'-(arylmethylene)-bis(3-methyl-1-phenyl-1H-pyrazol-5-ol)s using .

[TMEDSA][HSO4]2

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[TMEDSA][HSO₄]₂-Catalyzed, Solvent-Free Synthesis of Symmetrical *N*,*N*'alkylidenebisamides by Reaction Between Aldehydes and Amides

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Abstract

The notability of amides in biology, chemistry and technology is well recognized due to presence of this functionality in many natural products, proteins, pharmaceuticals, and therapeutic drugs. During the course of drug discovery almost 16% of all reported reactions are amide bond formation and over 50% of all drug candidates contain at least one amide bond functionality.¹

Among the amides, symmetrical and unsymmetrical *N*, *N'*-alkylidene bisamides and their derivatives are found as key structural subunits for the construction of peptidomimetic frameworks [16]. Other advantage of this amids consist of HIV inhibitors, antihypertensive, antitumor, antibacterial, anti-inflammatory agent, calcium channel blockers, α -adrenergic and neuropeptide Y antagonists.²

lonic liquids including the Lewis and the Bronsted acid have been proven to be efficient catalysts for various reactions because of various exclusive advantages such as environmental friendly, chemical and thermal stability and very low vapor pressure.³⁻⁵

In the present work, *N*,*N*,*N'*,*N'*-tetramethylethylenediaminium-*N*,*N'*-disulfonic acid hydrogen sulfate ([TMEDSA][HSO₄]₂), a protic acidic ionic liquid has been applied as a highly effective and homogeneous catalyst for the solvent-free preparation of symmetrical *N*,*N'*-alkylidenebisamides via the one-pot multicomponent reaction of arylaldehydes with benzamide/acetamide in solvent free conditions (Scheme 1). This protocol offer advantages such as high yields, short reaction times, generality, cost effective, simple procedure for the catalyst preparation and environmentally benign.



 $[TMEDSA][HSO_4]_2 = \begin{bmatrix} Me_{1}^{HE}_{1}^{He_{1}^{HE}$

Scheme 1. The production of N,N'-alkylidene bis-amides using [TMEDSA][HSO4]2

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Synthesis of spiro[indolo[2,1-*b*]quinazoline-pyrano[2,3-*c*]pyrazole] *via* Sequential Four-Component Reaction

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Abstract

Pyrano[2,3-*c*]pyrazoles, a fused heterocyclic five-member pyrazole ring to a six-member pyran ring, possess various biological and pharmacological activities which play an important roles in the field of medicinal chemistry.¹

The indoloquinazoline compounds are fascinating fused heterocyclic skeletons which are widely distributed in natural products, bioactive compounds, and synthetic molecules. Due to the special importance of them in synthetic and medicinal chemistry, they have attracted the attention of synthetic chemists.²

Considering the importance of two above motif parts and their significant properties, combination of two compounds in one molecular structure is very attractive which maybe leads to further biological screening. Herein, an efficient synthesis of a novel series of functionalized spiro[indolo[2,1-*b*]quinazoline-pyrano[2,3-*c*]pyrazole] derivatives via reaction between tryptanthrines, malononitrile and 3-methyl-pyrazol-5(4*H*)-ones is reported in CH₂Cl₂, in the presence of Et₃N at room temperature (25°C), in 62% - 83% yields (Scheme 1). Mild reaction conditions, short reaction time, simple purification and no chromatographic process, are notable advantages of this protocol which make it attractive.



Scheme 1: synthesis of spiro[indolo[2,1-b]quinazoline-pyrano[2,3-c]pyrazole] derivatives

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Synthesis of spiro[indolo[2,1-*b*]quinazoline-pyrano[2,3-*d*]pyrimidine] and spiro[indolo[2,1-*b*]quinazoline-pyrido[2,3-*d*]pyrimidine] via Sequential Four-Component Reaction

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Abstract

Pyrano[2,3-*d*]pyrimidinones and pyrido[2,3-*d*]-pyrimidines are analogues of uracil, which show considerable pharmacological properties and biological activities.¹ On the other hand, the indoloquinazolines constitute an important class of compounds which exhibit a wide range of biological and pharmacological activities. These compounds have been reported to be protein kinase CK2 inhibitors and poly (ADP-ribose) polymerase-1 (PARP-1) inhibitors. they have attracted the attention of synthetic chemists due to the versatile properties and importance of them in synthetic and medicinal chemistry.²⁻³

Considering the importance of such compounds and their significant properties, it is realized that the connection of these above compounds can enhance their inherent pharmaceutical activities in new derivatives. Herein, we report an efficient synthesis of functionalized spiro[indolo[2,1-*b*]quinazoline-pyrano[2,3-*d*]pyrimidine] derivatives and spiro[indolo[2,1-*b*]quinazoline-pyrido[2,3-*d*]pyrimidine] via reaction between tryptanthrines, malononitrile and some CH-acids including barbituric acid/ thiobarbituric acid/ 4(6)-aminouracil in CH₂Cl₂, in presence of Et₃N, under reflux condition, in high yields.



Scheme 1: Synthesis of spiro[indolo[2,1-b]quinazoline-pyrano[2,3-d]pyrimidine] derivatives and spiro[indolo[2,1-b]quinazoline-pyrido[2,3-d]pyrimidine]

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One-Pot Synthesis of Melamine Based Porous Organic Polymers

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Abstract

Porous organic polymers (POPs) are a class of multi-dimensional porous network materials, which are built via strong covalent linkages between various organic building blocks. They can be divided into two categories based on their degree of long-range order, including amorphous and crystalline.¹They have been used as gas storage materials for energy applications, solid supports for catalysis and other intriguing applications.²

Here, we report the synthesis of melamine-based polyamides by one-pot polycondensation strategy and Schiff-base reaction under mild conditions with constant molar ratio of melamine and binary benzoic acid/aldehyde without catalyst, respectively (Scheme 1). The prepared POPs were characterized by Fourier transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TGA), X-ray diffraction (XRD), fieldemission scanning electron microscope (FESEM), and BET analysis. The obtained polymers showed poor solubility in most solvents such as water, acetone, ethyl acetate, dimethylformamide, chloroform, tetrahydrofuran and 1,4-dioxane. However, improved solubility observed for isophthalic acid-based POP in 1,4-dioxane and chloroform due to the less rigid and less linear structure.



Scheme 1: The structure of prepared melamine based porous organic polymers

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Synthesis of Novel Diamondoid-Containing Pyrimidines

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Abstract

Diamondoids are cage hydrocarbon molecules that can be described as fully hydrogen-terminated nanometer-sized diamonds.¹ Adamantane molecule, corresponding to $C_{10}H_{16}$ formula, is the smallest Diamondoid. Derivatives of adamantane have found numerous applications in medicinal chemistry. The adamantyl group is present in eight compounds in current clinical use for the treatment of neurodegenerative disorders, viral infections and type-2 diabetes. Having the "lipophilic bullet" (adamantane is often viewed as providing the critical lipophilicity) readily available as an "add-on" for known pharmacophors, it was used in the modification of drugs. The adamantane modifications were chosen to enhance lipophilicity and stability of the drugs, thereby improving their pharmacokinetics.²

Dihydropyrimidinones (DHPMs) have widespread pharmacological activities, and are regarded as one of the most important groups of drug-like scaffolds.³ The Biginelli reaction is ranked as one of the most powerful tools for the facile synthesis of these scaffolds.

In this work, novel diamondoid-modified pyrimidines were synthesized in two steps. Firstly adamantlycontaining active methylene compound **1** was synthesized by the reaction of amantadine (1aminoadamantane) with ethyl acetoacetate. Then Biginelli reaction of **1** with thiourea **2** and benzaldehyde derivatives **3** afforded pyrimidines **4a-h**. All synthesized compounds were completely characterized by FT-IR, ¹H and ¹³C NMR spectroscopy.



R= H, 2-Me, 3-Me, 4-Me, 2-OMe, 3-OMe, 3-NO₂, 4-NO₂

Scheme 1: Synthesis of diamondoid- containing pyrimidines 4

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Methyl-2,4-dioxo Pentanoate with Aldehydes in the Presence of Indole

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Abstract

Considering the importance of indole derivatives as drugs affecting cancer cells and various other drug effects, in this study, new derivatives of methyl 2,4-dioxopentanoate and aldehydes adjacent to indole (including 4-nitro benzaldehyde, 3-nitrobenzaldehyde), and in the presence of piperidine at 80-90 degrees Celsius using acetone as solvent, in this reaction, acetylacetone was used instead of methyl 2,4-dioxopentanoate and aldehydes in the vicinity of indole. The products were detected by FTIR spectroscopy, ¹H NMR, ¹³C NMR.

Below is a general overview of these reactions:



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Green, Rapid and Efficient Synthesis of Chalcone Derivatives in the Presence of Novel NCP@SO₃H as Catalyst

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Abstract

The Chalcone derivatives are the subject of experimental and theoretical investigations. These flexible molecules appear in various conformations, and their properties depend on a suitable ring substitution as well as on the presence of the unsaturated ketone moiety.¹ Chalcones belong to the flavonoid family which constitutes one of the major class of naturally occurring oxygen heterocyclic compounds.² The unsaturated carbonyl system of chalcones possesses two electrophilic reactive centers allowing them to participate in addition reactions *via* attack to the carbonyl group or involving the carbon (1,4-conjugate addition), leading to the synthesis of promising bioactive heterocyclic compounds.³

Catalytic approaches might be considered as green since specific chemical transformation could be achieved within very short time with the addition of very little catalysts, significantly reducing production cost as well as health and environmental risks. Nowadays, silica, carbon, clay, zeolite, metal oxide polymers, and other mesoporous materials are being used as inorganic solid supports.⁴⁻⁶

In this research, preparation of α , β -unsaturated carbonyl system through reaction of indandione with various aldehyde has been investigated. Due to the efficiency of nano catalysts in the organic syntheses, initially, novel nano acid catalyst synthesized through treatment of synthetic nano clinoptilolite and CISO₃H. In continuation of our research, catalytic activity of synthetic NCP@SO₃H studied for preparation of desire products (Scheme 1). As a results, in the presence of this catalyst (0.011 g), the 2-arylidene-1H-indan-1,3(H)-dione drivatives obtained with excellent yields and short reaction times. The low cost and availability of catalyst, novel and green procedure makes this strategy more useful for the preparation of these α , β -unsaturated carbonyl compounds. The structure of synthetic nano catalyst confirmed by various analytical techniques such as; FT-IR, XRD, FE-SEM and EDS.



Scheme 1. Synthesis of chalcones in the presence of NCP@SO $_3H$

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Atom Transfer Radical Photopolymerization and Copolymerization of Monomers with Fluorescein Photocatalyst in Aqueous Media

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Abstract

Radical polymerization of photo-induced atom transfer (ATRP) is one of the most efficient polymerization methods designed to synthesize controlled molecules with low molecular weight and low dispersion. This process is environmentally friendly and can be used on an industrial scale.¹ The metal-free of this polymerization and the use of organic compounds instead of complexing intermediate metals as catalysts allow the use of these polymers in fields such as electronics and medicine.² Also, the light-oriented nature of the ATRP process saves energy and controls the polymerization rate by changing the light intensity.³ In this study, styrene monomer and fluorescein photocatalyst in water, which is a green solvent and has no problems with the use of organic solvents, were successfully polymerized and finally a copolymer was prepared to prove the viability of the reaction. The effect of reaction time and light intensity on the product efficiency was studied and the results of the research were evaluated using nuclear magnetic resonance spectroscopy (NMR) and infrared (IR) spectroscopy.

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Pyrrole-Schiff Base Complex of Palladium Supported Into Mesoporous Channels of MCM-41 as an Efficient, Reusable and Selective Catalyst in Suzuki and Heck Reactions

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Abstract

C–C bond formation is an interesting tool for the synthesis of natural products, advanced materials, biologically active compounds, hydrocarbons, UV screens, and polymers. C–C coupling reactions are commonly reported with palladium catalysts including phosphine ligands. The use of phosphine ligands leads to toxicity, high-cost, and also moisture or air sensitivity of the previously reported procedure. Herein, a phosphine-free and efficient method is reported for C-C coupling reactions such as Heck and Suzuki reactions in the presence of pyrrole Schiff base complex of palladium immobilized on mesoporous of MCM-41 (Pd-Pyrrole-MCM-41). The synthesis method of this catalyst is easy and it is prepared from available starting materials. The catalyst was characterized by FT-IR, TEM, XRD, SEM, BET and ICP-OES techniques. This catalyst has a high surface area therefore it has a higher catalytic activity than older catalysts. The protocol proves to be efficient and environmentally benign in terms of high yield, easy of recovery and reusability of catalyst. Also, a good selectivity was indicated in the C-C coupling reactions in the presence of Pd-Pyrrole-MCM-41 as catalyst. This catalyst is heterogeneous in nature therefore Pd-leaching under reaction conditions does not occur as a result, This catalyst can be reused for several runs.



Scheme 1: Pd-Pyrrole-MCM-41catalyzed the Suzuki and Heck reactions

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Manganese Supported on Modified MCM-41 with 5-Nitro Salicylaldehyde as a Recyclable and Chemoselective Nanocatalyst in Oxidation of Sul Oxidative Coupling of Thiols

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Abstract

The synthesis of sulfoxides and disulfids are two important transformation in organic chemistry, because these materials are useful in the synthesis of drugs, enzymes activation, natural products, germicides, and in medicinal chemistry such as antibacterial, anti-ulcer, antifungal and anti-atherosclerotic agents. Among the various oxidants; H₂O₂ was commonly used for this transformation as an inexpensive and environmentally benign oxidant. 5-Nitro salicylaldehyde Schiff-base is a bidentate ligand which have two donor atoms which allow them to bind to a central metal atom or ion at two points. In this work, manganese Schiff base complex of 5-Nitro Salicylaldehyde has been immobilized into mesoporous channels of MCM-41 (Mn-5NSA-MCM-41) and further applied as an excellent, recyclable and chemoselective nanocatalyst for the oxidation of sulfides to sulfoxides and oxidative coupling of thiols to corresponding disulfides. The catalyst was characterized by FT-IR, XRD, BET and TGA techniques. Also this catalyst can be recovered and reused for several times. The manganese Schiff-base complex is immobilized with strong bonds on the MCM-41, therefore the Mn-metal is not released in the reaction mixture and the reactions are performed under heterogeneous conditions, as well as the catalyst can reused for several times. Recyclability, easy synthesis, biocompatibility, high stability, selectivity and high catalyst activity are the advantages of this catalyst.





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Synthesis of Novel Ionic Liquids Bearing2,4-Thiazolidinedione Core as Potential Therapeutic Agents

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Abstract

Due to the unique biological activities of thiazolidinedione (TZD, **1**, Figure 1) derivatives, synthesis of novel TZD substrates has attracted considerable attention for drug design and discovery. Compounds containingthe thiazolidinedione core are used as antibacterial, antifungal, anti-inflammatory, aldose reductase inhibitors anti-diabetic, antimalarial, monoamine oxidase B (MAO-B) inhibitor, antiproliferative,MurD ligase inhibitor, antioxidant, and antitumor agents.^{1,2}

Many of the drugs used to treat a variety of diseases are in solid form, which can cause problems such as low solubility, instability, low efficacy, low absorption in the body and other side effects. Drug solubility is an important issue in the synthesis of new drugs. One way to increase the solubility of the drug is to use charged groups and synthesize the drug in the form of salt (i.e.: ionic liquids).^{3,4}Along this line, numerous drugs and active pharmaceutical ingredients are used as their ionic liquids, as instances morpholine salicylate, 1-butyl-3-methylimidazolium salicylate, and 1-butyl-3-methylimidazolium ibuprofenate. Inspired by numerous biological activities of TZD derivatives and application of ionic liquids in different era of science especially medicinal chemistry, herein, we report the synthesis of structurally divers ionic liquids bearing 2,4-thiazolidinedione core as potential therapeutic agents. The general structure of the synthesized ionic liquids **2** is shown in Figure 1. To synthesize compounds **2**, treatment of the presynthesized carboxylic acid derivatives with secondary amines in proper solvent at room temperature affords the desired products in good yields. The biological activities of title compound are under investigation and will be reported.



Figure 1: Structure of TZD (1) and synthesized ionic liquids (2)

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Green Synthesis and Characterization of Mannich Bases in the Presence of Nano Clinoptilolite under Solvent-Free Conditions

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Abstract

Multicomponent reactions have gained considerable attention in recent times. These reactions have avoided the tedious steps of protection and deprotection of functional groups, isolation of intermediates, thereby reducing the generation of waste.¹⁻³ The classical Mannich reaction is one of the most important carbon–carbon bond-forming reactions in organic synthesis because of its atom economy advantages and application in biologically active molecule syntheses. However, a three-component condensation between structurally diverse substrates containing at least one acidic hydrogen atom, an aldehyde component and an amine reagent leads to Mannich bases.⁴ Coumarin is a lactone compound which is widely distributed in plants and can be extracted, among others, from Anthoxanthum odoratum, Melilotus officinalis and Dipterix oppositifolia. Its derivatives are used as daylight fluorescent pigments, brighteners, fluorescent dyes, fluorescent sensors, laser dyes, drug carriers and drug delivery agents. Recently, various medicinal effects, such as anticoagulant, analytical fluorescence indicator, anti-inflammatory, and antioxidant properties have been reported. Recently, nanomaterial-based catalysts as prominent heterogeneous catalysts are widely used in different fields such as; organic synthesis.⁵⁻⁷ The low cost and special features of clinoptilolite make it valuable in many applications such as catalyst in organic synthesis.⁸

In connection with our consistent interest in the development of efficient synthetic methodologies, we report herein a new, green and efficient protocol using nanoclinoptilolite catalytic system to access the synthesis of some novel phenyl amine derivatives containing with hydroxyl-cumarin moiety through three component reaction under solvent-free conditions. Initially, an Iranian clinoptilolite tuff was pretreated and crushed by a mechanical method to obtain nanoparticles during a ball milling process and then mixture to one drop acetic acid. Then, three component reaction of hydroxycoumarin, various aromatic aldehyde and aniline investigated in the presence of acidic NCP under solvent-free conditions and heating at 60 °C temperature (Scheme 1.). As a results, using acidic NCP 4-hydroxy-3-(aryl (phenyl amino) methyl)-2H-chromen-2-one derivatives obtained in high yields and short reaction times. The structure of catalyst and products characterized using various analytical techniques.



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Synthesis of Modified Magnetic Nanoparticles with Some Organic Compounds and Their Applications in the Removal of Direct Red 16 Dye From Textile Industry Wastewater

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Abstract

In this work, magnetic iron nanoparticles were synthesized by co-precipitation method¹ and coated ² with some fatty acids (such as oleic and palmitic acid) and surfactants [such as sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB)]. Then the coated magnetic nanoparticles were identified by various analysis methods (FT-IR, SEM, VSM, EDS and XRD).³

In the next step, the application of these adsorbents in neutral and alkaline environments for separate the Direct Red 16 dye from the textile industry effluent was compared.^{4,5}

UV-VIS device was used to determine the amount of dye adsorption by nanoparticles. The results of the analysis showed that nanoparticles are active to absorb dyes under optimized conditions. The highest adsorption was recorded for iron oxide nanoparticles coated with cetyltrimethylammonium bromide (Fe₃O₄@CTAB) with 99.51% in neutral environment. Easy to use, reusability, use of inexpensive modifiers, use of environmentally friendly support as well as stability of nanoparticles up to at least 5 times in a row without significant activity loss, are some of the significant advantages of these nanoparticles.



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Pd Nanoparticle Immobilized on Fe₂O₃@SiO₂ Core-Shell Hollow Sphere Decorated by Cyclodextrin-Nanosponge: An Efficient Catalyst for Suzuki Coupling Reaction

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Abstract

Core-shell magnetic nanoparticles have a wide range of applications in many research areas due to their unique properties such as high magnetic sensitivity and high surface area. These nanoparticles can lead to the formation of separable magnetic catalysts that can be easily recovered using an external magnet, making chemical synthesis cleaner and more economical. Among these, hollow sphere material is a good magnetic substrate for immobilizing palladium nanoparticles.¹

One of the most important organic reactions performed by palladium-based catalysts is C–C coupling reaction. The reaction of aryl halide and boronic acid to form C-C bonds performed by palladium-containing catalysts is called Suzuki–Miyaura cross-coupling reaction, which has many applications in organic chemistry to synthesis of natural products.² The use of homogeneous palladium catalysts with co-catalyst and ligand is one of the classic methods of coupling reactions. In addition, the emergence of novel catalysts, that didn't require use of co-catalyst and ligands that could promote these reactions in non-toxic solvents has attracted attention of industry enthusiasts.⁴

Following the work of our research group^{1, 3}, herein, the catalytic activity of palladium-containing magnetic catalyst was described. This palladated magnetic-hybrid system, h-Fe₂O₃@SiO₂–CDNS@Pd, as a heterogeneous catalyst was synthesized according to the previously reported method.¹ The catalytic activity of h-Fe₂O₃@SiO₂–CDNS@Pd was investigated for ligand and copper-free Suzuki coupling reaction, Scheme 1. Finally, the recyclability of this catalyst was also studied. The catalyst could be successfully removed from the reaction mixture by using an external magnet and also recycled for several consecutive reaction times with slight loss of the catalytic activity.



Scheme 1. Suzuki coupling reaction catalyzed by h-Fe₂O₃@SiO₂-CDNS@Pd.

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Pd@Hal-CDNS-g-C₃N₄ As an Effective Catalyst for Promoting Ligand and Copper-Free Suzuki Coupling Reaction

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Abstract

Heterogeneous catalysis plays a part in the production of more than 80% of all chemical products. It is therefore essential that all chemists and chemical engineers have an understanding of the fundamental principles as well as the applications of heterogeneous catalysts.¹ The palladium-catalyzed reaction of aryl halide and boronic acid for the formation of C-C bonds so-called Suzuki-Miyaura cross-coupling reaction has many applications in Modern Synthetic Organic Chemistry.² Halloysite nanoclay (Hal) is a tubular clay (Al₂(OH)₄Si₂O₅·2H₂O) composed of tetrahedral siloxane on outer surface and aluminol groups on inner surface. The water molecules in the structure of Hal are located between the interlayer spaces. The properties of Hal are very similar to those of Kaolin. However, the porous morphology of Hal as well as some other features of clay such as inert entity, bio-compatibility, high mechanical, chemical stability and surface area, make this clay as a unique candidate for various applications such as drug delivery purposes, separation, catalysis and energy storage. Mostly, this naturally occurring clay is modiifed through surface functionalization. To date, various functional groups has been introduced for tuning the surface chemistry of Hal. Moreover, Pd-catalysts used for promoting these chemical transformations were mostly homogeneous and in some protocol use of costly or toxic solvents and bases was inevitable. Hence, development of an eco-friendly, eiffcient and cst-effectiv model for C C coupling reactions has received growing attention. In this line, disclosing of heterogeneous catalysts and development of ligand and copper-free methods in aqueous media were focused. Following the work of our research group on heterogeneous catalyst ³, herein, Pd@Hal-CDNS-g-C₃N₄ was applied for promoting ligand and copper-free Suzuki reactions in aqueous media (45-95%), Scheme 1. This catalyst was synthesized according to the previously reported method.⁴ Furthermore, the recyclability of Pd@Hal-CDNS-g-C₃N₄ was investigated. The catalyst could be successfully removed from the reaction mixture by simple filtration and also recycled for several consecutive reaction times with slight loss of the catalytic activity.



Scheme 1. Suzuki coupling reaction catalyzed by Pd@Hal-CDNS-g-C₃N₄

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Palladium Nanoparticles Doped on Magnetic Covalent Hybrid of Graphitic Carbon Nitride and Graphene Oxide: An Efficient and Recyclable Catalyst for A³ Coupling Reaction

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Abstract

On of the best way to control and stabilize the Pd nanoparticles is dispersing small-size Pd nanoparticles on appropriate supporting materials, such a carbon materials. In particular, graphitic carbon nitrides with the layered structure and rich nitrogen content are promising heterogeneous catalyst supports. Graphene that is a two dimensional carbon sheet exhibits low catalytic activity. Mostly, to improve the catalytic activity of graphene, it can hybridized with other materials. The results confirmed that hybridization of graphene and $g-C_3N_4$ can be considered as a solution for circumventing the drawbacks of these two carbon materials.¹⁻²

Propargylamines can be obtained from three component coupling reaction of amines, aldehydes and alkynes, referred to as the A³ coupling reaction. Propargylamine derivatives are key intermediates which are broadly applied for the synthesis of a diverse range of natural products and biologically active nitrogen containing chemicals. Despite developing some promising methodologies, some of them require a toxic solvent such as toluene, or expensive media, like ionic liquids. Therefore, development of a novel, efficient and heterogeneous catalyst for this process is a great idea. In continuation of our attempts ³⁻⁴, herein, we wish to disclose a novel efficient hybrid catalyst for promoting A³ coupling reactions under mild and green reaction conditions (75-95%), Scheme 1. This palladated magnetic covalent hybrid of graphitic carbon nitride and graphene oxide, Pd@g-C₃N₄-Fe-GO, was synthesized through multi-step procedure according to the previously reported method ². Furthermore, the catalytic recyclability of Pd@g-C₃N₄-Fe-GO, was also examined. The catalyst could be successfully removed from the reaction mixture by using an external magnet and also recycled for several consecutive reaction times with loss of catalytic activity.



Scheme 1. A³ coupling reaction catalyzed by Pd@g-C₃N₄-Fe-GO

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The Application of Copolymer-Coated Magnetic CNT in the Synthesis of Spiro [indolin-3,4`-pyrano [2,3-c] pyrazol] Derivativess

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Abstract

Spiro [indolin-3,4'-pyrano [2,3-*c*] pyrazol] derivatives are important heterocyclic compounds and represent a wide range of biological and medical activities. Anti-allergic, anti-inflammatory and anti-fungal effects have been reported for this heterocycles.¹ In addition, they are used in agriculture as insecticides, pesticides, herbicides and fungicides.²

One of the most useful methods that can be used for the preparation of spiro [indoline-3,4'-pyrano [2,3-c] pyrazol] compounds is multi-component reaction. Multi-component reaction is a powerful tool for the preparation of multi-functional products with high structural diversity in which three or more starting materials combine together in a one-pot, one-step reaction to give a single product.³

In this study, a new copolymer coated magnetic carbon nanotube was synthesized and characterized by FT-IR, SEM, VSM and EDS analyses and satisfactorily used in the multi-component preparation of spiro [indoline-3,4'-pyrano [2,3-c] pyrazol] derivetives. The catalytic activity of this new magnetic nano catalyst was compared with similar nano composites as catalyst.



Scheme1: synthesis of spiro [indoline-3,4'-pyrano [2,3-c] pyrazol] derivetives using Poly(Py-co-Ani)@CNT-Fe₃O₄ magnetic nanocatalyst

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CaFe₂O₄@SiO₂@SO₃H as a High Efficient, Durable, and Heterogenous Recovarable Magnetic Nanocatalyst for the Green Synthesis of Quinolines.

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Abstract

As a continuous attempt in the laboratory toward the advancement of new procedures for the high-speed synthesis of biologically relevant heterocyclic compounds, we became interested in developing a one-pot mechanism of the Friedlander synthesis.¹ The derivatives of Quinolines are one of the N-heterocyclic compounds and their derivatives have shown different pharmaceutical and physiological activities such as antibacterial, anti-inflammatory, antimalarial, anti-asthmatic, anti-hypertensive, analgesic agents, and anticancer. They were also employed in natural products, drugs, and chemistry.² Among the different ways for the synthesis of Quinolines, the Friedländer annulation is a common and easy method for the preparation of multifunctional quinolines. This method involves a condensation-cyclization between 2-aminoaryl ketones and an active carbonyl compound bearing a reactive α -methylene group that is catalyzed by an acid or base.³ Various Lewis acid and Brønsted acid-based catalysts as well as transition metal catalytic systems have been reported previously for the synthesis quinoline.⁴

On the development of useful synthetic methodologies, recently we have observed that $CaFe_2O_4@SiO_2@SO_3H$ catalyzes the Friedländer mechanism to form the corresponding Quinolines under mild conditions. These benefits have led to mild conditions for the preparation of quinolines, that is water as solvent at room temperature.



Figure 1: Quinolines Synthesis with CaFe₂O₄@SiO₂@SO₃H

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GO-NH₂-Cu²⁺ as a Novel, High Efficient, Heterogeneous Catalyst for the Green Synthesis of Suzuki-Miyaura Coupling Reaction in Aqueous Media.

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Abstract

The cross-coupling reaction is one of the fundamental reactions in the pharmacological industry and synthesis of organic compounds. The Suzuki-Miyaura reaction is the most convenient and efficient mechanism to form C–C bonds. Coupling reactions are used in the synthesis of pharmaceutical, natural products, materials science, biological, medicinal, supramolecular chemistry, coordination chemistry, polymer synthesis, complex molecules, and are also used in catalysis. Suzuki-Miyaura reaction is catalyzed by homogeneous catalysts and the reaction should be in high temperatures and toxic solvents. Recently, the synthesis of efficient green catalysts was received more attention. The reaction was usually catalyzed by noble and transition metals, such as Ni, Pd, Ru, Au–Pd, Au–Ag–Pd, and Pd–Ni. The metals (such as palladium) are not recommended, because Pd cannot be industrialized exclusively due to its high cost and other important factors, such as scarce storage capacities. The toxicity and high cost of Pd catalysts restrict their applications. Recent studies suggest that metal copper has a unique reactivity. The metal copper changes its oxidation states and easily undertakes radical reactions.¹⁻³

Modified graphene was used as a support for MNPs and applied in the coupling reactions. In this research, the preparation of the Cu supported on polyamine modified graphene oxide (GO-NH₂-Cu²⁺) by simple method for application as a robust heterogeneous catalyst for the Suzuki-Miyaura coupling reaction of phenylboronic acid and (bromoethynyl)benzene. The procedure was led to produce 1,2-Diphenylethyne derivatives compounds in excellent yields from 71% to 95%.⁴



Figure 1: 1,2-Diphenylethyne derivatives Synthesis

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Novel and Efficient Method for Synthesis of 3,3,6,6-tetramethyl-9-aryl-3,4,5,6,7,9-hexahydro-1H-xanthene-1,8(2H)-dione by Using NCP@-PMSi-HMTA as a Catalyst

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Abstract

MCRs provide a powerful and efficient approach to the synthesis of various heterocyclic compounds which mimic some natural heterocyclic compounds such as xanthenes.^{1, 2} Xanthene derivatives are very important chemicals with tremendous biological application. In medicinal applications these compounds share an important part. xanthene derivatives have moderate to excellent activities against number of biological targets. With changing substituents on the xanthene nucleus the biological targets vary from microbial diseased to viral problems and variety of cancerous cells. Xanthene derivatives target different biological problems by interacting with enzymes and proteins.³⁻⁶ Due to their wide range of applications, these compounds have received a great deal of attention in connection with their synthesis. Recently, nanomaterial-based catalysts as prominent heterogeneous catalysts are widely used in order to accelerate catalytic processes, particularly because they are accompanied with the principle of the green chemistry. Clinoptilolite is abundantly available in many regions around the world. The low cost and special features of clinoptilolite make it valuable in many applications. Clinoptilolite is used not only in its initial form but also in its modified form. It was pointed out that the area of application could be intensively expanded by the functionalization of external as well as internal surfaces of clinoptilolite. The modification can be conducted by various chemical reagents such as surfactants, organic compounds and inorganic substances.⁷ Herein, in order to achieve a more efficient synthetic process, minimize by-products, decrease the number of separate reaction steps, improving the yields and reaction times we wish to report a clean and environmentally friendly approach to the synthesis of xanthene derivatives via reaction of aldehydes and dimedone in the presence of functionalized nano clinoptilolite under solvent free conditions. Initially, basic NCP synthesized through reaction of synthetic NCP, chloropropyltrimethoxysilan and HMTA. In continuous of our research, preparation of xanthene derivatives investigated in the presence of this nano base solid catalyst (Scheme 1). The low cost and availability of catalyst, excellent yield of products, short reaction time, novel and green procedure makes this strategy more useful for the preparation of desire products. The structure of catalyst characterized using various techniques such as; FT-IR, XRD, FE-SEM and EDS.



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Cu@Furfural Imine-Decorated Halloysite as an Effective Heterogeneous Catalyst for the Preparation of Pyranopyrazoles *via* One-pot and Four-component Reaction in Green Media

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Abstract

Halloysite nanoclay (Hal) is a tubular clay $(Al_2(OH)_4Si_2O_5\cdot 2H_2O)$ composed of tetrahedral siloxane on outer surface and aluminol groups on inner surface, which applied in various fields such as drug delivery purposes, separation, catalysis and energy storage due to its unique properties. Copper nanoparticles as an eco-friendly and comparatively inexpensive metal-based nanoparticles play a significant role as catalyst in the field of organic transformation. Cu-based nanoparticles have been extensively examined as highly selective catalysts for the generation of carbon-carbon and carbon-heteroatom bond forming reactions.¹ Among them, multicomponent reactions (MCRs), proceeded with heterogeneous Cu-based nanocatalysts have undergone an explosive growth in recent years.²

In the following of our attempt to introduce heterogeneous and recoverable catalysts or promoting different organic reactions and developing eco-freindly methods for effective synthesis of chemicals,³⁻⁷ herein we report the methodology for the one-pot synthesis of pyranopyrazoles catalyzed by Cu@Hal-T-F as a heterogeneous catalyst. Cu@Hal-T-F was synthesized through multi-step procedure according to the previously reported method (6). To this propose, Hal was substituted with (3-chloropropyl) trimethoxysilan and subsequently treated with thiosemicarbazide and furfural to provide furfural imine functionalized Hal, which could serve as an effective support for immobilization of copper species. Next, the catalytic activity of Cu@Hal-T-F was evaluated in the synthesis of different 1,4-dihydropyrano[2,3-c]pyrazoles (**5a-j**) *via* four-component reaction of hydrazine hydrate, ethylacetoacetate, malononitrile and aromatic aldehydes involving electron-withdrawing or -donating substituents (ortho-, meta-, and para-functionlized) in H₂O as solvent under reflux conditions. The remarkable merits of this strategy are high yields (75-99%) of the expected products, short reaction times (4-60 minutes) and easy workup procedure. Notably, the nanocatalyst was readily recovered, and reused seven times without significant decrease in the yield of the product of model reaction.



Scheme 1: Synthesis of 1,4-dihydropyrano[2,3-*c*]pyrazoles (5a-j) in the presence of Cu@Hal-T-F. **References**

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Investigation of the Effect of UF and PVAc Resins on the Physical Properties of Cotton Fabrics

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Abstract

Fabric intended for the manufacture of garments needs to possess certain specifications. For example, some interlining fabrics have superior properties such as stiffness, crease resistance, wash fastness and suitable soft handle. The most widely stiffener used in textile is Polyvinyl acetate (PVAc) due to suitable and durable adhesion now. Among many polymeric adhesives used in industry polyvinyl acetate has a rather wide application.¹ The urea formaldehyde (UF) resin with low formaldehyde emission is important in industry as well. The ultimate performance of a fully cured amino resin same as UF largely depends on its synthesizing parameters including mole ratio, viscosity, water resistance and so on.²

In this study, a mixture of UF and PVAc in special finishing of cotton for producing interlining cotton fabrics properties has been investigated.

To find the role of UF and PVAc in this study, some physical properties of fabric such as bending length, crease recovery angle, wettability time and were studied with different concentrations. Bending length and wettability time of cotton fabrics increased by increasing the PVAc and UF concentrations as shown in the following diagram. But, crease recovery angle decreased by increasing PVAc concentration but increasing UF concentration improved the crease recovery angle again.

On the other hand, it is expected that PVAc as stiffener, increase the bending length and time of wettability of fabric. But crease recovery angle of finished fabric has been reduced with increasing of PVAc concentration; therefore, the UF resin was used to overcome this issue because UF as a cross-linking agent can increase the bending length, wettability time and crease recovery angle of finished fabric. Therefore, PVAc and UF play an important role in the physical properties of finished fabric.



Effect of UF concentration on wettability time of the fabric

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Investigation of the Relationship Between Décor Paper Type and Properties in Quality of Impregnated Paper

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Abstract

Paper impregnated and coated with thermosetting resins is commonly used as a decorative and rotective laminate for wood composites. The paper laminates are manufactured in a paper treater by impregnating décor paper with resin which is then cured.¹ So the treatment process, type of the paper and resin are significant parameters for surface properties. Décor paper improve the surface of wood panels by providing an excellent surface for use in the production of furniture, laminate flooring and other architectural panels.² In this study, effects of type of the raw paper on the surface quality has been investigated with some methods same as water absorption capacity (stands for the capacity of paper to absorb water), tensile stiffness test(to optimize process parameters such as wet pressing and drying), air permeability (define as the time it takes for a given volume of air to pass through certain surface area of paper under constant pressure), breaking length(to characterize the strength of the paper) and pore size(define the min and max open surface).

The raw papers were provided from 5 different suppliers: Schattdecor (Sc),Kingdecor(Ki), Shaddecor(Sh), Impress(Im), Technocel(Te) and impregnated with Melamine Formaldehyde (MF) and Urea Formaldehyde (UF) resin with 70:30 ratios and compared together.

By increasing the resin applying into the raw paper, the physical parameters of the impregnated decor paper were decreased comparing with the raw paper.

For example, the air permeability and pore size value were decreased about 85% and 65%, respectively because resin applied into the fibers and flowed on the surface. As classified in the following table, by comparing the different paper suppliers in impregnation processing, the quality of "Te" were found to be better. So it means this type can be suitable for laminating fiberboard (MDF) and particle boards (PB).

Type of the impregnated paper	water absorption capacity	tensile stiffness test	air permeability	breaking length	pore size
	g/m2	kNm/g	m3/min	km	micro meter
Sc	12	6	17	2.0	0.9
Ki	10	4	8	1.7	1.0
Sh	13	9	19	2.2	1.2
lm	13	9	12	2.3	0.8
Те	13	10	10	2.9	0.9

The quality comparing of impregnated film in different paper

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Non-Thermal Plasma Approach for Direct Hydroxylation of Toluene

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Abstract

Over the last several years, substantial efforts have been devoted to the synthesis of hydroxytoluenes, commonly called cresols, using different starting materials, reagents and experimental conditions. The use of appropriate catalysts, the application of high temperatures, and the implementation of multi-step processes are challenges faced by researchers in the synthesis of these compounds. Among the proposed synthetic methods, direct hydroxylation of the benzene ring in toluene appears particularly attractive.¹ One of the most promising and environmentally friendly approaches to this target is based on plasma systems, specifically non-thermal (also called cold) plasmas. Non-thermal plasmas are readily produced by electric discharges in a gas, notably air, at ambient temperature and atmospheric pressure and do not require for their action either catalysts or additional chemicals. The advanced oxidation of vaporized toluene in air nonthermal plasma has been extensively investigated in the search for novel green technologies for air purification, aiming at the complete mineralization of all organic carbon into carbon dioxide.² Way less studied and more difficult to achieve is instead the fine tuning of conditions for the application of non-thermal plasma for the synthesis of selected specific organic compounds. Notably, the conversion of toluene into hydroxytoluenes, has been investigated in a few studies which pointed out the occurrence of competing reactions leading to the formation of by-products including a few major ones due to oxidation of the methyl group.³⁻⁴ Herein, we present and discuss the preliminary results of a study we carried out on the one-pot non-thermal plasma induced direct hydroxylation of vaporized toluene in air at room temperature and atmospheric pressure using a dielectric-barrier discharge (DBD) reactor available from previous work⁵ and suitably adapted for the present task. The results show that cresols do form in the process, alongside with benzaldehyde, benzyl alcohol and phenol (Scheme 1). The discharge generated reactive species, including notably O atoms and OH radicals, will be discussed and mechanisms will be proposed for their reaction with toluene leading to the observed oxidation products.



Scheme1. The treatment of gaseous toluene and synthetic air in DBD plasma

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Synthesis of Dibenzosulfide and Dibenzosulfoxide Podands with Terminal Coumarin Moieties

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Abstract

Podands are of crucial significance in supramolecular chemistry due to their nonrigid structures. Indeed, these compounds can be effectively applied as molecular sensors.¹ The acyclic supramolecular ligands, commonly called podands, as host molecules, are able to be complexed with various anionic, cationic, and molecular guests.² Coumarins are also known as a momentous group of heterocyclic compounds due to their great biological importance.³ The complexation of bis coumarin podands with cations in acetonitrile has yielded attractive fluorescence spectral results in the presence of some alkali cations and Pb²⁺.⁴ In this study, dibenzosulfide and dibenzosulfoxide podands (compounds 1 and 2) were synthesized by the reaction of dibenzosulfide or dibenzosulfoxide with 3-(N-substituted) amino coumarins with high yields (Figure 1). The structures of these podands were confirmed using IR, ¹H NMR and ¹³C NMR spectroscopy.



Figure 1: The preparation of dibenzosulfide and dibenzosulfoxide podands containing 3-(N-substituted) amino coumarin moieties

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Palladated Porous Nitrogen-doped Mesoporous Carbon: A Recyclable and Effective Catalyst for Suzuki Coupling Reaction

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Abstract

heterogeneous catalysts are solid compounds that are added to liquid or gas reaction mixtures. heterogeneous catalysts can be separated from the reaction mixture in a straightforward manner, such as by filtration. In this way, these catalysts can be easily and effectively recovered, which is an important consideration for industrial manufacturing processes.¹ The suzuki reaction is an important type of coupling reaction, a designation that encompasses a variety of processes that combine two hydrocarbon fragments with the aid of a catalyst. The reaction is able to combine a variety of aryl halides and alkenyl halides with alkenylboranes and arylboronic acids, and is thus an important method of synthesizing many styrenes, alkenes, and biphenyls. The Suzuki reactions have many desirable features such as requiring mild reaction conditions, high tolerance to different functional groups, easily accessible substrates and exhibiting low sensitivity to moisture. Within this context, a major of solid supports including metal oxides, polymers, silica as well as carbon structures have broadly been utilized and performed well for the construction of biaryl compounds in the Suzuki coupling reactions, which are widely recognized as the fundamental transformations in pharmaceutical and biochemical applications.² In this study, we describe the Suzuki coupling reaction catalyzed by Pd@C for the formation of Biphenyl derivatives. This heterogeneous catalyst was synthesized through procedure according to the previously reported method³. The catalytic activity of the Pd@C as a heterogeneous catalyst was investigated for Suzuki coupling reaction under mild reaction conditions (75-90%), Scheme 1. Furthermore, the catalytic recyclability of Pd@C was examined. The catalyst could be successfully removed from the reaction mixture by simple filtration and also recycled for several consecutive reaction times with slight loss of the catalytic activity.



Scheme 1. Suzuki coupling reaction catalyzed by Pd@C.

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A Highly Efficient Functionalized Cellulose as A New Nanomagnetic Reusable Catalyst for the Synthesis of 1,2,3-Triazole Derivatives

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Abstract

In to decade, magnetic nanoparticles (MNPs) have attracted a great deal of attention due to their easy preparation, large surface-to-volume ratio, and easy separation by an external magnet. Today, organic chemists have used these characteristics of magnetic nanoparticles to design efficient catalysts for the synthesis of organic compounds.¹ Recently, the use of natural compounds such as cellulose, chitosan, and starch as part of the catalyst used in carbon-carbon coupling reactions and click chemistry, such as the synthesis of 1,2,3-triazoles, has received much attention from chemists.² 1,2,3-Triazoles are an essential group of heterocyclic compounds, the most important of which is their role in the pharmaceutical industry.³ In this study, a novel magnetic nanocatalyst based on Fe2O3 nanoparticles was modified by modulating its surface with cellulose and eventually converting it to a suitable magnetic ligand to form a complex with copper metal, as an effective catalyst for the synthesis of 1,2,3-triazoles at room temperature and using green solvent, ethanol.



Scheme 1: Synthetic procedure of novel core-shell magnetic nanocatalyst and its applicability in one-pot three component synthesis of 1,2,3-triazole derivatives

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Synthesis of Isatin-Derived Schiff Bases *via* the Reaction of Isatin and Cyanoacetohydrazide

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Abstract

The oxindole structure has long been distinguished as a "privileged motif" in a diversity of bioactive natural compounds and drugs. Especially, the 3-amino-3-substituted oxindole scaffold has been noticed by organic chemists in the last few years as it exists in numerous drug compounds. Numerous articles have been published related to the reaction of isatin imine during the last years, which demonstrates the significance of this scaffold.¹ Isatin-derived ketimines formed *via* the reaction of isatine and hydrazides are inexpensive, readily accessible, and stable precursors that have been increasingly used in the synthesis of a class of enantioenriched 3-substituted-3-aminooxindole products.² The chemistry of the carbon-nitrogen double bond of hydrazone is a suitable backbone of condensation reactions in benzo-fused *N*-heterocycles, which also constitute a valuable class of structure for the development of the novel drugs. Between various commercially available substituted hydrazides, cyanoacetic acid hydrazide has attracted the most attention recently, displaying a versatile and convenient intermediate for the formation of a broad diversity of heterocyclic products. This precursor can operate as an ambident nucleophile, that is, as both an N- and C-nucleophile.³

We are interested in reporting an eco-friendly methodology to produce isatin-derived Schiff bases **3** *via* the reaction of isatine derivatives **1** and cyanoacetohydrazide **2** as versatile substrates in the presence of trichloroacetic acid (TCAA) as a Brønsted-Lowry acidic catalyst as illustrated in Scheme 1 which can be used for the synthesis of valuable heterocyclic compounds such as 2-(2-oxo-3'*H*-spiro[indoline-3,2'-[1,3,4]oxadiazol]-5'-yl)acetonitrile.



Scheme 1: Synthesis of isatin-derived Schiff bases and spiro indoline oxadiazol acetonitrile 4.

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Silver Nanoparticles Immobilized on Halloysite-tetrazole Hybrid: An Efficient and Reusable Catalyst for the Synthesis of Tetrahydro-4*H*-chromene Derivatives through Three-component Reaction

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Abstract

Multicomponent reactions (MCRs) are very mostly tagged as an atom-economic, step-efficient with high exploratory power with regard to chemical space, processes. Employing the MCRs principles, fast and easy access to organic moieties with high diversity can be performed.¹ Lastly, inexpensive, low-toxic and abundant metals such as Ag have increased attention of the synthetic community. Many significant usages of organosilver compounds in organic chemistry have been identified for a long time, i.e. using silver reagents in the various reactions for example: cyclization, cycloaddition reactions, C-H functionalization and coupling reactions.² In the following of our attempt to introduce heterogeneous and recoverable catalysts and developing eco-freindly methods for effective synthesis of chemicals^{3,4}, herein we report the methodology for the one-pot synthesis of tetrahydro-4*H*-chromenes catalyzed by Ag@Hal-T as a heterogeneous catalyst. Ag@Hal-T was prepared *via* functionalization of halloysite nanotube with 1*H*-1,2,3-triazole-5-methanol and subsequent immobilization of silver nanoparticles through bio-assisted method employing Arctiumplatylepis extract.

Next, the catalytic activity of Ag@Hal-T was examined in three-component reaction between different aromatic aldehydes, dimedone, and malononitrile in water under reflux conditions. These results confirmed that the catalyst could promote the reaction to provide the desired tetrahydro-4*H*-chromenes in high yields (75-98%) in short reaction times (3-60 minutes). Additional features of this approach contain an efifcient, fast, and ec_friendly reaction process, easy workup, easy sepration, and recyclable green catalyst. It should be mention that, the catalyst could be recovered and recycled for eight reaction runs with slight loss of the catalytic activity.



Scheme 1: Preparation of tetrahydro-4H-chromenes in the presence of Ag@Hal-T

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Magnetic Heterogeneous Catalyst Based on Decoration of Halloysite with Ionic Liquid-containing Dendrimer: A Recyclable and Efficient Magnetic Nanocatalyst for One-pot Synthesis of Spirooxindoles

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Abstract

Magnetic nanoparticles have a nano size and interesting magnetic properties, which combines the properties both from homogeneous and heterogeneous catalysts. Some of these features include high activity, easy recycling, high reproducibility and repeatability.¹

It is shown that multicomponent reactions are effective tools to direct the construction of complex structures from the simple starting materials. Because of some outstanding features like the high atomic economy, less waste generation and high convergence, this type of reaction have been frequently used in the synthesis of organic material, natural product and biologically active molecules.^{2,3} Classic multicomponent methodologies contained use of homogeneous or expensive catalysts under harsh reaction conditions. Moreover, disclosing new catalysts, which didn't require use of expensive catalyst and could promote the reactions in non-toxic solvents, has attracted intensive attention. In the following our study and research group^{4,5}, herein, we describe the synthesis of spirooxindole derivatives by using magnetic catalytic system. The Fe-Hal-PAMAM-IL was synthesized through multi-step procedure according to the previously reported method.⁶ A heterogeneous magnetic catalyst, Fe-Hal-PAMAM-IL, was synthesized by growing dendrimer of generation of 3 on the surface of amine-functionalized Hal followed by modification of dendrimer terminal groups with IL and incorporation of Fe species. The catalytic activity of Fe-Hal-PAMAM-IL as an efficient catalyst, was investigated for the synthesis of spirooxindole under green reaction conditions (50-97%), Scheme 1. Furthermore, the catalytic recyclability of Fe-Hal-PAMAM-IL was examined. The catalyst could be successfully removed from the reaction mixture by using an external magnet and also recycled for several consecutive reaction times with slight loss of the catalytic activity.



 $R_2 = CN, CO_2Et$



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The Effect of Adsorption Types on Electronic Transport of 1,2-Bis(2,4-dimethyl-5phenyl-3-thienyl)perfluorocyclopentene as an Optical Molecular Switch

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Abstract

Application of molecules as components in atomic-scale circuits has become an attractive field.1,2-Bis(2,4-dimethyl-5-phenyl-3-thienyl)perfluorocyclopentene, which changes between open and closed forms under the excitation of light radiation (Figure 1) can be a good option for a molecular switch device, It is a member of diarylethenes.¹ The investigation on electron transfer in a diarylethene attached to Au atoms show that these compounds can be used as molecular switches.²

The transport properties of a diarylethene as a molecular switch can be studied using nonequilibrium Green's function formalism (NEGF) combined with first-principles density functional theory (DFT).

From the I–V characteristics, on-off ratio, it can be estimated that there is a significant difference in the conductivity of these two (open and closed) forms, and this molecule can be used as a molecular switch. The results showed that as the molecule changes from open form to closed form (open \rightarrow closed), conductivity changes from off state (low conductivity) to on state (high conductivity). It can be seen that the switch behavior is clearly dependent on the adsorption types (bridge, hollow, and top).



Figure 1: Chemical structures corresponding to closed and open forms of 1,2-Bis(2,4-dimethyl-5-phenyl-3-thienyl)perfluorocyclopentene

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The Effect of Electrode Materials on I–V Characteristics of 1,2-Bis(2,4-dimethyl-5phenyl-3-thienyl)perfluorocyclopentene as a Molecular Switch

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Abstract

In recent years, with the advancement of techniques for manipulating individual molecules, electronic devices based on single molecules have been considered one of the most promising candidates for today's silicon-based devices both for their novel physical properties and potential for device applications, such as negative differential resistance (NDR), switches, latches and rectifiers.^{1,2}

In this research, using nonequilibrium green's function (NEGF) integrated with density functional theory (DFT), the electronic transport properties of a diarylethene, 1,2-Bis(2,4-dimethyl-5-phenyl-3-thienyl)perfluorocyclopentene molecular wire, was investigated. This molecule can be converted from open form to closed form.³

The electronic transmission factors, spatial spreading of molecular projected self-consistent Hamiltonian (MPSH) orbitals, on-off ratio, I–V characteristics, the alteration of the electrode materials, Y, (Y =Au, Ag, and Pt), and HOMO–LUMO gaps relevant to these forms are thoroughly discussed. It can be concluded that due to the deformation of the mentioned molecule, there is a noticeable change in conductivity. The current in this electron device is significantly dependent on the electrode material. Both open and closed forms with diferent electrodes exhibit almost similar behaviors and regardless of the electrode type, the current in the closed form is always greater than that in the open form. The results showed that the title compound has the best switching performance in the Au electrode (Figure 1).



Figure 1: Current switching ratio as a function of applied bias with different electrodes

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Synthesis and Characterization of Novel Pyrimidine-Based Organometallic Dyes With High Efficient Light-Harvesting Properties for DSSC

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Abstract

Among renewable energy solutions, dye-sensitized solar cells (DSSC) have attracted wide attention as a biocompatible alternative for energy production.¹ In DSSCs, the photoactive dyes play a critical role, which not only anchor firmly on the semiconductor (TiO₂) surface, but also have optimal photochemical and charge transfer properties to enhance light-harvesting ability of the cells. Typically, transition metal complexes have received considerable attention for DSSC application because of their broad absorption spectra, long-life time excited state, favorable photovoltaic properties and high thermal and photochemical stability.^{3,4} The central metal ion is therefore a crucial part of the complex in which ancillary ligands can be tuned by different substituents (alkyl, aryl, heterocycle, etc.) to change the photophysical and electrochemical properties and thus improve the photovoltaic performance.

In this research, for the first time, a novel metal complexes has been synthesized and used as an efficient sensitizers in DSSCs. The organometallic complexes were obtained from Cu(II) salt and boron trifluoride with the synthesized pyrimidine derivatives as ligand with the mole ratio of 1:2, Figure 1. The presence of transition metals in the structure of azo dyes have led to prominent properties such as high molar absorption coefficient, broad absorption in the visible region and excellent photochemical stability. To achieve high efficiency and reduce the amount of charge recombination in the fabricated DSSCs, we introduced bulky moleties in the electron donor part of the dyes. The bidentate linkage was formed between (-N=C-OH) groups and TiO₂ surface which enhanced the efficiency of electron injection to conduction band of TiO₂. The optical and electrochemical properties of these dyes were fully evaluated.



Figure 1: Structure of the synthesized organometallic dyes

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Synthesis of N-benzoiel-1,3-diaryl-2-(para formyl) Azaphenalene Derivatives via Solvent-free Reactions and Evaluations of the Antibacterial Activity

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Abstract

Synthesis of α -aminobenzylnaphthol derivatives in which an aromatic aldehyde, ammonia, and 2-naphthol are combined in one-pot procedure according to the Betti reaction.¹⁻² This reaction has been created by using version N sources, substituted benzaldehydes or formaldehyde³ and 1-naphthol.⁴ Potential application of Mannich-type phenolic bases has been devoted to aminoalkylation of naphthol derivatives ⁵ which can be used as intermediates for the synthesis of derivatives with substantial antibacterial, hypotensive, and bradycardia activity.⁶



In this study, n-benzoiel-1,3-diaryl-2-(para formyl) azaphenalene derivatives have been synthesized by a onepot condensation reaction of the aromatic dial, 2,7naphthalenediol, carboxylic acids and aqueous ammonia (25 %). Different aromatic and aliphatic carboxylic acids and aromatic dial have been used in the reaction and the products were always obtained in good to high yields. All the synthesized compound were isolated, purified and the structures of the newly synthesized hybrid molecules were characterized by TLC, M.P., FT-IR, ¹H NMR, and ¹³C NMR. Taking the environment and economy into consideration, the work presented here has the merits of environmental friendliness, high yields, simple work-up, easy operation and the avoidance of the organic solvents and inexpensive catalysts. The antimicrobial activity of the newly isolated azaphenalene derivatives was evaluated against Gram-positive and negative bacteria. Most of the compounds showed a moderate degree of potent antimicrobial activity

Keywords: 2-Azaphenalene, One-pot synthesis, Multi-component, solvent free, antimicrobial activity

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Pd (0) Nanoparticles Immobilized on Magnetic Sepiolite Clay as an Efficient and Reusable Catalyst for Suzuk-Miyaura Coupling Reaction in Natural Deep Eutectic Solvent

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Abstract

Natural deep eutectic solvents (NADESs) are biodegradable and biocompatible mixtures of natural compounds, namely, sugars, organic acids and bases, amino acids, sugar alcohols, and polyalcohols. The components of a NADES interact through hydrogen bonding and liquefy if combined in specific molar ratios.¹ The low melting points of these mixtures are considerably lower than those of their individual ingredients and far below ambient temperature, make them suitable for suing as green solvents in various organic transformations.² Compared to the conventional solvents, NADESs are recognized as nonflammable, thermally stable, biodegradable, highly soluble, non-toxic, and non-volatile.³

Clays are inexpensive, nontoxic, abundant, and have great potential as catalytic carriers for supporting transition metals. Sepiolite is a type of natural clay mineral in the form of a magnesium silicate hydrate. Due to its special pore structure and unique one-dimensional nanoscale fibrous shape leading to high surface area, sepiolite has been widely used as adsorbent and support for transition metals.⁴

In this study, sepiolite was used as a support and ligand for the heterogenization of palladium (0) on the surface of Fe_3O_4 nanoparticles and the resulting system (Pd@Fe_3O_4-SEP) was employed as a novel, highly efficient, reusable and DES-compatible catalyst for Suzuki-Miyaura cross-coupling reaction in choline chloride/glycerol (1:2) NADES as solvent. The reaction proceeded with 1.5 mol% of Pd@Fe_3O_4-SEP, without need for ligands or an inert atmosphere. Various aryl halides react with boronic acids and corresponding products were obtained in good to excellent yields (Scheme 1). This protocol represents a promising alternative to the organic solvents routinely used for such coupling (e.g., DMF, DMSO or 1,4-dioxane). Finally, the catalyst could be separated from the reaction mixture simply using an external magnet and reused at least for four consecutive cycles with a minimum loss in its catalytic activity and performance



Scheme 1: Suzuki-Miyaura cross-coupling reaction of aryl halides with boronic acids using Pd@Fe₃O₄-SEP catalyst in NADES.

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Laccase Catalyzed Synthesis of 5,6-dihydroxyindoles

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Abstract:

Recently, laccases (benzenediol: O₂ oxidoreductase E.C. 1.10.3.2.) which are multicopper oxidases have attracted much attention in the synthesis of divers organic compounds. This approach due to the use of aerial oxygen as the oxidant and as a result water as its only by-product taken into consideration.¹ The 5,6-dihydroxyindoles are catecholic indoles which play an important role in the biosynthesis of eumelanins, the characteristic dark pigments of skin, hair, eyes and melanomas. Besides the biological importance of 5,6-dihydroxyindoles in human pigmentation, interest in these compounds derives from their increasing applications in cosmetics and medicinal chemistry.² Their has always faced with difficulties due to the oxidation and polymerization reactions, so there is an urgent need to protect hydroxyl groups.³ In this study for the first time, 5,6-dihydroxyindoles were prepared using laccase and available raw materials, with good efficiency and without the need to protect the hydroxyl groups of catechol. This reaction is carried out at room temperature in an aqueous medium (phosphate buffer pH 8) in the presence of ethyl acetate as a co-solvent, which can be important from the point of view of green chemistry principles.



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1,3-Dipolar Cycloaddition of Isatin-Derived Azomethine Ylides With Nitro Ketenes

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Abstract

Among the introduced synthetic methods to date, the 1,3-dipolar cycloaddition as the Huisgen reaction is considered as one of the most noteworthy procedures for the synthesis of pharmaceutically valuable fivemembered N-heterocyclic products. 1,3-Dipolar cycloaddition of ylidic types such as isatin-derived azomethine ylides with electron-deficient carbon-carbon double bonds demonstrates a powerful procedure to achieve the spirooxindole scaffold and also for the formation of pyrrolidine cores with important biological properties.^{1,2}

The biological and pharmaceutical activities of isatin and its derivatives have led to the wide application of these scaffolds as main precursors in organic synthetic reactions. Isatin is a motif constituent of various alkaloids and medicines as well as dyes, pesticides, and analytical reagents. So, isatins with their multifunctionality and diversity of transformations are synthetically versatile substances and numerous attempts have been done for the synthesis of drugs based on isatin-derived azomethine ylides.³

Considering that isatin is a valuable building block in organic reactions, and as regards that there are numerous methods that use isatin in the formation of heterocyclic products, in this paper the focus is on the reaction of isatin-derived azomethine ylides **1** derived from isatin derivatives and *L*-proline with nitro ketenes **2** derived from ethylene diamine and 1,1-bis(methylthio)-2-nitroethene to produce dispiro product **3** in isopropanol as solvent and room temperature condition as represented in Scheme 1.



Scheme 1: 1,3-Dipolar cycloaddition of isatin-derived azomethine ylides with nitro ketenes

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Sensitive Fluorescence Sensing of Sulfate by an Uncharged Lower Rim 1,3-disubstitutedcalix[4]arenes Receptor

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Abstract

Sulfate dianion is one of the important inorganic anions that plays a vital role in different biological processes and environmental activities.¹ High metallic sulfates concentrations in drinking water are undesirable that cause diarrhea and cathartic effects in consumers.² In addition, the changes in sulfate concentration of the blood cause various diseases.³ As a result, the synthesis of artificial sulfate hosts is essential.

The arena of anion recognition in supramolecular chemistry uniquely helps us in terms of selective sulfate recognition by binding to synthetic molecular receptors via non-covalent interactions.⁴

By utilizing calixarene chemistry as well as dithiocarbamate chemistry⁵ through multi-component reactions, the novel uncharged reinforced molecular sensor **1** was synthesized (Scheme 1) and its structures were characterized by NMR and HRMS.

The compound **1** exhibit highly sensitive fluorescent recognition towards sulfate dianion unexpectedly among **20** various anions. The satisfying association constant of the compound **1** with sulphate in 99%acetonitrile+ 1%water was determined $1.64 \times 10^{6} \, \text{M}^{-1}$ by titration flurescence sepctroscopy.



Scheme 1: Description of synthesis route

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Synthesis of Lower Rim 1, 3-Dimethylcarbamodithioate Calix[4]arenes as a Sensitive Fluorescent Sensor of Au³⁺ Ions

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Abstract

Dithiocarbamates (DTCs) are a topic of interest in organic chemistry, owing to the frequent presence of these structural units in herbicides, fungicides, and pesticides compounds.¹ Their important roles as a ligand in coordination chemistry to stabilize various transition metals are significant.² The attendances of organic dithiocarbamate functional groups on macrocyclic molecules such as the calixarene framework have attracted much attention in host-gust chemistry field.³

During the last two decades, calix[n]arenes which are produced by the condensation of p-substituted phenols with aldehydes have been used extensively in host–guest chemistry and specially design applied sensors.⁴

we applied the optimized lower rim 1,3-disubstitutedcalix[4]arenes synthesis with the structural benefits of the dithiocarbamate moieties to design crab ligands that allow the formation of stable complexes with Au^{3+} ions. Compound 1 as a sensitive fluorescent sensor exhibits high recognition towards Au^{3+} ions unexpectedly among 20 various cations by none covalent interactions. The formations of complex 1 properties with Au^{3+} ions were proven by fluorescence and NMR titration methods with a binding constant of 2.6 ×10⁵ M⁻¹.



Scheme 1: Calixarene Complexe

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Synthesis and Supporting of 5-ethoxycarbonyl-6-methyl-3-buthyl ferrocene-3,4dihydropyrimidine-2(1H)-one on rGO Nanocamposite for Investigation of High-Performance Supercapacitor Energy Storage

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Abstract

Recently, since the supercapacitors have drawn conciderable attention, a vast study have been triggerd in order to develop efficient electrodes for responding to the increasing demand of supercapacitors.the present work describes the synthesis and characterization of 2-buthyl ferrocene dihydropyrimidinone supported on rGO, scheme1.



Scheme1: Synthesis of 5-ethoxy-6-methyl-3-buthyl ferrocene3,4dihydropyrimidine-2(1H)-one and supported on rGO.

The results showed that a interaction via double bonds between rGO and of 5-ethoxycarbonyl-6-methyl-3-buthyl ferrocene-3,4-dihydropyrimidine-2(1H)-one was thermodynamically stable.

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Exploiting Solid Acid Catalyst Based on Periodic Mesopousos Organosilicas (PMOs) in the Synthesis of *N*,*N*'-Diarylformamidines

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Abstract

Antitubercular, hypotensive, bactericidal, fungicidal and localanesthetic are examples of fascinating biological and pharmaceutical features of organic compounds that contain formamidine skeleton in their structure^{1,2}. These compounds can act as protecting groups for primary amines ³, chelating/bridging bonding modes via coordination with metal center ⁴. Besides, they are useful as support linkers in solid phase synthesis. Up to now, several homogeneous and heterogeneous catalytic systems have been described ⁵. Despite this efforts, some key factors still remain a challenge. Therefore, introduction of a new catalyst which contains features including high activity and selectivity, easy separation and recovery for the synthesis of these compounds still can be a problematic.

In this work, we prepared a highly porous ionic liquid based periodic mesoporous organosilica catalyst through the following steps: (i) preparation of PMOs containing a linear amine precursor and (ii) reaction of perchloric acid with amine groups for having ionic liquid structures inside pore walls. The prepared catalyst displayed highly catalytic ability toward the synthesis of *N*,*N*'-diarylformamidines through the reaction of amines and triethylorthoformate (Scheme 1).



Scheme 1: Synthesis of *N*,*N*'-diarylformamidine derivatives catalyzed by PMO-NH₂⁺ ClO₄⁻ under solvent-free conditions

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Study of Kinetic Degradation of Fluorouracil (5-FU) by Ozonation Process

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Abstract

In this study, kinetic degradation of *Fluorouracil* (*5-FU*) by ozonation processes in a fine bubble system has been evaluated. This research forwards the determines the reaction kinetic of Fluorouracil (*5-FU*) degradation. In the ozonation system of organic compounds, if the amount of applied ozone is in excess and reaches a constant value after a while,the ozone concentration can be assumed to be constant and as a result the reaction kinetic is considered as pseudo-first order (Eq. 1):

$$r_{A} = \frac{d_{C_{M}}}{dt} = -k'C_{M}$$

Here, r_A is the reaction rate, C_M is the concentration of the desired compound and k' is the pseudo-first order reaction rate constant of ozone and the desired compound.

Generaly, In aqueous solutions, the organic compound M reacts directly with ozone and indirectly with OH° and its rate equation is written as Eq. (2):

$$\frac{d[M]}{dt} = -\left\{k_{O_3}[M][O_3] + k_{OH^{\square}}[M][OH^{\square}]\right\}$$

Where, $k_{OH^{\circ}}$ is the reaction rate constant of M with OH[°] and k_{O3} is the reaction rate constant of M with O₃. Considering that in the ozonation process at pH< 12, the reaction of molecular ozone with organic compounds is predominant¹⁻², so the effect of the concentration of OH[°] is omitted and Eq. (2) is converted to Eq. (3)

$$\frac{d[M]}{dt} = -k_{O_3}[M][O_3]$$

And if the ozone concentration is excess, the second-order reaction rate changes to pseudo-first order reaction³ as Eq. (4):

$$\frac{d[M]}{dt} = -k_{O_3}[M][O_3] = k'[M]$$

The linear form of Eq. (4) is Eq (5):

$$Ln \frac{[M]_0}{[M]} = k't$$

It is found that the first-order rate constant for the reaction of O3 and *Fluorouracil* (5-*FU*) is obtained in the 10^4-10^7 s^{-1} .

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Adsorption Equilibrium, and Thermodynamic Studies of β -Carotene Adsorbed by Mn/Fe₃O₄/Graphite Adsorbent

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Abstract

β-Carotene (Fig. 1) is an organic, strongly colored red-orange pigment abundant in fungi, plants, and fruits.¹ It is a member of the carotenes, which are terpenoids (isoprenoids), synthesized biochemically from eight isoprene units and thus having 40 carbons. Carotene is also used as a substance to color products such as juice, cakes, desserts, butter and margarine. It is approved for use as a food additive in the EU (listed as additive E160a).²⁻³ Excess β-carotene is predominantly stored in the fat tissues of the body. The most common side effect of excessive β-carotene consumption is carotenoderma, a physically harmless condition that presents as a conspicuous orange skin tint arising from deposition of the caroteneoid in the outermost layer of the epidermis.⁴ In this paper, the enhanced adsorption of β-carotene on Mn/Fe₃O₄/Graphite in aqueous solution was researched. The adsorption performance was determined by adsorption equilibrium, and thermodynamic parameters. The β-carotene adsorption capacity was obtained from Langmuir, Freundlich, and Temkin isotherm models, and Langmuir isotherm was found to best fit model. Several thermodynamic parameters such as enthalpy, Gibbs free energy, entropy ($\Delta S > 0$), and adsorption activation energy were calculated which demonstrated the feasibility, spontaneity ($\Delta G < 0$) and exothermic nature of ($\Delta H < 0$) of the β-carotene adsorption process. It was revealed, the adsorption process was controlled by a physical mechanism, and the maximum adsorption capacity was found to be 105 mg/g.



Fig. 1. Structure of β-Carotene

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Effect of Glycerol on the Stability of Immobilized Lipase Enzyme

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Abstract

Candida Antarctica B (CALB) enzyme was immobilized on octyl-agarose and amino glutaraldehyde-agarose beads [1-3]. Both immobilization strategies follow completely different immobilization mechanisms. The effect of glycerol (at different concentrations: 0, 15%, 30%, 45% and 60%) on the stability of all immobilized biocatalysts was studied at pH 5.0, 7.0 and 9.0, using temperatures where the inactivation courses showed a reliable inactivation rate. Octyl-CALB (Fig. 1a) at pH 5.0, in 15 and 30% of glycerol destabilized the immobilized enzyme compared to the inactivation course in absence of glycerol. The progressive increase of glycerol improved the immobilized enzyme stability, and by using 45 % glycerol, the stability became slightly higher compared with no glycerol, also the enzyme was clearly more stable in 60 % glycerol. Using glutaraldehyde-CALB (Fig. 1d), the presence of glycerol gradually increased the enzyme stability progressively (Fig. 1b) increased when increasing the glycerol concentration, reaching a maximum in 45 % glycerol, the use of 60 % of glycerol produced no significant changes. In the inactivation of glutaraldehyde-CALB (Fig. 1e), the use of low concentrations of glycerol produced a more significant stabilization effect that using octyl-CALB. Again stability was the highest using 45 and 60 % glycerol. At pH 9.0, glycerol stabilized octyl-CALB (Fig. 1c), but without a

clear trend. During the initial times the highest enzyme stabilization is obtained using 15 % glycerol, while at the last steps of the inactivation, the highest residual activities were obtained using 60 % glycerol. Using glutaraldehyde-CALB (Fig. 1f), glycerol shows a small but progressive stabilizing effect, reaching the maximal stabilization using 60 % glycerol.



Fig. 1. Effect of glycerol and inactivation pH on the stability of different immobilized preparations of CALB. Octyl-CALB: (A) pH 5.0, 88 °C; (B) pH 7.0, 80 °C; (C) pH 9.0, 60 °C. Glutaraldehyde-CALB: (D) pH 5.0, 72 °C; (E) pH 7.0, 70 °C; (F) pH 9.0, 64 °C. Dotted line, empty squares: references; full squares: 15 % glycerol; full triangles: 30 % glycerol; full circles: 45 % glycerol and empty circles: 60 % glycerol.

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Molecular Simulation of Graphene Dispersion Using Gemini Surfactants

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Abstract

Graphene nanosheets have a unique structure and excellent mechanical, thermal, optical, and electrical properties. They can be therefore potentially used in various fields.^{1,2} The successful preparation of stable suspensions of graphene nanosheets is a significant step toward the effective use of features of this rare. Due to Gemini surfactants special structure, they have a high charge capacity, high hydrophobicity and unique self-assembly properties compared to single-chain surfactants. Therefore, the Gemini surfactants with their little concentrations are expected to disperse and stabilize graphene nanosheets in aqueous solutions more effectively.³⁻⁵ Molecular dynamics simulations were performed to assess self-assembly and morphology of assemblies formed by the single-chain and double-chain cationic surfactants on graphene surface in the aqueous phase. The results showed that the morphology of assemblies formed on graphene surface is affected by the surfactant structure. The increasing surface coverage, especially for double-chain surfactant, leads to a transmission in the adsorption mechanism and most surfactants head groups tend toward the aqueous phase and prevent water molecules from accessing graphene surface. It can be concluded from morphological assessments that Gemini surfactant is more effective than single-chain surfactant in stabilizing aqueous suspensions of graphene nanosheets.

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Adsorption of Cu (II) Ions From Water by Carbon Nanotube and Hybrid Graphene-Carbon Nanotube

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Abstract

As important parts of industrial wastewater, heavy metal ions have caused many environmental problems. Toxic heavy metals encountered in industrial wastewater treatment include lead, chromium, cadmium, mercury, arsenic, nickel, copper, and zinc. Copper is one of the most important heavy metals in industrial and agricultural processes and can enter the environment from many sources.¹ Although copper is needed for metabolism of organisms, its excessive accumulation in organisms can cause several problems such as: hypertension, respiratory, renal, and liver dysfunction, seizures, cramps, vomiting and even death.² Adsorption is one of the most common ways of removing metallic ions, which uses materials with high bonding tendencies and capacity for elimination or even tracking of undesirable chemicals.³ In the present study, molecular dynamic simulation was used to investigate copper adsorption by carbon nanotube (CNT) and hybrid graphene-CNT functionalized with OH and COOH functional groups. The results showed that COOH functional group on CNT and hybrid graphene-CNT can significantly boost Cu (II) adsorption. The simulation results showed that more Cu (II) ions are adsorbed by hybrid graphene-CNT than by CNT alone. Of the nano-structures investigated, hybrid COOH-graphene-CNT showed the greatest Cu (II) adsorption in aqueous solution. Interaction between Cu (II) and hybrid COOH-graphene-CNT is stronger than interaction between Cu (II) and COOH-CNT. The strong π - π interactions between CNTs and graphene sheets form conjugations between graphene and CNTs, resulting in a hierarchical network of structures with open pores leading to increased available adsorption sites. Furthermore, inherent wrinkles on graphene nanoflakes causes heterogeneity of charge distribution on graphene sheets with concentration of charges in wrinkles, resulting a more desirable areas for adsorption of Cu (II) ions. Hence, it can be concluded that graphene-CNT hybrid structures have greater Cu (II) adsorption ability than CNT, which agrees with the experimental observations by Dichiara et al., who showed that SWCNT-graphene hybrids perform better in the process of Cu (II) adsorption.⁴

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Antimony-Modified Nickel Ferrite: An Efficient Magnetically Nanocatalyst for Knoevenagel Condensation of Aryl Aldehydes with Malononitrile

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Abstract

Benzylidene malononitriles (BMN) are one of the valuable organic intermediates which are utilized for synthesis of biologically active materials such as enzyme inhibitors, carbohydrates and heterocycles.¹⁻³ In addition, certain derivatives of benzylidene malononitriles have also been exhibited various optical, electrical and biological activities. BMN are generally prepared through the condensation reaction of aryl aldehydes with malononitrile in the presence of a catalyst. This subject prompted us to prepare NiFe₂O₄/SbF_x (0.045 gr) as an efficient reusable nanocatalyst towards synthesis of benzilidenmalononitrils in refluxing ethanol (Fig. 1). This method has the advantages in terms of mild reaction conditions, short reaction times high yields of the products and reusability of the prepared catalyst system. Nickel spinel ferrites are the widely used magnetic metal oxides because of nontoxicity, biocompatibility, high thermal stability up to 900 °C without losing magnetic property, and effective catalytic activity in various processes. These super characteristics cause them susceptible to consider as the best candidates to adjust their surfaces with different metal species for the promotion of various organic transformations.



Fig. 1 Synthesis of Benzylidenemalononitrile with NiFe₂O₄/SbF_x

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An Efficient Synthesis of 2*H*-chromene Derivatives by a One-pot, Three-Component Reaction

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Abstract

The development of multicomponent reactions (MCRs) has attracted much attention from the vantage point of combinatorial and medicinal chemistry. Many important heterocycle synthesis are multi-component reactions. Recently, the synthesis of 2*H*-chromenes and derivatives have attracted great interest in their biological and pharmacological activities. The 2*H*-chromene derivatives show various pharmacological properties such as spasmolytic, diuretic, anticoagulant, anticancer, and antianaphylactic activities.

In the beginning, we design and synthesize new 2*H*-chromenes using the multicomponent reaction of aldehyde derivatives (1) (1 mmol), ethyl acetoacetate (2) (1 mmol), and dimedone (3) (1 mmol) in EtOH (Scheme 1). Favorably, the reaction proceeds well and resulting in the expected 2*H*-chromenes product which was further confirmed by spectral techniques such as IR, ¹H & ¹³C NMR. Initially, we tried to carry the reaction without catalyst in EtOH at reflux conditions. But the reaction did not proceed well and results in a very low yield of product. After screening of various type of catalysts in compression with the model reported reaction (that used 40 mol% of various catalyst). The new catalyst we designed and synthesized preformed a good yield with easy separation. Therefore, we found that out of all catalysts screened, KU₂ (Scheme 2) drags the desired reaction with a higher yield in less reaction time. Therefore, the final optimized reaction conditions for the present protocol are in EtOH at 80 °C. With these optimized reaction conditions in hand, such as 0.1 gr of KU₂, the generality of the protocol was assessed using a variety of substituted aldehydes with electron-donating and electron-withdrawing groups. As a result, the expected products with good to excellent yields were synthesized in a comfortable procedure in the presence of this IL-catalyst.



Scheme 1: Multicomponent synthesis of Chromene derivatives

Scheme 2: KU2

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Green Synthesis of New Azepane Containing Compounds Under Solvent-Free Conditions

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Abstract

Exploring diverse functionalities of heterocyclic compounds in relation to medicinal field is a hot research area. One such type of group is azepane, with strong reactivity to capture CO2. This nature of it is of important development values in medicinal chemistry and has attractive in recent years.¹ The azepane motif is in the top 100 most frequently used ring systems for small molecule drugs.² Tolazamide **1** and Glypinamide **2** are FDA approved antidiabetic drugs with azepane moiety.³ Therefore, Green routes and ecological methodologies are required in the synthesis of N-heterocycles, due to the remarkable importance of these compounds in medicinal chemistry.⁴ On the other hand hydrazides are important intermediates in organic synthesis, especially in the preparation of pharmaceuticals and agrochemicals. Their synthesis has attracted significant attention due to their utility as building blocks in many synthesis.⁵



Scheme 1. Synthesis route of N- (azepan-1-yl) benzamide derivatives under solvent free condition.

In view of the above and in continuation of our interest in study of acyl hydrazide reaction in solvent-free media ⁶, Here in we report the green synthesis of new azepane derivatives with alkylation reaction of various acyl hydrazides and 1,6-dibromohexane in the presence of K₂CO₃ as basic catalyst and TBAB as reaction media.

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Synthesis and Characterization of MgFe₂O₄/CaO.C Catalyst for Biodiesel Production

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Abstract

MgFe₂O₄/CaO.C catalysts were prepared and applied to the esterification of oleic acid with ethanol . Magnetic nanoparticles due to their easy separation and reusability are important intermediates in organic catalyst synthesis.¹⁻³ Characterizations such as X ray diffraction(XRD), field emission scanning electron microscopy(FESEM) (Fig.1), energy dispersive spectroscopy(EDS) and Brunauer–Emmett–Teller (BET) were performed. In order to optimize the reaction conditions, various parameters such as catalyst weight percentage, temperature, alcohol to oil ratio, and time were investigated. By carrying out the reaction at 70 C for 4 h with 5% wt of catalyst and a molar ratio of oil to ethanol of 1:12 . for the first run, the catalyst presents a yield of 85%. This process shows potential application for esterification of oleic acid for the green production of biodiesel. due to the fact that the catalyst is a two-factor, it is expected that this catalyst will also participate well in the transesterification reaction and have acceptable activity.



Fig1. FESEM image of MgFe₂O₄/CaO.C

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Fe₃O₄@SiO₂@Pr- (NH₄)₆Mo₇O₂₄ @Cu Magnetic Nanocomposite: An Efficient and Magnetically Recoverable Nanocatalyst for the Efficient Synthesis of Benzothiazoles

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Abstract

Polyoxometalates have a unique application in the field of catalysis, medicine, reduction, and oxidation due to their supreme redox potential and their nanometer scale. In the present research, a novel copper polyoxomolybdate nanoparticles coated iron oxide magnetic nanocomposite (Fe₃O₄@SiO₂@Pr-(NH₄)₆Mo₇O₂₄@Cu) is prepared, and tested in the application to the preparation of benzothiazoles derivatives from various aldehydes and aminothiophenol that resulted in a product with higher efficiency, high reaction speed and high selectivity. The hole properties of the synthesized nanocatalyst, The chemical composition, magnetic properties, crystalline structure, morphology, and particle size of this nanomaterial, prove the presence of all expected elements, and thermal stability was studied by using Brunauer–Emmett–Teller technique (BET), Fourier transform infrared (FT-IR) spectroscopy, vibration sample magnetometer (VSM) analyses, powder X-ray diffraction (PXRD), *Field Emission Scanning Electron Microscopy* (FESEM), energy dispersive X-ray spectroscopy (EDS), and thermogravimetric analysis-differential thermal analysis (TGA- DTA). The findings indicated that copper and (NH₄)₆Mo₇O₂₄ synergetic effects in the synthesis of benzothiazoles. The current study provided a rational design and synthesis of multifunctional catalysts for the development of "green chemistry" and "green technologies".



Figure 1: Synthesis of Benzothiazoles in the presence of nanocatalyst

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Asymmetric Arylation of Imine in the Presence of L-proline@Fe₃O₄

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Abstract

Recently, the investigation of chiral nanoligand on asymmetric synthesis is getting much importance. These nanoligands offer a powerful method for the preparation of optically active molecules that can act as precursors for other useful organic compounds.¹ One of the best economic and environmental ligands are amino acids, which contain both nitrogen and oxygen acceptor groups. Amino acids have the ability to perform several asymmetric catalytic reactions due to their direct availability, easy preparation and high stability. Other hand, the magnetic property, separation effect, and the high activity during cyclic utilization of Fe₃O₄ nanoligand are evaluated and indicated they could be used in various organic reactions.²

Chiral amines are found in the structure of important pharmacologically active compounds, as well as biologically active for example neurotransmitters. Due to the high importance of amines, several methods have been developed for their synthesis such as the addition reaction of imines.³

In this work, in order to develop an innovative approach toward the design of recoverable and reusable asymmetric nanoligand for C-C bond formation reactions, we have investigated the catalytic activity of Lproline-functionalized Fe₃O₄-nanoparticle catalyst on arylation of imines 1 by boron reagents 2 which have produced the chiral amines 3 (Scheme 1).

The structure and morphology of prepared nanoligand L-Proline@Fe₃O₄ were characterized by EDAX, SEM, and FT-IR. The structure of chiral products is investigated by melting point, IR, ¹H NMR, and ¹³C NMR spectroscopies. The enantiomeric excess (ee) of chiral products is also detected by the polarimeter.



Scheme 1: Synthesis of chiral amins by arylation of imines

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A Unique Strategy for the Synthesis of C/N Co-doped P25-TiO₂ as a Vigorous Photocatalyst for Selective Blue LED-Driven Conversion of Benzyl Alcohol to Benzaldehyde

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Abstract

Hexamethylenetetramine (HMTA) as a promising dopant source was efficiently deployed to produced carbon and nitrogen co-doped P25-TiO₂ *via* the facile sol-gel method. The low visible light absorption of TiO₂ is rooted in its wide band gap, therefore, the effectual green approach of this work was applied to promote the photoactivity traits of P25-TiO₂. The unstable surface of Ti³⁺ would grab the major focus in TiO₂ modifications. Accordingly, the C/N co-doped P25-TiO₂ possessing surface stable Ti³⁺ would lead to escalate the charge transfer with inhibit the recombination of photogenerated electron-hole pairs. As a consequence, these attributes empower the photoactalyst to absorb approximately the full visible-light spectrum.

The C/N co-doping would generate the intragap localized states positioned above the TiO2 valance band. Moreover, the formation of carbonate species on the surface of TiO₂ could be employed as the photosensitizer. The predominant feedstock of benzaldehyde with high additional value is considerably utilized in the chemical industry. Designing and synthesizing of C/N co-doped P25-TiO₂ as a superior photocatalyst improved the photooxidation of benzyl alcohol along with highly selective benzaldehyde formation under exposure to the light source of blue light-emitting diode.

This environmentally friendly procedure has demonstrated many merits such as manageable, simplistic, nonspecific, and inexpensive process bringing about considerable light absorption spectrum with the adjustable band gap, prominent surface area with plentiful reaction active sites and rapid charge separation.

This study can open a new horizon for alternative co-doped processes to upgrade the optical features by alleviating band gap energies from 3.1 eV to 2.4 eV which introduces a new class of surface engineering.



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C-C Bond Formation on Unactivated Arenes via Metal-Organic Frameworks

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Abstract

In the past decades, the synthesis of metal-organic frameworks in which organic ligands act as metal ion linkers and their use as heterogeneous catalysts in a variety of organic chemical reactions has been considered by chemists. The size of the pores, high reactivity, large surface area, active sites, the ability to adjust the network for different reactions has greatly influenced this type of catalyst.

This report describes the modification of an organic metal framework based on iron and carboxylate with another transition metal.¹

We found that it can be used to catalyze the reaction which produced the new carbon-carbon bond.² This reaction occurs between different aldehydes containing electron-donating and electron-withdrawing groups with arenes. (Fig 1)

The aldehydes are arylated by C-H activation of simple unactivated arenes after decarboxylation by the synthesized metal-organic framework.³



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Efficient Synthesis of β -Hydroxy Carbonyl Group by Metal Oxide Nanoparticles with Ultrasonic Irradiation

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Abstract

The β -Hydroxy Carbonyl Group is an important synthon for natural products and biologically active organic molecules. In order to construct the functionally, various transformations have been developed and among them, aldol reaction is recognized as the most efficient and convenient method. Many efforts have been devoted to the development of catalytic and asymmetric aldol reactions^{1,2}, but almost all of them require a reconversion of the ketone or ester moiety into a more reactive species, using no less than stoichiometric amounts of reagents. On the other hand, with recent progress in nano materials, organic synthesis catalyzed by nano-particles (NPs) has attracted much attention, and a large number of useful catalytic reactions have been discovered.³ Among the NPs, metal oxide NPs are attracting attention⁴, as they appear able to promote a diversity of new transformations never observed with classical metal catalysts.

In this research, the synthesis of β -Hydroxy ketones using the aldehydes and ketones were developed in the presence of catalytic amount of metal oxide NPs under extremely mild conditions and good yields with ultrasonic irradiation. The results show that ultrasonication can reduce the time of metal oxide NPs-catalysed aldolization to 3 Minutes. The advantage of this methodology is using small amounts of catalyst, the reduction of formation of the aldol condensation product and aldehyde self aldolization.

The structure of all synthesized compounds were confirmed with spectroscopic methods (FTIR, ¹HNMR, ¹³CNMR).

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Synthesis and Routine Production of ^{99m}Tc-L,L-ethylenecysteine Dimer to Assess Regional Cerebral Blood Flow

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Abstract

The synthetic scheme for the L,L-ethylenecysteine dimer (L,L-ECD) is given in Fig 1. L,L-ethylenecysteine dimer (L,L-ECD) compound was synthesized with an overall yield 56.8% and a melting point 197-198°C. A systematic study has been carried out on the labelling of L,L-ECD with technetium-99m by ligand exchange via 99mTc-EDTA. The produced ^{99m}Tc-L,L-ECD complex is stable, neutral and lipid soluble. Radionuclidic purity was over 99.9 %. Labeling yield and radiochemical purity were >99 %. Biodistribution studies have shown complete retention of injected radioactivity at the administration site up to 72 h. The 99mTc-L,L-ECD complex penetrate the blood-brain barrier following intravenous injection in the tail vein of mice with an initial brain uptake equal to 0.9% at 2 minutes and a slow washout equal to 0.65% after 25 minutes. High uptake in the gastrointestinal tract (GIT) was observed. These results indicate that this ligand is suitable for brain imaging and has a tendency to be excreted via liver and GIT due to its lipophilicity Fig 2.



1-thiazolidine-4-Carboxylic acid N.N-bis-L-(1-carboxy-2-mercapto) N.N-bis-L-(1-carboethoxy-2-mercapto)ethylethylendiaminedihidro chloride. L.I.-ECD

Fig. 1. Reaction scheme for the synthesis of L,L-ethylenecysteine dimer (L,L-ECD).



Fig. 2. ^{99m}Tc-ECD brain perfusion SPECT image of a 6-year-old boy with Landau-Kleffner syndrome.

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Synthesis, Characterization, Structural, Optical and Thermal Analysis of New Ni(II) 1-D Coordination Polymers at Single Crystal and Nanometer Sized, New Precursor for Preparation of NiO Nanoparticles

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Abstract

One-Dimensional Ni(II) coordination polymers $[Ni_3(\mu - BTCA)_2(\mu^3 - 0)]_n[Na(0H)_3]10H_20$ at bulk and nanosized synthesized by simple solvothermal method.¹

These new coordination polymers of Ni(II) complexes with bridging 1, 3, 5-benzene three carboxylic acid ligand, have been synthesized and characterized by elemental analysis, FTIR, thermal gravimetric analysis and single crystal X-ray diffraction.²

In these CP (CP=Coordination Polymers) and NCP (NCP=Nano Coordination Polymers), Ni(II) ions are bridged by two situations of BTCA (BTCA=1, 3, 5-benzene three carboxylic acid) ligands forming linear chains, which are also further coordinated by neutral BTCA and Oxygen ligands into a one-dimensional polymeric chain. This polymeric precursor has been used to prepare NiO nano-particles using calcination of NCP. The prepared Ni(II) Oxide nano-structure was characterized by scanning electron microscopy and X-ray powder diffraction and studied with optical properties. Figure1



Figure 1: SEM image of nanoparticles of NCP as produced by solvothermal proses.

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Synthesis of Ag₂O and Ag₂S Nanoparticles from New Mixed Ligand Ag(I) 1-D Zig-Zag Coordination Polymers, Characterization, Thermal, Antimicrobial and Optical Analysis

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Abstract

Nanopowders and single crystal of new Ag(I) One-dimensional coordination Polymer, [Ag (µ-4-PCA)(SAC)]n were synthesized by a impel sonochemical and branched tube methods. The new nanostructures of Ag(I) coordination Polymer was characterized by single crystal X-Ray crystallography analysis (X-RAY), Scanning Electron Microscopy (SEM), X-Ray powder diffraction (XRD), Transmission Electron Microscopy (TEM) and IR spectroscopy. The crystal structure of this compound consists of onedimensional zigzag polymeric units. The thermal stability of compounds was studied by Thermal Gravimetric Analysis (TGA) and Differential Thermal Analyses (DTA). Ag₂S and Ag₂O nano-structures were obtained by calcinations of the nano-structures of this coordination polymer at 800 °C.

The inborn antibacterial property of silver nanoparticles has been studied against Escherichia coli and Pseudomonas aeruginosa. The tests conducted have illustrated that the nanoparticles of this coordination polymers better than bulk simple and also nanoparticles of Ag₂O and Ag₂S better than other samples.



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Synthesis of Novel 1,2-Diol Mono-esters Containing 2,4-Thiazolidinedione Core as Potential Therapeutic Agents

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Abstract

The thiazolidinedione derivatives are important substrates in organic and medicinal chemistry. Compounds containing the thiazolidinedione moiety exhibit numerous biological activities. Among them, 5-arylidene derivatives have attracted considerable attention due to their unique biological activities. 5-Arylidene thiazolidinedione derivatives display different biological activities such as COX-2 inhibitor, antidiabetes, antibacterial, anticancer, anti-HIV, and antifungal activities.¹

Epoxides are extensively used to synthesize structurally diverse organic compounds via its ring opening reaction with different nucleopholes. The ring opening reaction of epoxides with carboxylic acids affords 1,2-diol mono-esters which play an important role in the pharmaceutical and perfume industries, oil and gas industries, coating and polymer industry, and synthesis of biopolymers and other organic compounds.²⁻⁴ The epoxides are generally reacted with carboxylic acids in the presence of protic/Lewis acids and bases which suffer from one or more drawbacks such as low yield, harsh reaction condition, tedious work-up procedure, isomerization of the desired product, the use of expensive and nonreusable catalysts as well as limited substrate scope. Thus, the development of facile and applicable methods with suitable generality for synthesis of 1,2-diol mono-esters still remains of great importance. Inspired by the uniqe biological activities of thiazolidinedione derivatives and importance of 1,2-diol mono-esters, herein, we report the synthesis of compound **1** via the ring opening reaction of epoxides with the preformed carboxylic acids in the presence of a novel and neutral silica-based heterogenous nanocatalyst. The effect of different parameters on progress of the reaction have been studied. The structure of synthesized compounds were confirmed by NMR and IR.



G = H, Me, OMe, Cl, ... R = alkyl, aryl, aryloxy, alkyloxy, ...

Figure 1: The general structure of synthesized compounds.

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Design and Exploring Physicochemical Properties of the New Class of Tunable Ionic Liquids Using Computational Chemistry

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Abstract

lonic liquids (ILs) are a novel class of chemical compounds with a wide range of applications. These materials have unique properties such as low melting points, negligible vapor pressure, extremely low volatility, non-flammability, unusual solvation and resistant to oxidation, particularly in the presence of air and moisture.¹⁻⁴ By tuning sterically and electronically characteristics of the both cationic and anionic parts of the ILs, physicochemical properties of an ionic liquid could be developed. Standard ionic liquids based on imidazolium cation carry two alkyl chains, which are limited to inductive effects. The aim of the present research is to determine the influence of the various anions and saturated and unsaturated aliphatic groups at the cation part on their physical, chemical and electronic properties which are explored by using quantum chemical calculations at M06-2X/AUG-cc-pVDZ level of theory. Three series of the designed ionic liquids composed of 1-phenyl-3-ethyl imidazolium ([PEIM]⁺), 1-phenyl-3-vinyl imidazolium ([PVIM]⁺)and 1-phenyl-3-ethynyl limidazolium ([PEnIM]⁺) cations and (Y1-4 = [CH₃CO₂]⁻, [NO₃]⁻, [BF4]⁻ and [ClO₄]⁻) anions are taking into account. Based on these sets of the cations and anions and also electrostatic potential maps of them, twelve ion pair configurations named as [PEIM][Y1], [PEIM][Y2], [PEIM][Y3], [PEIM][Y4], [PVIM][Y1], [PVIM][Y2], [PVIM][Y3], [PVIM][Y4], [PEnIM][Y1], [PEnIM][Y2], [PEnIM][Y3] and [PEnIM][Y4] ILs were proposed and undergo further investigation. Primary results show that the anions of [Y3]⁻ and [Y4]⁻ locate above the imidazolium ring (on-top configuration), while anions of [Y1] and [Y2] locate nearly in the plane of the imidazolium ring. In addition ILs including Y1 and Y2 anions with [PVIM]⁺ cation as well as the ILs including Y3 and Y4 anions with [PEIM]* cation have the highest interaction energy within the studied ILs. In continue some physical characteristic of the studied ILs such as melting point, surface tension, viscosity and etc. are predicted and discussed stand on the obtained results.

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Biosynthesis and Characterization of Iron Nanoparticles Utilizing Zosima Absinthifolia Leaves Extract and its Antibacterial Activity

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Abstract

The interest in synthesizing Nanoparticles in an easy and environmental friendly way has been increasing in the recent years. Physical and Chemical methods are conventionally used for synthesis of Nanoparticles, however due to limitations of these methods, the focus of research has been recently shifted towards the development of clean and eco-friendly synthesis protocols.

The green synthesis of Iron Nanoparticles has been achieved using environmental acceptable plant extract. It was observed that zosima absinthifolia leaf extract can reduce Iron ions into Iron Nanoparticles at room temperature. The aim of this study is to synthesize Iron Nanoparticles using zosima absinthifolia extract in an environmental and sustainable way.

The synthesized Iron Nanoparticles were characterized using Scanning Electron Microscope (SEM) and Fourier Transform Infrared (FTIR) analysis. This study shows that the Iron Nanoparticles can be synthesized using zosima absinthifolia leaf extract as a antibacterial active. Keywords: FeNPs, Biosynthesis, Nanoparticles, Green method, SEM, XRD

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Characterization of Copper Nanoparticles Utilizing Falcaria Vulgaris Leaves Extract

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Abstract

Copper oxide nanoparticles were synthesized using *falcaria vulgaris* leaves water extract and copper nitrate as a source of copper by green synthesis at 80 ° C. This method has many advantages such as nontoxic, economic viability, ease to scale up, less time consuming and environmental friendly approach for the synthesis of CuO nanoparticles without using any organic chemicals. The synthesized CuO nanoparticles were characterized by powder X-ray diffraction(XRD), scanning electron microscopy (SEM) and Fourier Transform Infrared Spectroscopy (FTIR).^{1,2}

Crystallite size of CuO nanoparticles was calculated using Scherrer formula. The Xray powder diffraction (XRD) analysis revealed the formation of monoclinic phase CuO with average particle size of 22-39 nm.



Scheme 1. Falcaria Vulgaris

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Loading and Release of Curcumin by Hydroxyapatite

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Abstract

Curcumin (Figure 1), the bioactive molecule found in turmeric, possesses a board spectrum oftherapeutic effects, especially antioxidant, anti-inflammatory, and anticancer activities. It promotes apoptosis induction in various tumor cells without harming normal cells. Numerous studies revealed that curcumin directly modulates the growth of cancer cells via interfering with several signaling pathways including cell proliferation and survival, caspase activation, tumor suppressor, and mitochondrial pathways.^{1,2}

The loading of curcumin onto hydroxyapatite was optimized by response surface methodology (RSM). The RSM-optimized results demonstrated that the maximum curcumin loading efficiency was about 75% at a hydroxyapatite amount of 1 g, curcumin concentration of 50 mg L⁻¹, and a pH of 7 within 60 min.

To evaluate the curcumin release behavior in the gastrointestinal tract and blood plasma, evacuation of curcumin from hydroxyapatite was tested during 24 h at 37 °C at three different pHs, i.e. 1.2, 7.4, and 8.5, inspired by the acidic, neutral, and alkaline pHs of the stomach, blood plasma, and intestine, respectively. Approximately 78, 19, and 57% of the loaded curcumin was severally released under acidic, neutral, and alkaline conditions in the first hour, while these values reached up to 98, 53, and 67% at the end of the study, respectively.



Figure 1: Curcumin

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Calcium ferrite nanoparticles loaded with clove essential oil

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Abstract

Cloves (Figure 1) are the dried flower buds of clove tree and contain a number of bioactive compounds which some of them are highly effective antioxidants and antimicrobials. Clove essential oil (CEO) contains mainly phenylpropanoids such as eugenol and its derivatives, along with minor levels of β -caryophyllene and α -humulene organic compounds.^{1,2} CEO has various applications in the food, sanitary, biomedical, pharmaceutical, active packaging and cosmetics industries due to its biological properties including antioxidant, antimicrobial, antiseptic, pesticide, analgesic and anticarcinogenic activities.³

In this research the loading of CEO onto calcium ferrite was studied. The results showed that the maximum CEO loading efficiency was about 63% at a calcium ferrite amount of 2 g, CEO concentration of 25 mg L^{-1} , and a pH of 5.

The cytotoxicity of calcium ferrite and calcium ferrite nanoparticles loaded with CEO on A549 cell lines were evaluated using the MTT (3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide) colorimetric assay. The results demonstrated that the samples slightly affect the mortality even at higher concentrations, inferring the biocompatible nature of them.



Figure 1: Cloves

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Investigation of Antioxidant Properties of Iranian Berberis

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Abstract

Free radicals are the highly reactive molecules that cause great damage to cell membranes and DNA, resulting in inducing oxidation and mutations of DNA, which lead to cancer, degenerative, and other diseases. Antioxidant compounds could be of great benefit in prevention and treatment of these diseases.¹ Natural antioxidants are more safe and healthier than synthetic ones.² Barberry fruits are found to be rich in antioxidant compounds and this study aimed to examining the antioxidant properties of 55 accessions of Iranian barberry fruit.^{3,4}

Fruit sample of plants were collected from barberry collection garden of Mashhad and different natural habitats of barberry from various provinces of Iran. The samples were air dried, finely ground, and extracted by methanol: water (80:20) for 1 h by shaking. The extracts were filtered and dried by vacuum. Then, radicals neutralizing effects of extracts were examined by means of DPPH method.⁵

The results showed significant difference between antioxidant properties of various extracts, at probability level pf 1%. The highest and lowest rates of free radical scavenging DPPH were 59.06% and 12.3%, respectively.

Difference in antioxidant activity was observed for samples of barberry fruit extract produced from different barberry samples. This differences probably reflected phenolic and anthocyanin composition of barberry fruit extracts.

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Synthesis of Hydro Acenaphtho[1',2':4,5]pyrrolo[2,3-d]pyrimidine Derivatives via One-Pot Three-Component Reaction

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Abstract

Multi-component reactions (MCRs) have emerged as a highly efficient synthetic tool in organic and medicinal chemistry because of their ability to synthesis pharmaceutical compounds and their productivity, high atom economy, step efficiency, molecular diversity, and operational simplicity.¹ In the past decade, new MCRs have been developed and used for the construction of important complex molecules.²

pyrrole is a heterocycle of great importance because of its presence in numerous natural products such as heme, chlorophyll, vitamin B₁₂, and various cytochrome enzymes.³

Initially, the three-component reaction of acenaphthoquinone **1**, barbituric acids **2** and aminouracil derivatives **3**, in ethanol at reflux for 3 h, afforded a series of hydro pyrimidine acenaphtho[1',2':4,5] pyrrolo[2,3-*d*]pyrimidine **4a-4h** in 79-94 % yields (Scheme 1).



Scheme: Synthesis of hydro acenaphtho pyrrolo pyrimidine derivatives

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Synthesis of Acenaphtho[1,2-b]indol-11b-yl)-1H-indene Derivatives via Four-Component Reaction

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Abstract

Over the past few years, multi-component reactions (MCRs) have been designed to be efficient and potent tool and have become a significant area of research in organic chemistry. MCRs are used for the synthesis of biologically active compounds in medicinal chemistry and complex product from simple and readily available starting materials without isolation of intermediates in short time with high purity, maximum selectivity and in a minimum number of synthetic steps and good yields.¹⁻²

Herein, we report an efficient synthesis of acenaphtho[1,2-*b*]indol-11*b*-yl)-1*H*-indene derivatives via fourcomponent reaction of 5,5-Dimethylcyclohexane-1,3-dione (dimedone), arylamines, acenaphthoquinone and indondione in refluxing ethanol under catalyst-free conditions is described (Scheme 1). In this work, the structures of all compounds were deduced from their analysis, IR, ¹H NMR,¹³CNMR spectra. The mass spectrum displayed the molecular ion peak at the appropriate m/z value, which is in agreement with the proposed structure.



Scheme 1: synthesis of acenaphtho indol indene derivatives

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Solubility of Insoluble Dyes in Organic Solvents Using Amphiphilic Polyurethane Reverse Micelle

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Abstract

Reverse micelles are nanometer-sized aggregates of amphiphilic molecules surrounding a microscopic water core in a nonpolar solvent.¹ Their core-shell structure provides good solubilization for hydrophilic guest molecules in nonpolar organic media.²⁻³

In this approach, to investigate solubility of hydrophilic dyes using amphiphilic polyurethane reverse micelles (APU), the desired polymer was prepared by the reaction of polyethylene glycol, isophorone diisocyanate (IPDI), PCL-PEG-PCL (PCEC) triblock copolymer and one drop of dibutyl tin dilaurate (DBTL) as a catalyst (Figure 1). The synthesized polymer showed a self-assembled structure in nonpolar organic media by direct dissolution method. The aggregation point (RCMC) of APU was determined by turbidimetry and viscometry methods The morphologies of these nanoparticles were investigated by field emission scanning electron microscopy (FE SEM), atomic force microscopy (AFM), dynamic light scattering (DLS), ¹H NMR spectroscopy and water contact angle (WCA) measurement. The solubility of different dyes (e.g., Rhodamine B, Fuchsin, Malachite green and Lackmus reinst (Figure 1)) were studied by UV-vis measurement. The percentage solubility of dyes in organic phase increased with increasing the amphiphilic polymer concentration.



Figure 1: Structure of amphiphilic polyurethane and solubility of insoluble dyes in toluene solvent

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Impact of Magnetic Field on Cell Growth and Antimicrobial Activity of Haematococcus Lacustris Algae

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Abstract

Magnetic field is a physical factor which can stimulate membrane permeability and ion currents and induced growth parameters and secondary metabolite production.¹ In the present study, impact of various magnetic fields were investigated on the cell growth and antimicrobial activity of Haematococcus lacustris alga. Alga stock was prepared from biotechnology institute of Mashhad, cultured in BBM-specific culture medium, and the suspension cultures were exposed to various magnetic fields (0, 4, and 8 mT) for 1 hour during continuously three days.²

Optimal density (750 nm), cell number, and antimicrobial activity were investigated after three weeks. Results showed that magnetic field changed the cell growth and number of H. lacustris and the highest mentioned parameters were observed at 8 mT. MIC test showed the inhibitory impact of H. lacustris extract on Staphylococcus aureus bacteria. However, there wasn't observed growth inhibitory effect of extract on Staphylococcus and MCRS bacteria. The resulted suggested effect of magnetic field on the antibacterial activity of algae which may associate with the rise of antioxidant capacity of algae by magnetic field.^{3, 4}

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Antibacterial Activity of *in vitro Physalis Alkekengi* Seedlings Under Different Concentrations of Iron Nanoparticles

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Abstract

Physalis alkekengi is a medicinal plant from Solanaceae family and has various pharmaceutical properties, including antioxidant and anti-inflammatory properties.¹ Nanoparticles have small size, high surface area, and high adsorption capacity by plant cells and cause to stimulate plant growth and yield (Torabzadeh et al. 2019). In this study, the effect of iron oxide nanoparticles (Fe2O3 NPs) on the growth parameters and antibacterial activity of Physalis alkekengi seedling under in vitro condition was investigated. Physalis alkekengi seeds were strillized with sodium hypocloride for 10 min, alchohol (70%) for 2 min, and then washed three times with distilled water. The disinfected seeds were cultured in Murashig and Skog medium containing different concentrations of Fe2O3 NPs (0, 10, 20 and 30 mg L⁻¹) and trasfered to culture room. Seedlings were harvested for physiological and biochemical analyzes after 4 weeks. Results showed that Fe2O3 NPs up to 20 mg L⁻¹ significantly increased growth parameters such as fresh weight, dry weight and relative water content. Increase of Fe2O3 NPs level (30 mg L-1) decreased water content and growth parameters. By contrast to growth parameters, antibacterial activity of Physalis alkekengi extract increased under Fe2O3 NPs. MIC analysis showed the inhibitory effect of extract for Escherichia coli and MRSA bacteria, but didn't affect on Escherichia coli and MRSA bacteria. Plant grown under Fe2O3 NPs (20) showed the highest MIC activity. It seems that impact of Fe2O3 NPs on antibacterial activity may relate to changing the antioxidant capacity by iron NPs.^{2, 3}

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Synthesis Of Novel Schiff Base Derivatives Containing Diamonded Adamantane Moiety

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Abstract

Schiff bases, named after Hugo Schiff, are formed when any primary amine reacts with an aldehyde or a ketone under specific conditions.¹ Schiff bases with the general structure $R_2C=NR'$ ($R' \neq H$) are found to be a versatile pharmacophore for design and development of various bioactive compounds. Many aromatic Schiff base compounds have developed as antibacterial, antitumor and antibiotic drugs in recent years.² In chemistry, diamonded are variants of the carbon cage molecule known as adamantane ($C_{10}H_{16}$), the smallest unit cage structure of the diamond crystal lattice. Diamonded also known as nano diamonds or condensed adamantanes may include one or more cages.³ A diamond combines several very useful properties, such as extreme mechanical hardness, stability against chemical reagents, broad optical transparency, wide band gap, high radiation hardness, and high thermal conductivity [4]. Diamonded, also have many properties of diamond, therefore molecules with diamonded moiety contain modified properties. Thus, we have attempted to prepare Schiff bases with diamonded adamantane moiety. For this purpose, salicylaldehyde derivatives **1** was treated with amantadine (1-amino adamantane) **2**, as the primary amine, to obtain amantadine- Schiff base hybrids **3** (Scheme 1).



Scheme 1. Synthesis of amantadine- Schiff base hybrids

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Amphiphilic Polyurethane Nanomicelles as Drug Delivery Systems

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Abstract

Recently Amphiphilic polymers (APs) have been interesting class of polymers that are applicable in many area including nanoencapsulation, phase transfer, nano-reactors, drug delivery and biomaterials synthesis.1-3

We have recently reported a synthesis of amphiphilic polyurethane (APU) with hydrophilic and hydrophobic moleties, Figure 1.⁴ Such architecture can induce the polymer to behave as a micellar host. In order to evaluate the probable capability of the APU nanomicelles in drug encapsulation and delivery, paclitaxel (PTX) and doxorubicin hydrochloride (DOX-HCL) were used as probe. Preparation of nanoparticles containing DOX-HCL or PTX was performed using the double emulsion solvent evaporation technique. The dye loaded APU nanomicelles showed suitable physical stability, negative zeta potential charge and with low level of critical micelle concentration (CMC). The cytotoxicity of their degradation products was evaluated using methyl thiazole tetrazolium (MTT) assay in vitro. These nanomicelles significantly inhibited the growth and proliferation of the human breast cancer MCF-7 cells. Drug release studies showed controlled release of drugs from nanoparticles that was mainly driven by diffusion-based mechanism.

Based upon these findings, we propose that the amphiphilic polyurethane nanomicelles can be used as an effective nanocarrier for drug delivery.



Scheme 1: Structure of amphiphilic polyurethane

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Decoration of Palladium NPs on the Functionalized Cellulose as A Novel Support in Suzuki Reaction

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Abstract

Due to its remarkable properties, Cellulose is an attractive and promising candidate that could be used as an efficient, renewable, and biodegradable support for catalysts.¹ In addition, cellulose is stable in most organic solvents, inexpensive, and has a high surface area. Typically, functional groups present in cellulose backbone participate in bonding with metals. In this study, for increasing the functional groups of Cellulose, the Cellulose p-toluenesulfonate (Cell-OTs) was synthesized via a methods reported in the literature.² Afterward, Cell-OTs was reacted with melamine via the nucleophilic substitution of Cell-OTs with NH₂ groups of melamine. In order to improve the catalytic performance, OTs⁻ was exchanged by Cl^{-,3} The resulting support was then decorated with palladium nanoparticles (Pd NPs) to give the final catalyst.⁴ The synthesized Pd NPs were used as a catalyst for suzuki cross coupling reaction (Figure 1). After optimozing the reaction condition in the reaction of phenylboronic acide and iodobenzen as a model reaction, the catalytic activity of Pd NPs was studied in the Suzuki cross-coupling reaction of various aryl halides with phenylboronic acid. The results exhibited that this catalyst efficiently catalyzed Suzuki cross-coupling reactions and gave the corresponding products in good to excellent yields and also the catalyst showed good activity after 5th cylces.



Figure 1: Suzuki cross coupling reaction of aryl halides with phenyl boronoc acid

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Functionalized Cellulose for Removal of Cd(II) From Waste Water

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Abstract

Due to their remarkable properties, cellulose nanomaterials are emerging materials for wastewater treatment.¹ In this study, both pristine cellulose nanomaterial and modified cellulose nanomaterial with Polyethylenimine were prepared from the wood of the *Corn plant* for the removal of Cd(II) ions from waste water. After charactrizing the adsorbents, The effect of initial concentration, contact times, adsorbent dose, temperature, solution pH on Cd(II) ions removal was studied. Langmuir and Freundlich adsorption isotherms² were certainly fixed to a maximum Cd(II) ions uptake capability (Qmax) of 88 and 170 mg g⁻¹ by Cellulose and modified Cellulose adsorbents, respectively. The pseudo-second-order and pseudo-first-order kinetics model was well fitted to the uptake process.³ Results revealed that the percentage removal (%R) of Cd(II) ions from the adsorbent by the addition of HCl, and the regenerated sorbent was reused as an adsorbent for at least 6 successive cycles.⁴ The results indicated excellent recycling capabilities, and the adsorbent was used as adsorbing material for the removal of Cd(II) ions from modified Cellulose after 6 successive cycles without significant efficient loss.

				/ I		
Metal ion	Pseudo-first-order kinetics			Pseudo-second-order kinetics		
Cd(II)	q e,cal	k₁ (1/min)	R ²	q e,cal	k₂ (g/mg	R ²
	(mg/g)			(mg/g)	min)	
Cellulose	80.1	0.083	0.93	82.42	0.01559	0.99
Modified	124	0.040	0.94	165	0.0037	0.99
Cellulose						

 Table 1: The values of parameters of pseudo-first-order, pseudo-second-order

Acknowledgements

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Synthesis of CuO@UiO-66 and its Application in Henry Reaction

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Abstract

Metal-organic frameworks (MOFs) are a category of compounds with both organic and inorganic parts.¹ Between these large families, Zr-based MOFs, which also are known as UiO family, have been attracted more attention than the other MOFs because of their high thermal and chemical stability. One of these porous materials, UiO-66, has received remarkable attention due to its easy synthesis, high relative stability, high specific surface area, large porosity and leading properties for a wide range of applications in different fields.² According to the high surface area feature, the UiO-66 can also be used as support. Metal oxide nanoparticles that show great catalytic activity can simply be loaded in the pores of UiO-66.³ Henry reaction is one of the C-C bond forming reactions in organic synthesis, which produces β -Nitroalcohols.⁴

In this work, CuO@UiO-66 was prepared by solvothermal method and characterized by several techniques such as FT-IR, XRD, SEM, EDX, TEM, and BET-BJH (Scheme 1). Then, the catalytic activity of CuO@UiO-66 was examined in the Henry reaction and the resulting products were obtained with high yields in short time of reaction (Scheme 2).



Scheme 1: Incorporation of CuO into UiO-66



X: H, CI, NO₂, OMe, OH

Scheme 2: CuO@UiO-66-catalyzed Henry reaction of benzaldehyde and nitromethane

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Enantioselective Copper(I)-Catalyzed Henry Reaction Using Chiral Heterogeneous Oxazoline Based Ligands

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Abstract

The coupling reaction of a nitroalkane and the carbonyl group of an aldehyde or ketone in the presence of a base, is called Henry (nitroaldol) reaction. This reaction with no doubt, is one of the most effective methods for carbon-carbon bond formation in organic synthesis.¹

The development and design of highly efficient and selective ligands are important factors in coppercatalyzed asymmetric Henry reactions.²

Preparation of chiral heterogeneous catalyst by immobilization of chiral ligands onto an inorganic mesoporous substrate such as SBA-15, has attracted a lot of attention in recent years.³ In this work, chiral amino oxazoline ligands were synthesized from chiral amino alcohols and cyanogen bromide.⁴ Next, by immobilization of them on mesoporous silica SBA-15, chiral heterogeneous ligands (OX-R-SBA-15) were synthesized and then characterized by using FT-IR, XRD, SEM, EDX, TGA, and BET-BJH techniques (Scheme 1). Finally, the obtained chiral heterogeneous ligands in the presence of copper salts were examined in enantioselective Henry reaction (Scheme 2). The resulting chiral β -nitroalcohols were obtained in high yields and good enantioselectivities.



Scheme 1: synthesis of chiral heterogeneous ligands OX-R-SBA-15



X= H, Me, CI, NO₂

Scheme 2: Enantioselective Henry reaction using of copper salts and chiral heterogeneous ligands

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The Synthesis of Chiral Betti Bases and Their Applications in Asymmetric Allylic C-H Bond Oxidation of Olefins

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Abstract

Allylic oxidation of alkenes to produce allylic alcohols and allylic esters is one of the most important reactions in organic chemistry. In this reaction, because of the specific nature of the allylic C-H bond, a new functional group is created without the involvement of the double bond. The stereochemistry of this reaction can be controlled by the use of asymmetric methods.¹ Among these methods, providing a chiral environment especially by using chiral catalysts, has attracted much attention because they can use in small amounts and produce enantioenriched compounds. The Betti reaction produces racemic and non-racemic aminobenzylnaphthol ligands. Non-racemic aminobenzylnaphthols can be used as chiral ligands or chiral auxiliaries in asymmetric synthesis.² In this work, first, racemic Betti bases were synthesized by the multicomponent reaction of 2-naphthol, benzaldehyde, and ammonium acetate. Then, the resulting enantiomers were separated by the diastereomeric crystallization method using (L)- tartaric acid in ethanol and methanol (Scheme 1).^{3,4} Finally, the synthesized chiral Betti bases were used as chiral ligands in allylic oxidation of olefins for the first time and the resulting products were obtained in high yields and moderate enantioselectivities (Scheme 2).



Scheme 1: Synthesis of chiral Betti bases by the diastereomeric crystallization method



X= H, Me, Cl, NO₂

Scheme 2: Enantioselective allylic oxidation of alkenes in the presence of chiral Betti bases

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Synthesis and Identification of Magnetic Gelatin-Polyvinyl Alcohol Hydrogel for Use in the Release of Furosemide Drug

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Abstract

Gelatin-based hydrogels have been used as a scaffolding biomaterial for tissue engineering of 'highly' vascularized organs and also in the cell-based therapies after heart failure.¹ Additionally, due to the presence of bioactive sequences², gelatin derivatives have shown promising applications for tissue regeneration³, cancer studies⁴ as well as for vascularization and angiogenic growth factor delivery.⁵ In this work, magnetic gelatin-polyvinylalcohol hydrogel was prepared using $K_2S_2O_8$ in aqueous media in the presence of *N*,*N'*-methylenebisacrylamide (Scheme 1). The magnetic gelatin-polyvinylalcohol hydrogel was characterized by FT-IR, SEM and thermal analysis. Then, loading and release of furosemide drug was investigated using magnetic gelatin-polyvinylalcohol hydrogel. The effects of temperature and pH on the loading and release of fluvoxamine maleate drug in magnetic gelatin-polyvinylalcohol hydrogel were studied. The results showed that the highest loading of the drug was achieved at room temperature after 4 hours. Also, the highest drug release was observed after 8 hours at room temperature in pH = 7.



Scheme 1: The synthesis of cross-linked magnetic gelatin-PVA hydrogel.

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Production, Purification and Activation of Flavin Reductase for Performing Promiscuous Organic Transformations

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Abstract

The utilization of biocatalysts for the synthesis of novel organic compounds has become an interesting field over the past few years. Enzymes are proteins that are responsible for almost all transformations that take place in-vivo.¹ Enzymes are well-known for their unique characteristics in chemical transformations such as chemo, regio, and stereo-selectivity. However, when an enzyme performs its catalytic functions using non-canonical substrate "substrate promiscuity" takes place, while "catalytic promiscuity" occurs when the active site catalyzed different types of reactions.² Biocatalytic promiscuity, a novel usage of enzymes, has attracted much interest and developed rapidly in recent years. The promiscuity has extended the application of enzymes as biocatalysts in different industries particularly the pharmaceutical industry. Therefore, developing novel promiscuous enzymes will introduce new methods for synthesizing daily chemicals.

Flavin reductase (EC 1.5.1.30) from *e.coli* is a NAD(P)H-dependent reductase that reduces riboflavin. In this work, recombinant flavin reductase has been produced. First, the gene of the enzyme was amplified using the PCR technique, then the amplified gene was cloned. Having done the gene expression, the enzyme turned out to be insoluble. However, the sequencing has demonstrated three undesired mutations. Therefore using molecular docking, structural investigations have been perform to explore the effect of these mutations on the structure of the enzyme, in particular on the active site. The docking has shown the structure of the enzyme was unaffected by mutations and they were far away from the active site, therefore the NADH interactions with the binding site of the flavin reductase were unaffected. The produced protein has activated and purified urea gradient and ion-exchange column chromatography. The recombinant flavin reductase has been used to catalyze promiscuous organic reactions to form C-C and C-N bonds and initial results have shown that flavin reductase is capable of catalyzing C-N bond formation in a very mild condition.

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Ef cient Removal of Copper from Wastewater by Using High Surface Area Carbon Nanostructure

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Abstract

Lack of clean water has been one of the most important problems and global effects on human society.¹⁻² In this study, the carbon nanostructure were synthesized by pyrolysis method from waste of Oil Refinery Company. The samples were characterized by XRD, BET, FESEM and EDX techniques and applied as an adsorbents for the removal of copper ions from industrial waste water. Also, the effect of different parameters such as adsorbent type, the amount of absorbent, the initial concentration of heavy metal, pH and adsorption time were investigated. The adsorption isotherm was well i tted with Langmuir mode [(figure 1) and the adsorbent (5 mg) was able to remove 99% of copper ions from 100ppm solution (50 ml) at acidic media in 1hour. Accordingly, the carbon nanostructure can be used as an effective adsorbent for rapid removal of Cu²⁺ ions from aqueous solution.



Figure 1. Langmuir Isotherm

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Using of Isocyanide Insertion for Synthesis of Aminobenzimidazoquinazolines

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Abstract

The importance of isocyanides because of their electrophilic and nucleophilic potential Compounds are in multicomponent reactions. Different reactions based on isocyanides Reactions such as: nucleophilic Substitution, electrophilic addition, Imidation, oxidation, etc.

In the field of organophilic chemistry, isocyanides generally act as ligands for transition metals. Coordination of isocyanides to metal centers alters the electron distribution of the isocyanide fraction, and as a result reaction paths become available, which is not possible in the absence of metal. The use of isocyanides in catalytic systems in reaction with various compounds, especially heterocyclic structures, leads to the production of structures that are biologically very valuable.

In this project, the aim is to synthesize biologically active compounds by isocyanide insertion. Here are an example of these reactions:



Scheme 1: Imidolition of 2-aminoaniline catalyzed by cobalt

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Arylation of Aromatic Aldehyde in the Presence of Nanomagnetic Organometallic Catalysts Based on Palladium and Dppe Ligand

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Abstract

The diaryl hydroxymethyl group has become an essential part of the development of the synthesis of many compounds. This structural unit has become the backbone of many chiral auxiliaries, drugs, chemicals, flavors, and materials used in the agricultural industry, ligands, as well as catalysts. These compounds which have the two aryl groups play a crucial role in maintaining or enhancing the stereoselectivity of the reaction¹ are also used for the kinetic resolution of racemic α -aryl propanoic acids, α -aryl butanoic acids, and β -substituted α -aryl propanoic acids.²

The catalytic activity of palladium nanoparticles is explained in various reactions. Separable nanomagnetic organometallic catalysts were synthesized by different processes through direct immobilization of ligand on Fe₃O₄ magnetic nanoparticles bearing metal.^{3,4}

In this research, heterogeneous nanomagnetic catalysts preceded the addition of arylboronic acids **2** to aromatic **1** aldehydes for C-C bond formation reactions with considerable excellent activity to the synthesis of diaryl hydroxymethyl **3** during a short time. These catalysts were easily recovered by the simple magnetic decantation and reused with no significant decrease in the activity several times (Scheme 1).

The structure of nanomagnetic organometallic catalysts is determined by FT-IR, VSM, TGA-DTA, TEM, SEM, EDAX, and X-ray diffraction (XRD) and The structure of products is confirmed by melting point, FT-IR, ¹H NMR, and ¹³C NMR spectroscopies.



Scheme 1: Arylation of aldehyde in the presence of nanomagnetic organometallic catalysts

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Michael Additions of Dihydropyrimidinons to α,β- Non-Saturated Esters Compounds Under Solvent Free Condition

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Abstract

Dihydropyrimidinones are known to exhibit a wide range of biological activities such as antiviral, antitumor , antibacterial and anti-inflammatory actions.¹ The various techniques of green chemistry, reaction under solvent free conditions emerge as a powerful approach for the synthesis of biologically molecules.² High efficiency and improved synthetic methodology for the preparation of 3-4-dihydropyrimidin-2(1H)-thios(Ethyl 6-methyl-4-phenyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate) and derivatives in the one pot multicomponent–Biginelli reaction by condensation of β -dicarbonyl compounds, thiourea, and aromatic aldehydes using concentrated HCI as a catalyst. this new method has the advantage of easy reaction condition, time, excellent yield, recyclable green catalyst, and absence of organic solvent.³ A simple and efficient method for the synthesis of N3-substituted 3,4-dihydropyrimidinon by aza-Michael addition reactions of 3,4-dihydropyrimidinones to α , β -non-saturated esters compounds under solvent free condition is described.⁴



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Identification of Secondary Metabolites of the Lichen *Diploschistes Ocellatus* from Iran Detected by High Performance Liquid Chromatography Mass Spectrometry (HPLC-MS)

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Abstract

Lichens are well known for their unique secondary metabolites and various applications such as in medicine, cosmetics and food. This study focuses on the chemistry of *Diploschistes ocellatus* (Fr.) Norman using acetone extract. Secondary metabolites of this lichen were identified using high performance liquid chromatography-mass spectrometry as powerful analysis method. 10 metabolites were identified. Based on the structure of the identified components, the presence of 5 depsides, 2 depsidone, 1 tridepside, 1 chromone, 1 Depsone was investigated.

No	Name	Metabolite	Structure	Molecular	Measured	Retention
	And Molecular	Type		weight	mass	time
	Formul	. , , , , ,		(g/mol)	(m/z)	(min)
1	Diploschistesic	Orcinol	но он он	334.3	356.7	20.4
	acid	Depside			(+Na)	
	C ₁₆ H ₁₄ O ₈	Dopoldo	Ч Ч он		(Thu)	
2	Lecanoric acid	Orcinol	ОНОНОН	318.28	313	16.48
	C ₁₆ H ₁₄ O ₇	Depside	но-			
3	Norstictic acid	β-Orcinol	HO	372.3	371.0	18.23
	$C_{18}H_{12}O_9$	Depsidone	0 <u> </u>			
			OH H			
			0 он			
4	Gyrophoric acid	Orcinol		468.4	468.8	18.65
	$C_{24}H_{20}O_{10}$	Tridepsid	он о С С ОН			
			но			
5	Atranorin	β-Orcinol		374.3	372.75	14.89
	$C_{19}H_{18}O_8$	Depside	но			
			<u>سر</u> کر ٥-			

Table 1. Identification of some secondary metabolites Diploschistes ocellatus by LC-MS

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Carbon Monoxide Hydrogenation to Valuable Products Over Cobalt Based Catalyst

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Abstract

Fischer–Tropsch synthesis (FTS) over Cobalt catalyst would be a structure-insensitive reaction and the activity of Cobalt catalyst would depend on the number of exposed Cobalt metal sites on the catalyst surface. Therefore, Cobalt was typically deposited on supports having high surface area (e.g. SiO₂, Al₂O₃, TiO₂ and carbon materials) in order to increase the number of active Cobalt metal sites.^{1,2} Thus, a small amount of noble metals e.g. Pt, Re, Ru, Pd, Ir, Au and Ag is often added to Cobalt catalysts, since they can facilitate the reduction of Cobalt oxide and increase the number of active Cobalt metal sites, presumably by hydrogen dissociation and spillover from the promoter surface.^{3,4} Co-Zr/γ-Al₂O₃ catalyst was prepared by a wet impregnation method. The Cobalt loading was 14 wt.% on the catalyst. The catalyst was dried at 120 °C for 24 h and calcined at 400 °C for 3 h. The catalyst was characterized using XRD, H₂- TPR and BET techniques.The catalyst was pressed into pellet, crushed and sieved . Prepared catalyst was tested in a fixed bed reactor at FTS conditions: Temperature of 210°C, GHSV of 2 l.h⁻¹. gcat.⁻¹,H₂/CO ratio of 2, and pressure of 25 atm. CO conversion and product distribution calculated using results of Gas chromatography that it was shown in Figure 1.



Figure 1: CO conversion and product distribution of the catalyst

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Synthesis of A New Sensor Modified by Silver Nanoparticles to Measure Vitamin B₁₂ Using The Rayleigh Resonance Scattering Technique

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Abstract

Vitamin B_{12} is stored in the liver of people for one year and reduces the risk of developing low blood pressure. Vitamin B_{12} plays an important role in DNA production and also keeping your nerves and red blood cells healthy. Vitamin B_{12} can cure many diseases and problems.¹ This vitamin treat diseases and problems such as anemia dependent to deficiency of vitamin B_{12} , fatigue, alzheimer, heart disease, breast cancer, high blood cholesterol, and sickle cell disease. Low levels of vitamin B_{12} in the body can cause fatigue, loss of appetite, memory and other nervous problems in the body.¹

At first, the sensor is prepared and modified by silver nanoparticles during synthesis, then it was used to measure vitamins B_{12} using the Rayleigh Resonance Scattering technique.² Various factors affecting the construction of the sensor, such as pH, type of buffer, buffer volume, time, amount of nanoparticles, etc. are optimized.



Figure 1: Structure of Vitamin B₁₂.

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MCM-41@Fe₃O₄ Catalyzed N-Arylation of Sulfonamides

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Abstract

Amines are found in the structure of important pharmacologically active compounds, as well as biologically active for example neurotransmitters. Due to the high importance of amines, several methods have been developed for their synthesis such as the addition reaction of amine compounds.¹ Nowadays, numerous organic compounds such as amines were synthesized through the reaction between amid derivatives and imines which the use of immobilized catalysts on various solid supports with the advantage of catalyst separation and recyclization is one of the suitably developed strategies in recent years. Among the different types of used supports in heterogeneous catalysis, mesoporous silica MCM-41 on Fe₃O₄ has been employed as useful and versatile nanomagnetic catalyst.^{2,3}

The use of boron reagents **1** as a source of anyl through the exchange of anyl groups between boron and metal is one of the most commonly used methods for the anylation of aldehyde 4.

In this work, amine derivatives were synthesized by *N*-arylation of *p*-toluene sulfonamide **2** in the presence of a nanomagnetic catalyst (MCM-41@Fe₃O₄) in the optimum condition in excellent yields and short reaction time (Scheme 1).

The structure of the catalyst was identified *via* SEM, EDAX, TGA and, FT-IR techniques, and the prepared products were characterized by melting point and IR, ¹HNMR, and ¹³CNMR spectral analysis.



Scheme 1: Synthesize of amine by N-arylation of p-toluenesulfonamide

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Synthesis and Optimization of Nitration Process of 2-Ethylhexyl Nitrate Using Central Composite Design of Experiment

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Abstract

2-Ethylhexyl nitrate (2-EHN) is an energetic additive used to increase the cetane number of diesel fuels, usually prepared by nitration of 2-ethylhexanol (2-EH).^{1,2} Many energetic material syntheses, such as nitration of alcohols, despite the simplicity of reaction routes, involve fast and highly exothermic liquid-liquid reaction process and have explosive potential. Also, they can easily volatilize and undergo a self-sustaining decomposition with an intensive heat release.³

In this research, a safe preparation of 2-EHN was investigated exprimentally by nitration of 2-EH in the mixed sulfuric-nitric acid nitration agent, and some important factors affecting on the performance and efficiency of the process have been modeled, analyzed and optimized using central composite design (CCD) of experiments by Minitab 16 software, to evaluate and demonstrate the characteristic of the nitration process of 2-EH alcohol. In addition, the required qualitative and quantitative analyses such as high performance liquid chromatography (HPLC), gas chromatography (GC), density, carbon-13 nuclear magnetic resonance spectroscopy (13C NMR), hydrogen nuclear magnetic resonance spectroscopy (1H NMR), and Fourier transform infrared spectroscopy (FTIR) were used for the evaluation of the quality of the product. Obtained results showed that four main factors affect on the yield independently are as follows; the nitration temperature, the amount of water in the mixed acid, the amount of nitric acid in the mentioned mixed acid and the reaction aging time. Practical studies and statistical analyses show a very good agreement between presented model and experimental data, and the reaction conditions were optimized.



Scheme 1: Proposed nitration mechanism of 2-EHN



Figure 1: Effect of nitric acid and reaction time on yield of 2-EHN

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Controlling of Polymorphs of Solid Cyclotetramethylene-Tetranitramine from α to β type in Nitration Process of Hexamine and DPT

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Abstract

1, 3, 5, 7-Tetranitro-1, 3, 5, 7-tetraazacyclooctane commonly known as Octogen or HMX (high melting explosive) is the most powerful military explosive in current military applications.¹ HMX explosive has four different crystalline polymorphs of α , β , γ , and $\delta \Box$ with orthorhombic, monoclinic, monoclinic, and hexagonal crystal lattice system, respectively. It is generally agreed that the friction and impact sensitivities are $\delta > \gamma > \alpha > \beta$, but it is dependent on the size and morphology of crystals.²

In the synthesis of hexamethylenetetranitramine (HMX) energetic material by nitration of hexamine in anhydride acetic-ammonium nitrate-nitric acid nitration system, the morphology of crude HMX products are needle-like with alpha polymorph. This crude product of α -HMX is very sensitive and unsafe relative to $\Box\beta$ -HMX. Here, a seeding strategy was developed in the synthesis process of HMX high explosive by hexamine and 1,5-dinitroendomethylene-1,3,5,7-tetraazacyclooctane (DPT) raw materials, to control the polymorphism of the crude products from $\alpha\Box$ to β type, and their morphology from needle-like to spherical shape. Therefore, the microparticles of β -HMX, as micro-seeds, were added to the nitrator in the various steps of products were characterized using X-ray diffraction spectroscopy (X-ray) and optical microscopy. The results show that this interesting technique can control the polymorph and structure of crude HMX from α to β type, and it improves the safety of crude product and its filtration time.



Figure 1. Optical microscopy and XRD of alpha (top) and Beta-HMX (bottom)

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Application of Response Surface Methodology for Optimization of MIL-(101)Cr by **Ultrasound and Traditional Methods**

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Abstract

This paper reports MIL101-Cr was synthesis with Cr (NO₃)₃.9H₂O and PTA (1, 4- benzenedicarboxylates) as an organic agent. MIL-101 is a kind of Metal organic frameworks (MOFs) crystal porous Material with high specific surface area, porous structure and adjustable pore size.1-3 Interactions between the three effective factors for the optimization process of MIL-101(Cr) were investigated using the CCD tab of the Design Expert Software. The factors were reaction time (A), temperature (B), and reaction vessel.

In this work the morphology and pore structure of the as-prepared product were systematically discussed through N₂ adsorption-desorption analysis and Scanning electron microscopy (SEM). The N₂ adsorptiondesorption analysis show that MIL101-Cr possessed microspore. The synthesized MIL-101(Cr) had surface area of 1035 m²/gr and total pore volume of 0.542 cm³/gr which are comparable to the one conventionally prepared with analytically pure Cr (III). SEM images shows that the MIL101(Cr) crystals are regular shaped octahedrons. And its thermal stability performance was measured by thermogravimetric(TG), the heating temperature is too high, the material structure easily damaged, MIL101(Cr) has the highest adsorption performance after activation at 420 °C.

In addition, the experiment studied the optimal activation temperature, MIL101(Cr) has the highest adsorption performance after activation at 420 °C.The steps of experimental synthesis are shown in Scheme 1.



Scheme 1: The steps of experimental synthesis

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Application of Response Surface Methodology for Optimization of MIL-(53)AI by Ultrasound and Traditional Methods

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Abstract

MIL-53(AI), as a typical metal organic framework (MOF) has been synthesized by conventional electric (CE) heating and by ultrasound (UTS) to develop rapid and energy efficient alternative synthesis techniques.¹⁻³ In order to optimize the synthesis of MIL-53(AI) a statistical approach using a two-level, multi-factorial design was utilized. Design-Expert 7.1.5 software (StatEase, Minneapolis, USA) was used to investigate the effect of each reaction parameter on the crystallinity and yield of synthesized samples.

MIL-53(Al) materials were prepared by, a clear solution of terephthalic acid (H₂BDC) and a double molar amount of NaOH was added over another clear solution of Al(NO₃)₃, under stirring at room temperature. The solution was then transferred either to a round bottom flask connected to a condenser or to a seald pressurized glass vessel and heated for a specific time (i.e. 2 or 15h) at a predetermind temperature (i.e. 100 or 150 °C) according to the experimental design. For UTS irradiation, 10 mL of the reaction mixture was added to a vial which was placed in the probe of an ultrasonic generator. These experiment were performed at a predetermined time (i.e. 10 or 30 min.), temperature (i.e. 20 or 60 °C) and power (60% of maximum power). Highly crystalline materials were synthesized in 15 min from UTS irradiation. The product yields from UTS irradiation were observed to be less than those obtained from CE heating.



Scheme 1: Schematic illustration for the synthesis of MIL-53(Al).

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Synthesis and Characterization of a Novel Multi-Functionalized Nanomaterial Hybrid from Graphene Oxide

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Abstract

Recently, diverse methods have been established to design drug delivery systems. A wide variety of drug delivery systems such as nanoparticles, micelles, dendrimers, biopolymers have been established to afford targeted drug delivery carriers.¹ Graphene oxide (GO) is used as a carrier due to the high loading capacity of anticancer drugs through non-covalent forces and due to the release of the drug.² Dopamine (DA) receptors are over expressed on certain cancer cells.³ Thus dopamine functionalized graphene oxide can be used to specifically target cancer cells. Gold nanoparticles conjugated with antibodies are being developed as photothermal therapy agents that are used to kill cancer cells.⁴ pH-sensitivity of carrier is very important feature for cancer therapy which leads to reduced injury on healthy tissues.⁵ In continuation of our interest on the application of graphene oxide⁶ and its derivatives,⁷ in this work, we present a nanomaterial hybrid carrier (GO/DA/Au) which was prepared with targeted dopamine and gold on the surface of graphene oxide. Then, doxorubicin was used as a model antitumor drug and was encapsulated in the GO/DA/Au material to give a novel multi-functionalized GO/DA/Au/DOX nanomaterial hybrid. The GO/DA/Au and GO/DA/Au/DOX nanomaterial hybrid were fully characterized with Fourier transform

infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray (EDS), X-ray diffraction (XRD), transmission electron microscopy (TEM) and UV-vis absorption(Scheme1). Drug release behavior of this multi-functionalized nanomaterial hybrid was investigated under various pH. It was found that the rate of drug release from the nanomaterial hybrid depended on the pH of the solution.



Scheme 1: Structure of GO/DA/Au/DOX nanomaterial hybrid

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Synthesis and Thermal Analysis Study of Some Ionic Liquids with Diverse Counter Ions

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Abstract

lonic liquids are the compounds that have caused revolution in research institution and chemical industries. These compounds which are among green chemical materials as a solvent, have a significant role in redusing the using poisonous, baneful and risky compounds that damage the environment.¹ Ionic liquids can substitute many regular solvents in pharmaceutical industry. Todey ionic liquids are used for organic compounds which are formed from iones and its melting point below the boiling point of water.² In this research *N*-methyl imidazolium chloride (1) is used as a starting material for the synthesis of ionic liquids (2) and is shown in Scheme 1. Also in this work, the thermal degradation of compounds 2 have been probed with TG and DTA techniques (Fig1).



Scheme 1. Synthesis of ionic liquids 2.



Figure 1: TG thermograms of 2.

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NMR Investigation of Tautomeric Populations of Water Clustered 3-aryl-7-thioxo-7,8-dihydro-6*H*-pyrimido[4,5-*c*]pyridazine-5-ones

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Abstract

The importance of fused pyrimidines such as pyrimido[4,5-*c*]pyridazine-5,7(6*H*,8*H*)-diones, which are common sources for the development of new potential therapeutic agents, is well-known.¹ Some of this class of compounds plays new heterocyclizations based on S_N^H -methodology as $N_{(2)}$ -oxide and 3-alkylamino derivatives of 6,8-dimethylpyrimido[4,5-*c*]pyridazine-5,7(6*H*,8*H*)-dione.²

Herein, we have reported dynamic NMR investigation of tautomeric populations of water clustered 3-aryl-7-thioxo-7,8-dihydro-6H-pyrimido[4,5-c]pyridazine-5-ones (X.H₂O) at room temperature.



Figure 1: Formula structures and intermolecular hydrogen bond of **1a-g** with water protons assigned by H_b (b= bonding) and H_f (f = free)

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Synthesis of Dibenzyl Carbonotrithioate Derivatives Using Nano Composite (C3N4-LiOH)

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An efficient and straightforward method for synthesis of biologically active dibenzyl carbonotrithioate derivatives by the addition reaction of Benzyl chloride, CS₂ in the presence of nano composite (C3N4-LiOH) has developed. Using a magnetically recoverable acidic ionic catalyst allows eco-friendly and facile conversion and simplifies experimental setup and work-up procedure that enables the direct synthesis of dibenzyl carbonotrithioate derivatives under mild conditions. The designed catalytic system provides a broader scope under short reaction times in good to excellent yields. C3N4-LiOH could be simply recovered by magnetic separation using an external magnet, maintaining stable activity up to five cycles without appreciable loss of activity.



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Synthesis and Characterization of New Precursors for B-C-N Ceramics

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Abstract

Borazine $(B_3N_3H_6)$ is a very stable molecule under an inert atmosphere and called inorganic benzene because its structure consists of six elements with alternating boron and nitrogen atoms. The compound 2,4,6-tri-chloroborazine (TCB) **1** is known as a valuable precursor to prepare various derivatives of borazine and was synthesized using a modified and facilitated route in our laboratory.¹ Two new derivatives of borazine, the compounds 2,4,6-tri(phenylalkynyl)borazine **2** and 2,4,6-tris[2,3,5,6-tetramethylphenylalkynyl]borazine **3** were synthesized via the reaction of the Grignard reagent with TCB (Scheme 1). Tri(arylalkynyl)borazines **2** and **3** were characterized via ¹¹B-, ¹H- and ¹³C-NMR spectroscopy.



Scheme 1: Synthesis procedure for preparation of new tri(arylalkyl)borazines

These new borazine derivatives containing unsaturated groups can be considered as effective precursors for the preparation of boron carbonitride (BCN) in various structures including ceramic fibers, composite ceramics and coatings. In another word, the pyrolysis of these molecules under an inert atmosphere could provides an alternative route to B-C-N ceramics.² The relationship between the molecular structure and composition of the pyrolytic product is now being studied in our laboratory.

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Synthesis and Characterization of a Novel Ferrocene Based bis-Schiff-base

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Abstract

Since the discovery of ferrocene in 1951, ferrocene and its derivatives have attracted the attention of many researchers for use in various applications such as materials science, bio-organometallic chemistry, nonlinear optics, asymmetric catalysis, polymer science as redox-active polymers, electrochemistry, corrosion inhibition and molecular recognition as biosensors.¹ Schiff-bases are classical ligands for metal ions of p, d, and f blocks, which have significantly contributed to the development of coordination chemistry on both basic and applicative aspects, with a special reference to catalysis.² The chemistry of hydrazone-type Schiff-base compounds has gained intense attention due to their unique coordination and structural properties and various biological applications.³

The reaction between ferrocenecarboxaldehyd **1** and hydrazine (H₂N-NH₂) resulted in the formation of ferrocenyl hydrazone **2**. The Synthesis of Schiff-base **2** was confirmed by the disappearance of the aldehyde proton peak and also observation of two singlets at δ =7.48 and 6.21 ppm related to <u>H</u>C=N and N<u>H</u>₂, respectively in the ¹H-NMR spectrum.

The condensation reaction of compound **2** with1,4-benzenedicarboxaldehyde in a mole ratio of 2:1 led to the synthesis of a new bis-Schiff-base **3** (Scheme 1), which can be used as an attractive novel Schiff-base ligand to synthesis of new metal complexes and investigation of their properties and applications. In the ¹H-NMR spectrum of the new Schiff base **3**, there is no trace of the peak related to the NH₂. The peak of HC=N was observed at δ =8.67 ppm. Furthermore, the spectrum indicated a singlet for two identical Cp-H₅ rings at δ =4.30 ppm. Two other singlets were observed at δ =4.55 and 4.80 ppm attributed to the two kind of Cp-H₂ due to their different chemical environment.



Scheme 1: Synthesis of a novel ferrocene based bis-Schiff-base 3

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An Environmentally Friendly Method for Acetylation of Alcohols, Catalyzed by I₂ Generated in situ Using Fe(NO₃)₃·9 H₂O/Nal Under Neutral Condition

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Abstract

Esterification is a key and fundamental step to protect the hydroxyl groups during functional transformation in various organic synthesis.¹⁻³ So acetylation is one of the most essential transformations in organic syntheses. The acetylation of alcohols using ethyl acetate as an acetyl surrogate is intriguing despite its low electrophilicity. However, the use of ethyl acetate in the place of commonly used acetic anhydride can be complicated by reversible trans-esterii.cation⁴

Molecular iodine is a versatile reagent in organic synthesis ⁵, it is corrosive and toxic, making its use somewhat unattractive. To overcome these disadvantages with molecular iodine, we wish to describe a new procedure for acetylation of a wide variety of alcohols using ethyl acetate in the presence of I_2 generated in situ from Fe(NO₃)₃.9H₂O/Nal (Scheme 1). It should be mentioned that molecular iodine is generated in situ by oxidation of Nal using Fe(NO₃)₃.9H₂O.

$$R-OH \xrightarrow{Fe(NO_3)_3.9H_2O/Nal} \longrightarrow R-OAc$$
AcOEt, Reflux

Scheme 1

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Application of 1-(2-bromoethyl)-4-hydrogen-1,4-diazobicyclo-[2,2,2] octane bromide (BEDABCO-Br) for Synthesis of Alkyl Thiocyanate Under Solvent Free Condition

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Abstract

Alkyl thiocyanates are important synthetic precursors for preparation of the sulfur-containing organic compounds. Also, organic thiocyanates have been used extensively in synthetic organic chemistry, with a wide range of applications, particularly in biological and heterocyclic chemistry.¹⁻² Alkyl thiocyanates are generally prepared via nucleophilic displacement of leaving groups attached to C by thiocyanateion.³ In view of the versatility of thiocyanate group in the field of drugs and pharmaceuticals, the development of simple, convenient, and highly efficient approaches are desirable.

During recent decades, a wide range of synthetic methods have been developed for the construction of organic compounds and synthetic intermediates using Br_2 . In recent years, researchers tried to use tribromide-containing compounds instead of Br_2 to decrease the toxicity of molecular bromine. ⁴⁻⁵

Here, we report new and efficient solvent free procedure for the one-pot preparation of alkyl thiocyanates using 1-(2-bromoethyl)-4-hydrogen-1,4-diazobicyclo-[2,2,2] octane bromide (BEDABCO-Br) as catalyst (Scheme 1).

Scheme 1

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Computational Evaluation of Phagraphene Efficiency for Detection of Some Air Pollutants

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Abstract

The tracing of dangerous gases is very significant matter due to enhancing contamination in the environment and therefore gas sensing is very necessary technology in various industries.^{1,2} In order to explore the sensing capacity of Ga-doped phagraphene for some toxic gas molecules, interaction of NO, NO₂, NH₃, SO₂ and SO₃ molecules with Ga-doped phagraphene was investigated using density functional theory calculations in terms of HOMO level of energy, LUMO level of energy, HOMO-LUMO energy gap, adsorption energy, HOMO-LUMO energy alteration, gas/Ga-doped phagraphene charge transfer, Fermi level of energy, work function, work function alteration, molecular electrostatic potential profile and density of state plot. It was found that Ga-doped phagraphene can effectively interact with the NO and NH₃ molecules despite of NO₂, SO₂ and SO₃ molecules, so that their work functions are considerably changed upon exposure to these molecule. So, it can be said that doping the phagraphene with Ga atom may be a suitable strategy for designing appropriate sensors for detection of NO and NH₃ toxic molecules.



Figure 1: NO (left) and NH₃ (right) molecules adsorption on the Ga-doped phagraphene.

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Theoretical Assessment of Aminated C20 Fullerene in Identifying of A-234 Nerve Agent

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Abstract

The organophosphorus compounds are one of the main menaces to mankind, because of their capability to prevent the acetylcholinesterase enzyme action, which has an important role in the nervous system transmissions.^{1,2} The In this study, we investigated the interaction of A-234 molecule with the pristine, Si, Ge, Sc doped and aminated C20 fullerene using density functional theory (DFT). Adsorption of A-234 molecule on pristine C20 fullerene provides insufficient adsorption energy (-5.27 kcal.mol⁻¹) which makes it unsuitable sensor platform for detection of this molecule. When A-234 molecule is adsorbed on Si, Ge and Sc doped fullerene, the work function (Φ) alters properly (-18.78%, -25.69% and -70.43%, respectively). However, adsorption energies are very high (-104.16, -96.19 and -76.05 kcal.mol-1, respectively). In contrast, when a A-234 molecule is adsorbed from its P]O head on the C20HNH2 (aminated) fullerene, its work function is considerably decreased (-12.20%) demonstrating a appropriate sensitivity and the adsorption energy (-13.55 kcal.mol⁻¹) is small enough to provide short recovery time. In addition, the electron emission greatly increases which can be converted to an electronic noise and thus, C₂₀HNH₂ fullerene is a work function-type sensor for sensing and detection of A-234 nerve agent.



Figure 1: A-234 adsorption on the aminated A-234 C20 fullerene.

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A Ratiometric Fluorescent Sensor Based Azo Compound of 4-(dimethylamino)phenyldiazenyl-N-Arylbenzamide for Selective Detection of Ions

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Abstract

Recognition of metals has received much attention because of their undeniable role in biological and environmental processes.¹ In this regard, the design of sensors that are able to detect these metals is very valuable.² Azo compounds have been introduced as one of the valuable compounds for designing metal detection sensors due to their easy synthesis and color recognition.

New colorimetric and ratiometric azo dyes compounds 4-(dimethylaminophenyl)diazenyl)-N-(pyridin-2-4-(dimethylaminophenyl)diazenyl)-N-phenylbenzamide) yl)benzamide and were prepared and characterized. The optical sensing properties of the ligand toward different cations were studied by UV-Vis, fluorescence, and NMR methods. While, the synthesized compounds of 4-(dimethylaminophenyl)diazenyl)-N-(pyridin-2-yl)benzamide can acted selective sensor for Fe³⁺ as а ion, the 4-(dimethylaminophenyl)diazenyl)-N-phenylbenzamide compound demonstrated colorimetric sensing toward Hg²⁺, Cu²⁺, Fe³⁺ ion.



(E)-4-((4-(dimethylamino)phenyl)diazenyl)-N-(pyridin-2-yl)benzamide



(E)-4-((4-(dimethylamino)phenyl)diazenyl)-N-phenylbenzamide

Scheme 1: Structure of two sensors

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Environmental-Friendly Synthesis of α , β -Unsaturated Isoxazol-5(4H)-ones Under Aqueous Medium

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Abstract

The isoxazol-5(4H)-one, also called isoxazolone, ring systems represent important molecular structures, which have been employed as the precursors in the synthesis of interesting organic molecules.¹ They have been known to show antibacterial, antifungal, tyrosinase inhibitory, anticancer, anti-obesity, anti-androgen and insecticides activities.²

Also, the isoxazol5(4*H*)-one play an important role in the organic synthetic chemistry. Therefore, organic chemists are interested in the synthesis of such heterocycles in recent years. One of the most attractive methods of obtaining isoxazol-5(4*H*)-ones is the cyclocondensation of hydroxylamine hydrochloride with β -ketoesters and various aldehydes in the presence of various types of catalysts.³⁻⁶

Humic acid is a high-molecular weight polymer that is primarily derived from biodegradation of dead organic matter and appears mostly in peat, soil, coal, upland streams, dystrophic lakes and well water. Because humic acid is nontoxic, inexpensive and easily available, the study of its catalytic activity may be very important. Humic acid is an acidic catalyst owing to the presence of abundant carboxyl and phenolic hydroxyl groups in the structure of it. There are only very few reports in which catalytic activity of humic acid has been described.^{7,8} In view of the efforts toward development of the potential of humic acid as a catalyst, herein, we report an efficient one pot three-component synthesis of α,β -unsaturated isoxazol-5(4*H*)ones (**1a**–**j**) from less expensive and easily available starting material aldehydes along with hydroxylamine hydrochloride and β -ketoesters (Scheme 1).



Scheme 1.

The advantages of this work are clean, cost-effectiveness, easy work-up, high yields, environmental-friendly and the use of water as environmentally benign solvent.

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Humic Acid: A Catalyst From the Heart of Nature for The Synthesis of Benzochromeno-Pyrazole Derivatives

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Abstract

Green chemistry is a new field of chemistry with the goal of developing new eco-friendly and efficient procedures for the synthesis of chemicals by minimizing the waste and byproducts, using renewable resources, applying green solvents or solvent-less procedures etc.¹

In the last two decades, multicomponent reactions (MCR) have drawn special attention due to the advent of high-throughput screening techniques that enabled rapid identification of potential new medicines among large collections of organic compounds. This required the development of new approaches to the synthesis of organic compounds. The methods that would provide rapid access to high-quality compound libraries came to be in high demand. Multicomponent reactions ideally suited the new demand, and this, in turn, fueled more interest in the earlier developed reactions and in the invention of similar or even fundamentally new ones. In different reports, the potential benefits of MCR chemistry have been completely proved.²⁻³ Chromene compounds occupy an important place in the realm 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.⁴ Chromenopyrazoles are known to exhibit interesting biological properties.⁵ Some procedure for the synthesis of chromeno-pyrazole derivatives have been reported already: Abunada et al.⁶ studied synthesis of chromeno[3,4-c]pyrazole derivatives from hydrazonoyl bromides and substituted coumarins. Heravi et al.⁷ reported one-pot synthesis of benzochromeno- catalyzed by sulfamic acid. In this work, onepot synthesis of different benzochromeno-pyrazole derivatives has been reported via the condensation reaction of aldehydes, 3-methyl-1H-pyrazol-5(4H)-one and α -naphthol/ β -naphthol in the presence of humic acid. (Scheme1)



Scheme1. Humic acid as efficient catalyst has a good performance in the synthesis of benzochromeno-pyrazole derivatives.

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Using Ionic Liquid as Catalysts in the Process of Ester Oil Synthesis and Its Application in the Preparation of Metal Working Fluids

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Abstract

Metalworking fluids are used in metal removal processes such as cutting and grinding and in metal forming processes such as drawing, rolling, and stamping. Also, Metalworking fluids are used as a coolant to reduce the heat generated by the process.¹ Bio metalworking fluid (high degradability, optimal lubrication, high viscosity index, and oxidation stability could be mentioned as advantages of bio metalworking) is introduced as an alternative to petroleum products of metalworking.^{2,3} These fluids can be prepare from synthetic esters which include fatty esters. Fatty acid esters are prepared by the reaction of fatty acids with alcohol in the presence of an acidic catalyst.^{4,5} In this study, ionic liquids are used as solvents and catalysts in esterification processes and the obtained esters are used as a raw material in the bio metalworking fluids producing process.



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Preparation of SBA-16 / ZnO Nanocomposite and Kinetic Study of Temozolamide Adsorption on it

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Abstract

In this study, the adsorption kinetics of temozolomide on SBA-16 / ZnO nanocomposite as a drug carrier was investigated. For this purpose, in the first step, the SBA-16 mesostructured was synthesized using pluronic f127 as a structural determinant. XRD, SEM and FT-IR analyses were prepared from the synthesis samples. After mesopore correctness was confirmed, it was loaded on SBA-16 using in situ method with ZnO and acetate salt on two surfaces. The nanocomposite was prepared again from XRD, SEM and FT-IR analyses. Then the adsorption kinetics of temozolomide on the synthesized nanocomposite were investigated. In the second stage, using the test design software (DOE) by response surface methodology (RSM) and central composite model (CCD), the effect of parameters affecting the drug uptake process including pH, contact time, temperature, drug concentration and adsorbent dose were studied. And the optimal value for each parameter was obtained. Finally, to find the best kinetic model, two quasi-first-order and second-order quasi-second models were studied under optimal conditions and the results showed that the loading process of temozolomide on SBA-16 / ZnO nanocomposite is consistent with the second-order quasi-kinetic model.



Figure 1: Structure of the drug Temozolomide

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Synthesis of Oxazine Derivatives Under Mixed Metal Oxide Magnetic Nanocatalyst

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Abstract

In the present study, mixed metal oxide nanocatalyst have been explored as an efficient, cost-effective, and recyclable nanocatalyst for environmentally protocol and efficient synthesis of pharmaceutically interesting Naphtho [1,2-e] [1,3] Oxazine derivatives through a one-pot three-component condensation of aromatic aldehydes, β -naphthol and urea under green conditions in water solvent and short reaction time with excellent yields. The structure of products was approved by FT-IR, ¹H-NMR spectroscopy and melting point. The results of SEM imaging of nonacatalyst showed that all compounds have a spherical morphological structure with mean diameter of 16.50 ± 3.94. These nanoparticles are important in organic reaction with their ability to be easily separated and recycled by magnetic field.



Scheme 1: Structural formula for the synthesis of manganese oxide / iron oxide / zinc oxide nanocatalysts

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Surface Modification and Incorporating of Hyaluronic Acid with Organic Materials

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Abstract

Hyaluronic acid (HA) is a glycosaminoglycan (GAG) constituted with repeating units of a disaccharide that contains β -1,4-D-glucuronic acid and β -1,3-N-acetyl-D-glucosamine (figure 1). This study adhesive hyaluronic acid (HA) modified, decorated, incorporated with various carbon materials via a different functional group on the polysaccharide backbone with multiple anchoring mechanisms (amide bond through the dynamic Schiff base reaction, hydrogen bond, and physical interpenetration) .^{1,2} HA-based hybrid and surface modification exhibited significantly improved durability and stability within a humid environment. together with higher adhesive strength, as compared to other materials. The results of this review showed that HA-based hybrid and surface modification was biocompatible, nm in size, with improved stability, high drug encapsulation efficiency, low cytotoxicity and could be easily and rapidly prepared in situ and contain prominent application as well. The review article is mainly focused on clarify the recent advances on HA derived from the represented material which provides comprehensive knowledge about the various methods of preparing, advantages, and many applications in various fields such as bone tissue engineering and drug delivery systems, and so on.



Figure 1: Schematic illustration of Molecular structure of Hyaluronic acid and its incorporated with other material³.

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Synthesis of Fragrances by Polyoxometalate Catalysts Stabilized on Magnetic Iron Oxide Nanoparticles

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Abstract

Esterification of carboxylic acids is one of the basic reactions in organic chemistry that the rate of this reaction can be increased by increasing the acid catalyst to the reaction medium.

Tungsten phosphoric acid (TPA) stabilized on magnetic iron oxide nanoparticles used to ester carboxylic acids with alcohols to prepare aromatic Fragrances. The advantage of this method is the very easy separation of the catalyst from the reaction medium by the magnet. Polyoxometalate are used as catalysts of heteropolyacids fixed on a solid substrate, which gives the substrate a chance to heteropolyacid to spread over a wider surface. Acidic polyoxometalate and the stabilization of polyoxometalate such as phosphotangestic acid on a solid substrate, which is the same as iron oxide magnetic nanoparticles (Fe₃O₄), can be used as a heterogeneous catalyst for the synthesis of ester essential oils. By optimizing the temperature, time, the molar ratio of raw materials and the amount of catalyst, the best and highest efficiency for the synthesis of Fragrance in the esterification reaction was obtained.

In this research, firstly iron oxide magnetic nanoparticles were synthesized by thermal solvent method from iron (III) salt. further, with the fixation of polyoxometalate on iron oxide magnetic nanoparticles, a nanocatalist synthesized as a heterogeneous catalyst, capable of separation and reuse, to perform a esterification and synthesis reaction essences were used.

Initially, the catalytic role of polyoxometalate stabilized on iron oxide nanoparticles was investigated in the reaction of isoamyl alcohol with acetic acid, which resulted in the production of isoamyl acetate. The reaction of benzyl alcohol with acetic acid in the presence of a catalyst, which resulted in the production of benzyl acetate, was investigated. Some other esters or Fragrance that are similar to fruits are also studied.

The reaction of esterification under different conditions of temperature, time, raw material concentration and also the percentage of catalyst used was considered. After optimization, optimum temperature for reaction of 90°^c, optimum time in advance, reaction time of 2 hours and percentage of catalyst used In the reaction of esterification, 0.1 g was obtained.

RCOOH + R \circ \circ OH → RCOO R $^{-}$ + H₂O Scheme 1: esterification reaction

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Study of Noncovalent Interactions on Some of Phosphinophosphinidene Compounds

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Abstract

Noncovalent interactions have been studied in great detail through last century due to their importance in chemical and biological systems.¹ Recently, computations have revealed a new kind of interactions referred as pnicogen and chalcogen bonding.² They have attracted significant interest because of their wide applications in biology, supramolecular chemistry and crystal engineering. In 2020, a theoretical study on the pnicogen bonding in the binary and ternary complexes involving the substituted benzonitrile and PO₂F showed that the binary complexes had a medium strength interaction of pnicogen bonds toward the ternary complexes.³

In this paper, DFT calculation has determined that substitutions have dramatic effect on noncovalent interactions of studied phosphinophosphinidene compounds. Ab initio calculations have been carried out at B3LYP/6-311++G^{**} level with the Gaussian 09 pakage⁴ to investigate the bond interactions. The results showed that when the two groups, electron donating hydroxyl and electron withdrawing nitro ones, were placed in a complex, a powerful pnicogen bond was formed.



Scheme 1: Structure of the pnicogen bonding binary complex

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Energy Decomposition Analysis of the P...N Interactions in Some Phosphinidene Compounds

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Abstract

One of the newest members of the noncovalent interactions'family is the pnicogen bonding. ¹⁻² In this work, the nature of bonding interactions between P and N atoms (P...N) in some phosphinidene compounds have been studied via the energy decomposition analysis (EDA) based on the ETS-NOCV.

The focus of the EDA is the instantaneous interaction energy (ΔE_{int}) which is the energy difference between the molecule and the fragments with the frozen geometry of the complex. In this work the geometries of all compounds were fully optimized at the B3LYP/6-311++G** level of theory using the Gaussian 09 package.³ Also, Energy Decomposition Analysis (EDA) of P...N was performed using the program package ADF 2009.01 at BP86/TZ2P//B3LYP/6-311++G** level of theory with C₁ symmetry. ⁴ The interaction energy (ΔE_{int}) between two interacting fragments is divided into four steps, which can be interpreted as follows:

 $\Delta E_{int} = \Delta E_{elstat} + \Delta E_{pauli} + \Delta E_{orb} + \Delta E_{disp}$

The obtained results through EDA analysis show that main contribution in ΔE_{int} in phosphinidenes compounds studied here comes from ΔE_{orb} . Also, a comparison between the obtained results from above methods shows that the dispersion energy hasn't an important role in stabilization of all complexes studied in this work.

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Theoretical Study on the Noncovalent Interactions Between C₂₄ Small Fullerene and Isoniazid

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Abstract

The discovery of fullerenes has attracted considerable attention in the material science. After the experimental identification of C_{60} fullerene by Kroto et al. in 1985¹, many experimental and theoretical studies have been carried out on the structural and electronic properties of this fullerene and its derivatives.²⁻⁴ The C₂₄ fullerene is one member of the fullerenes smaller than C₆₀ which is studied in this paper. There have been some theoretical studies at different levels of theory on the structure and stability of the C₂₄ fullerene.⁵ In this work, the nature of interactions between the C atoms of the hexagonal and pentagonal rings in C₂₄ fullerene with H atoms of the Isoniazid were characterized using density functional theory (DFT) calculations. Therefore, three kinds of interactions between C₂₄ small fullerene and Isoniazid

were calculated. The geometries of all compounds were fully optimized at the B3LYP/SVP level of theory using the Gaussian 09 package. ⁶ Also in order to understand the nature of these interactions in these complexes, the Bader's theory of atoms in molecules (AIM) have been used. The data showed that the largest value of IE can be observed that when the H atoms of the Isoniazid interact with C atoms of the pentagonal ring in C₂₄ (Fig.1).



Fig. 1: optimized structure and selected bond lengths (A) of C24 and Isoniazid

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Production of Quinoline-2-ones with the Annulation of Ortho-heteroaryl Anilines and CO₂ in the Presence of FPS/[Cu(Bpy)₃]²⁺ Nano Catalyst

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Abstract

The transformation of CO₂ to beneficial organic chemicals as a research field has been highly investigated by scientists.^{1,2} CO₂ is known as a greenhouse gas emission and a waste compound in chemical industry and transportation sector as well as power plants.³ In addition, it is a non-toxin, non-flammable, inexpensive, and easily available carbon feedstock.⁴ However, CO₂ is not generally used in the industry because of its low reactivity. Carbon dioxide (CO₂) play a basic role as a sustainable feedstock during chemical synthesis. The considered approach should be moderated to be viable. Cu(II) trisbipyridine complex FPS/[Cu(Bpy)₃]²⁺supported over fibrous phosphosilicate (FPS) utilizing dipyridin ligands has been determined as highly valuable catalysts of cycloaddition of ortho-heteroaryl anilines with CO₂ during the synthesis of quinoline-2-ones (Scheme1). The mentioned materials possess various eco-friendly properties like high catalytic activity and easy to recovery from the reaction mixture using the method of filtration, and various reuse times without losing the efficiency.



Scheme 1 : Cycloaddition of ortho-heteroaryl anilines with CO2 at the attendance of FPS/[Cu(Bpy)3]²⁺

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Fe₃O₄/SiO₂/UiO-66/btb/Pd as a Stable Catalyst Reduction of 4-Nitrophenol Into 4-Aminophenol

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Abstract

In different industries, 4-aminophenol has been introduced as a significant chemical known as an intermediate for the pharmaceutical and dye industries and developer in the photography industry.¹ For instance, 4-aminophenol can be used as an intermediate for synthesizing paracetamol known as a medication utilized worldwide (in essential lists of the World Health Organization and also in the manufacture of azo dyes and sulfur shown to have significant applicability in the alimentary, textile and leather industries.^{2,3} sodium borohydride is used in The chemical reduction of 4-nitrophenol to 4-aminophenol considered as a model reaction to metal NPs (nanoparticles) because of its wellknown kinetics along with associated color changes.⁴ In order to synthesis 4-aminophenol, there are two different approaches including the nitrobenzene hydrogenation or the nitration of phenol that occurred commonly after the chemical reduction of the obtaining 4-nitrophenol using sodium borohydride. In addition, other different reducing agents like hydrazine were previously used.^{5,6} In order to synthesize highly sparse nanoparticles, Fe₃O₄/SiO₂/UiO-66-NH₂ can be utilized as appropriate support. It has great surface area, which is functionalized by 1,3bis(dimethylthiocarbamoyloxy)benzene compounds that can act as powerful performers, hence, the Pd (II) is a complex without aggregate over the Fe₃O₄/SiO₂/UiO-66-NH₂microspheres structures. Nitro-aromatic pollution in industrial waste streams threatens the wellbeing of water resources. The produced Fe₃O₄/SiO₂/UiO-66/btb/Pd nanocatalyst showed appropriate catalytic activity for reducing nitro-aromatic compounds in an aqueous solution (Scheme 1).



Scheme 1: Schematic illustration of the synthesize for Fe₃O₄/SiO₂/UiO-66/btb/Pd (II)

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A New Fluorescent Sensor Based on 5-(4-Dimethylamino-phenylazo)-isophthalic acid

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Abstract

Nowadays, recognition of metal cations due to their importance in biological processes as well as their role in the environment, have received much attention.¹ In this regard, the design and synthesis of colorimetric sensors that have the ability to detect metal cations by simple methods and especially by the naked eyes compared to expensive methods such as atomic absorption spectroscopy and inductively coupled plasma mass spectrometry, has been considered by researchers.²

An important group of organic compounds are azo dyes, which in addition to widespread applications in various fields such as liquid crystals, polymers, antibacterials and antivirals and lasers, as one of the important compounds in the synthesis of sensors to detect metal ions are used.^{3,4} These compounds have received a lot of attention due to their easy and inexpensive synthesis method and their color recognition. Due to the importance of metal detection, new sensors based on azo compounds were successfully synthesized and then their ability for detection of different metal ions were investigated.



Figure 1: Route of synthesis of sensors

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A Novel Fluorescent Sensor Based on 4-(4-Dimethylamino-phenylazo)-benzoic acid (dabcyl acid)

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Abstract

In recent years, metal cations have received a great deal of attention due to their influential role in biological systems and the environment, which has increased the importance of accurate identification and detection of them.¹ In this regard, the fluorescence method for detecting of metal ions, due to its outstanding advantages such as simplicity, cost-effectiveness, noninvasive property, high response speed, high sensitivity and selectivity has attracted the attention of many scientists.²

Recently, azo compounds have been considered as one of the suitable candidates for fluorescence sensors due to their color recognition with the naked eye as well as easy and fast synthesis method. These compounds, as the most important class of color compounds in industries, have a wide range of applications in various fields, including dyeing of textile fibers, pigments.^{3,4}

In this regard, due to the great importance of detection of cation ions, in this work, a novel colorimetric and fluorescence ligand based on azo compounds was successfully synthesized (Figure 1), which in particular have the ability to detect metal ions, and was characterized by IR, UV-Vis.



Figure 1: Route of synthesis of ligand

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Preparation of Nickel and Cobalt Ferrite Nanocomposites Based on Graphene Oxide for Solar Cells

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Abstract

Electricity supply causes serious problems in the environment. Energy and the environment are the most important challenges for the continuation of civilization. Among renewable energies, solar energy is the most promising source of energy to change the flow. Due to the properties of graphene oxide and metal nanocomposites (such as nickel, cobalt and iron) such as high mobility of charge carriers, good transparency, high electrical conductivity, flexibility and light weight, this material is suitable for use in cathodes and anodes. Solar panels are suitable. To prepare nickel and cobalt ferrite composites based on graphene oxide. Graphene oxide was first synthesized by modified Hummer method. Nickel and cobalt ferrite composites were prepared by co-precipitation method and placed in a furnace for calcination Then dispersed in ethyl alcohol and mixed with 2: 1: 4 ratios of 6-aqueous nickel nitrate and 6-aqueous cobalt nitrate and urea and transferred to an autoclave for 4 hours at 120 ° C. The resulting composite was washed and dried in vacuo. The nanocomposites were detected by X-ray diffraction and CV curves were plotted for them, and good oxidation and reduction were observed for them.



Figure 1: Schematic diagram of a solar cell

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Preparation of High Strength, Anti-Corrosion and Water-Resistant Coatings for Industrial Use

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Abstract

The new nanoparticle-based coatings have found a variety of applications, including protection against corrosion, light, retrofitting, wear and swelling. The aim of this research is to prepare graphene composite coatings to prevent corrosion of steel metal. For this purpose, graphene oxide was synthesized by Hammer method. First, graphene oxide (GO) and nickel chloride (NiCl₂.6H₂O) and cobalt chloride (CoCl₂.6H₂O) separately in proportions (1: 5: 5) Dissolved in deionized water and sonicated and the three solutions mixed together and refluxed for one hour and precipitated by soda. The precipitate was collected and dried. The work electrode used was made of steel metal and after degreasing, a spin coating machine was used to achieve a coating with uniform distribution throughout the electrode. To evaluate the corrosion resistance of the composite, first the strength of each component, namely the uncoated steel electrode, the electrode coated with epoxy resin only, nickel hydroxide, cobalt hydroxide, graphene oxide and finally the steel electrode coated with The prepared graphene composite was investigated. TOEFL polarization technique was used to evaluate corrosion. The application of nanocomposites in the preparation of coatings decreases with the change of cathodic and anodic slope and corrosion potential, flow and corrosion rate and finally corrosion resistance increases.



Figure 1: Schematic of anode and cathode reactions in the presence of graphene

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Magnetic Nanoparticles ZSM–5 as a Novel Mesoporous Catalyst for the Synthesis of α -Carbamato-alkyl- β -naphthols

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Abstract

H-ZSM-5 zeolites have been considered more attention in chemistry, due to their exclusive properties such as channel structure, thermal stability, shape-selective property, flexibility in tailor-making and physical-chemical performance.¹

After the first report of ZSM-5,² various investigations have been conducted on ZSM-5 as a catalyst. These catalysts have been obtained by encapsulation or exchanged different materials inside the crystalline walls of H-ZSM-5.³

In this study, we prepared Magnetic nanoparticles ZSM–5 (MNPs/ZSM–5) by hydrothermal method. In this method, Fe₃O₄-MNPs was doped directly into the pores nanozeolite (ZSM-5).

The structure of MNPs/ZSM–5 was confirmed by FT-IR, XRD, EDX, VSM, TEM, and N₂ adsorption/desorption techniques. In continuation, we used Fe₃O₄ MNPs/ZSM–5 for the synthesis of α -carbamato-alkyl- β -naphthols *via* a three-component reaction of β -naphthol, carbamates and aromatic aldehydes under solvent-free conditions at 100 °C (Scheme 1).



Scheme 1: Synthesis of α-carbamato-alkyl-β-naphthols using Fe₃O₄-ZSM–5 as a catalyst

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New Bis-SO₃H-functionalized Ionic Liquid: A Green Catalyst for Synthesis of β -Acetamido Ketones

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Abstract

Green chemistry is the original priority in organic synthesis. In this regard, ionic liquids have been used generally in organic chemistry; because they have insignificant vapor pressure and non-flammable nature.¹ The ionic liquids (ILs) have been used as catalysts and solvents in organic chemistry.² Among various lonic liquids (ILs), SO₃H-functionalized ILs, have attracted increasing interest in organic synthesis.³

in continuation of our researches with environmental synthetic methodologies, using green catalysts and ionic liquids⁴, herein we focused our notice on a simple, practical, and facial method for preparation of novel bis-SO₃H-functionalized ILs. In this work, 1,4-bis(4-sulfobutyl)piperaziniumbis(trifluoracetic acid)([(BS)₂pi][TFA]₂) was synthesized by easy and green procedure,(Scheme 1) for the first time and characterized with ¹HNMR, and FT-IR Spectroscopy.





For investigation of catalytic activity of $[(BS)_2pi][TFA]_2$, we applied this novel ionic liquid for the synthesis of β -acetamido ketones *via* a three-component reaction of aromatic aldehydes, acetamide, and dimedone under solvent-free conditions (Scheme 2).



Scheme 2: Synthesis of β -acetamido ketones using of [(BS)₂pi][TFA]₂ as a novel ionic liquid

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Microcellular Polyurethane Foam/ Nanoencapsulated Stearic Acid@SiO₂ as A Thermal Energy Storage Nanocomposite, Preparation and Characterization

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Abstract

Microcellular polyurethane foam (MPUF) provides many superior properties such as high thermal reliability, noise and vibration insulation, shock absorption, low thermal conductivity, light weight, high energy absorption, high fatigue life and high toughness in comparison with conventional foams, by having high cell density as well as small cell sizes.¹

Incorporating functional materials in MPUF matric leads to designing high performance nanocomposites. Phase change materials (PCMs) play a vital role in the subject of thermal energy storage which have high latent heat values.² Micoencapsulated and nanoencapsulated PCMs are attractive materials have been widely used in many fields like waste solar energy storage, food conservation, medical therapy, thermoregulated textile, packaging and buildings.³

This paper focuses on preparation and characterization of novel MPUF nanocomposite incorporated with nanoencapsulated Stearic acid with SiO₂ shell (SA@SiO₂) as PCM. The objective of this research was to develop a nanocomposite having thermal insulation characteristic coupled with thermal regulation properties. Nanoencapsulated SA@SiO₂ was synthesized *via* sol-gel process.⁴ Figure 1. According to FE-SEM images, nanocapsules had spherical shape with nano size mean diameter of about 500 nm. MPUF nanocomposite sheet samples loadings different percentage of nanoencapsulated SA@SiO₂ were prepared and characterized by FT-IR, TGA, DSC and FE-SEM. The DSC results for MPUF/SA@SiO₂ nanocomposite with the highest content of nanocapsules indicated that the thermal conductivity of new designed nanocomposite was improved.



Figure 1: Formation of the nanoencapsulated SA@SiO₂.

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Fabrication and Characterization of a High Performance Membrane Based on Sulfonated Polystyrene Modification with MIL-53(AI)-NH₂

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Abstract

In this study, we prepared a novel proton exchanger membrane based on sulfonated polystyrene modification with MIL-53(AI)-NH₂ for application in direct methanol fuel cell. In these membranes, different amount of MIL-53(AI)-NH₂ were used to prepare the membranes. The membrane is characterized by FT-IR, SEM and TGA. Water uptake, proton conductivity, oxidative resistance, ionic conductivity and methanol permeability are measured to evaluate its performance in a direct methanol fuel cell with cation exchanger membrane. The SPS-PE-MIL-53 (1:1:0.25 w:w:w) membrane showed relatively better performance than the other membranes. The selectivity factor for this membrane was 7.17×10^4 S.s.cm⁻³. The prepared membranes were used in a fuel cell to evaluate the performance. All membranes prepared, in the fuel cell performed well, but the SPS-PE-MIL-53 (1:1:0.25 w:w:w) membrane performed better than other membranes.



Fig. 1: Reaction scheme of homogeneous sulfonation: (A) the generation of acetylsulfate and (B) sulfonation of PS.



Fig. 2: Scheme of MIL-53(AI)-NH₂

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A Facile and Green Approach for One-Pot Synthesis of Highly Functionalized Pyrroline Derivatives by Reaction of Pyrrole, Ninhydrin and *B*-enaminocarbonyls

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Abstract

Multi-component reactions (MCRs), especially three-component reactions, offer apparent advantages over conventional linear-type synthesis because the combination of the reactants to generate new products in a single step is economic and easy.^{1,2} Pyrrole derivatives have viably been utilized as intermediates in preparing various natural products, agrochemicals, flavorings, dyes, and functional materials.³ In addition, ninhydrin has been used in a lot of heterocyclic preparations and is indeed a key building block in organic synthesis. A broad range of reactions includes ninhydrin in the synthesis of heterocyclic compounds.⁴ Pyrroline derivatives have been used as intermediates in the synthesis of biologically and/or medically active compounds.⁵ In this project we report a new and highly efficient method for synthesis of pyrroline derivatives **1** by reaction between pyrrole with ninhydrin and β -enaminocarbonyls derivatives in water as a green solvent under reflux conditions in the absence of any catalyst (scheme 1). The products were isolated by plate chromatography in good yields. All the products were characterized using the NMR and IR spectral and analytical data.



Ar = C_6H_5 , $CH_2C_6H_5$, 4- CIC_6H_4 , 4- $OCH_3C_6H_4CH_2$, 4- $CH_3C_6H_4$

 $R = CH_3$, OCH_3 , OCH_2CH_3

Scheme 1: Structure of Pyrroline Derivatives

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Catalyst-Free Microwave-Assisted Arylglyoxal- Based Three-Component Reaction for the Synthesis of Pyridazine Derivatives

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Abstract

Heterocyclic compounds are the most biologically active compounds in nature. Due to this finding, nitrogen Heteroatom-containing compounds are becoming more famous in recent researches and so is the development of new more potent drugs and newer derivatives of existing or currently used drugs without or minimum side e..ects 1 The pyridazine moiety is an important structural feature of different pharmacologically active compounds. Pyridazine derivatives have been reported² to possess a wide range of biological activities, these include antiviral and anticancer,³ antituberculosis,⁴ antihypertensive⁵ and antimicrobial⁶ activity. Therefore, continuing our interest in the synthesis of pyridazine derivatives, we decided to investigate the synthesis of 3-hydroxypyridazine-4-carbonitriles **3** by three-component reaction of arylglyoxals **1**, alkyl 2-cyanoacetates **2** and hydrazine hydrate in alcoholic media under microwave irradiation at room temperature (Scheme 1). Microwave synthesis provided excellent yields in short reaction times in the absence of any catalyst.



 $\begin{aligned} Ar &= C_6H_5, \ 4\text{-}ClC_6H_4, \ 4\text{-}BrC_6H_4, \ 4\text{-}IC_6H_4, \ 4\text{-}NO_2C_6H_4 \\ R &= OCH_3, \ OCH_2CH_3 \\ \end{aligned}$

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Silver Nanoparticles-Decorated 1-Vinylimidazole Functionalized New Magnetic Carbon Biomass: A Narrative and Proficient Catalyst for the Union of Spiro-2-Amino-4*H*-pyrans (spirochromenes) *via* Multicomponent Reactions

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Abstract

multicomponent reactions (MCRs) have interested an excellent bargain of intrigue both in the scholarly community and venture due to their specific manufactured viability, characteristic molecule budgetary framework, intemperate cleverness, and practical solidarity. Various and energizing heterocyclic structures, particularly those generous in combinatorial appeal as able embellishments in biologic disclosure, were better actinic through MCR. MCRs additionally are helpful for the sensible brought set up of chemical libraries of basically related, medicinally essential Pharmaceutical simple compounds. 2-Amino-4*H*-pyran subordinates (4*H*-pyrans) were synthesized through the three-segment reaction checking unique β -dicarbonyl compounds, subbed aromatic aldehydes startlingly malononitrile/ethyl cyanoacetate using Ag in EtOH/H₂O underneath reflux condition. In development, spirochromenes were synthesized through a three-segment reaction including isatins or acenaphthenequinone, malononitrile or ethyl cyanoacetate and distinctive 1,3-diketones (dimedone, barbituric destructive or ethyl acetoacetate) or 4-hydroxycoumarin/3-methyl-1*H*-pyrazol-5(4*H*)- one) inside the proximity of Ag in EtOH/H₂O under reflux condition. All reactions were finished on short occasions, and the things were gotten in incredible to excellent yields. The reaction medium can be reused a lot a couple of times with no efficiency incident.



Scheme 1. An efficient one-pot synthesis of functionalized spirochromenes

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A Facile and Effective Procedure for Synthesis of 1H-Indol-3-yl-Dihydroindeno Pyrrole-4(1H)-one Derivatives Under Mild Conditions

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Abstract

Multicomponent reactions are strong synthetic tools for the synthesis of complex organic molecules. The improvement of environmentally friendly chemical protocols is one of the basic principles of green chemistry. According to this fact, the selection of water as an environmentally benign solvent has received a lot of attention. It is cheap, readily available, non-toxic and non-flammable medium.¹ Indole and its derivatives because of their ability to inhibit quorum sensing and virulence factor production are considered as potential antivirulence compounds against antibiotic-resistant pathogens.² Ninhydrin reaction chemistry has many applications in the fields of food, medicine, and forensics. Several ninhydrin analogs have been synthesized and evaluated as alternatives to the conventional ninhydrin reagent for the development of latent finger marks on paper surfaces.³ In this project, we describe a green synthetic protocol from three-component condensation of indole **1** with ninhydrin **2** and β -enaminocarbonyls **3** in water under reflux conditions in the absence of any catalyst (Scheme 1). The afford project is a new and excellent method for synthesis of pyrroline derivatives **4**. The products were isolated by Plate chromatography in good yields. All the products were characterized using the NMR and IR spectral and analytical data.



Scheme 1: Reaction between indole, ninhydrin and β -enaminocarbonyls

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Unexpected Products in the Multicomponent Reaction of Arylglyoxals, Meldrum's Acid and Pyrrole

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Abstract

Multicomponent reactions, especially three component reactions, offer significant advantages over conventional linear-type syntheses, because the combination of the reaction components to produce novel products in a single step is economic and easy.^{1,2} Meldrum's acid (MA) is an organic compound, discovered in 1908 by A. N. Meldrum.³ MA can be easily Synthesized by the condensation reaction of malonic acid and acetone in acetic anhydride in the presence of concentrated sulfuric acid as a catalyst. Due to its high acidity (pKa 7.5), MA appears to be an Interesting reagent in synthesis of natural products.⁴

Substances of the Meldrum's acid group have been used therapeutically for many years. Due to the chemical structure of Meldrum's acid and its capability to make keto-enol form, it has a unique potential to be used as a valuable building block in various organic reactions.⁵ In continuation of previous works on the development of multicomponent reactions, we report a simple three component reaction between arylglyoxals **1a-g**, pyrrole **2** and Meldrum's acid **3** in water as a green solvent in the absence of any catalyst (scheme 1). The products **4a-g** were isolated by simple filtration in high yields. All the products are stable and the structure assignments of new products have been established based on spectral data, elemental analysis, and melting points.



Ar: Ph, 4-MeC₆H₄, 4-ClC₆H₄, 4-MeOC₆H₄, 4-FC₆H₄, 4-NO₂C₆H₄, 4-BrC₆H₄ **Scheme 1:** Reaction between arylglyoxals, pyrrole and meldrum's acid

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Assembly of Indole Cores through a Palladium-Catalyzed Metathesis of Ar–X σ -Bonds

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Abstract

Phosphines play a crucial role in most transition-metal- catalyzed cross-coupling reactions in stabilizing the active metal center and fine-tuning the selectivity of the conversion.¹ The initially formed aryl palladium species, however, have been reported to frequently undergo an undesirable aryl/aryl interchange with the aryl substituents of triarylphosphine ligands via C-P bond scission, leading to undesired scrambled side products and deactivation of the catalyst.² Accordingly, early studies were focused on shutting down this side trail. However, by the accumulation of mechanistic data, new avenues for developing various catalytic reactions through the strategic utilization of the metathesis of Pd-C and P-C bonds have been recently opened.³ creating a suitable catalytic system to provide an appropriate platform for a productive ligand exchange would find great applications in organic synthesis. Inspired by recent advances in this area, we set out to identify reaction conditions to construct indole scaffolds with the benzoic ring built by the aryl section of simple triarylphosphines via the metathesis of Ar-X σ -bonds. Aryl's attachment to phosphorus can be activated via a controlled exchange between P-Ar and Pd-Ar, and it can participate in a cascade annulation reaction for the purpose of the construction of more complex molecules, which is unprecedented to the best of our knowledge and would be very attractive. This transformation exploits palladium-catalyzed reversible oxidative addition/reductive elimination chemistry to offer the synthesis of a diverse array of highly functionalized indoles in high yields and opens a new window for the application of simple phosphines in the assembly of indole cores.

We describe the development of a new method for the construction of highly substituted indole scaffolds through the strategic utilizing of the metathesis of Ar-X σ -bonds based on the dynamic nature of palladium-based oxidative addition/reductive elimination. A suitable and simple catalytic system has provided an appropriate platform for a productive ligand exchange and consecutive carbopalladation/C-H activation/amination of phosphine ligands with alkynes and aromatic/aliphatic amines for construction of structurally diverse indoles.



Scheme 1: Synthesis of diverse indoles *via* the carbopalladation/C-H activation/amination cascade References

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Investigation of Production Management and Disposal Methods of Acid Sludge Due to Vaseline and Paraffin Purification Process

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Abstract

Vaseline and paraffin are petroleum derivatives that are part of the downstream market in this industry. These products must be refined and converted to saturated hydrocarbons to enter the consumer market, Figure 1.¹

In the industry, various methods are used for purification, including chemical¹, adsorption², and hydrogenation. Acid sludge is a by-product of the chemical treatment of Vaseline and paraffin raw materials. In addition to having adverse environmental effects, this sludge ultimately increases the cost of products and reduces the company's competitiveness in the market.

In this research, the methods of production management and disposal of acid sludge are investigated. Suggested solutions, in summary, are treatment optimization with the help of experiment design³ before each loading of treatment tanks for production, improvement of treatment equipment to control the parameters affecting the process, neutralization of sludge, and depot it in the locations designated by the Environment Agency.



Figure 1: Process flow diagram of paraffin and Vaseline production

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Synthesis of Sulfonated Amine-Tripod as A New Dispersing Agents

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Abstract

Here, we report the synthesis of a new sulfonated dispersing amine-tripod agent from the reaction of cyanuric chloride, 4-hydroxybenzaldehyde and several amines.¹⁻⁴ The resulting amine-tripod were sulfonated with excess chlorosulfonic acid. The structures of target sulfonated dispersing amine-tripod and related intermediate material were identified by TLC, MP, IR, ¹H NMR and ¹³C NMR. The synthesized compounds could be used in industry as anti-dispersant agent either for organic compounds as well for inorganic compounds.



Scheme 1: Synthesis of sulfonated dispersing amine-tripod

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A New and Efficient Synthesis of Nanocarboxymethyl Starch

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Abstract

Starch, the second most abundant biomass material, is a natural, renewable, and biodegradable polymer produced by many plants as a source of stored energy.¹ Carboxymethyl starch (CMS) is a water-soluble starch derivative having wide applications in various fields such as pharmaceutical, paper making, textile, adhesive and absorbent.² Nanocrystalline starch and functionalized natural starches are ideal for the reinforcement of a biopolymer compared to amorphous starch and they can generally be attractive supports in industrial and medical aspects.³ Now, due to these applications, efforts have been made to create nano carboxymethyl starch to cover the shortcomings of starch.

In this research, at first, CMS was prepared according to the literature. In order to synthesize nanocarboxymethyl starch, the produced CMS was dissolved in distilled water. The aqueous solutions of sodium hydroxide and urea were prepared separately and then these solutions were slowly added to the CMS and stirred at 35 ° C for one hour. After cooling the reaction vessel to room temperature, 10 ml of the obtained solution was introduced to a 100 ml beaker and 10 ml of ethanol was added dropwise for 20 to 30 minutes under stirring. The nanoparticles of carboxymethyl starch were obtained by centrifuging of obtained suspension for 30 minutes and then ultrasonic treatment of them. The produced nanoparticles were washed twice with ethanol.

The results of DLS analysis showed that with increasing the time of centrifuge from 10 min to 30 min, the particle size was so smaller.



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Synthesis of Bis(3-indolyl)pyridines *via* Vinylogous Anomeric Based Oxidation by Using as a Novel Cobalt-Based Metal Organic Framework with Sulfonic Acid Tags

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Abstract

In recent years, metal-organic frameworks (MOFs) are valuable materials because of their applications on the preparation of adsorption, catalysis, sensors, electronics, selective separation, fuel cells, petrochemistry, large scale of industrial products and drug delivery.¹⁻² Recently, application of solid acids with sulfonic acids tags as catalysts comprehensively reviewed. The research and application of various multi-SO₃H functionalized solid acids are interesting due to their nano structures, Bronsted acidic and environmentally friendly, good candidates for replacing of conventional solid acids, which could be used as a catalyst and reagent.³ In this paper, cobalt-based metal organic framework as a novel and heterogeneous catalyst with sulfonic acid tags was synthesied and fully characterized by using various analysis techniques. We wish to develop vinylogous anomeric based oxidation mechanism at the preparation of bis(3-indolyl)pyridines from aryl aldehydes, 3-(1*H*-indol-3-yl)-3-oxopropanenitrile and ammonium acetate in the presence of a catalytic amount of cobalt-based metal organic framework under mild conditions (Scheme 1). The major advantages of the described method are high yields, short reaction times and reusability of the catalyst. The obtained results from this research will be by the idea of rational designs, syntheses and applications of task-specific catalysts.



Scheme 1: Preparation of bis(3-indolyl)pyridine derivatives using Co-based MOFs

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Synthesis and Catalytic Application of a Novel Magnetic Metal-Organic Frameworks of Fe₃O₄@MIL-101(Cr)-N(CH₂PO₃)₂ in One Pot Preparation of New Pyrazolo[3,4b]pyridine-5-carbonitriles *via* a Cooperative Vinylogous Anomeric Based Oxidation

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Abstract

Metal organic frameworks (MOFs) are a class of ultraporous materials fabricated by assembling metal ions with organic ligands in appropriate solvents, which have been attracted considerable attention because of their exceptionally high accessible surface area, diverse structural topologies as well as tunable functionalities. These characteristics make them show remarkable capabilities in a variety of application areas, including gas storage, separation, catalysis, and drug delivery.¹⁻² Another material that has been the center of attention among researches who work on new materials with new applications is magnetic nanoparticles (MNPs). To synthesis MNPs, several methods have been developed depending on the target compounds.³ The combination of functional MNPs with MOFs results in the formation of magnetic frameworks composites (MFCs) which is in the center of attention among most of the scientists who work in this field to improve their properties.⁴ In this paper, Cr-based magnetic metal organic framework as a novel and heterogeneous catalyst with phosphorus acid tags was synthesized and fully characterized by using various analysis techniques. This magnetic metal-organic frameworks (MMOFs) were applied in the synthesis of new pyrazolo[3,4-b]pyridine-5-carbonitriles.



Cat. = Fe₃O₄@MIL-101(Cr)-N(CH₂PO₃)₂ ABO = Anomeric Based Oxidation

Scheme 1: Preparation of novel mono and bis and tris pyrazolo[3,4-*b*]pyridine carbonitriles using Fe₃O₄@MIL-101(Cr)-N(CH₂PO₃)₂.

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Novel Nano-Architectonic of Hybrid Carbon Quantum Dots (CQDs) with Phosphorous Acid Tags as Catalyst for the Synthesis of New Pyridines and 1,4-Dihydropyridines

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Abstract

Carbon quantum dots (CQDs) material or blocks spherical are including organic compound as nuclei with semiconductor nano-crystals below 10 nm, that is based on graphene (QGDs) and carbon quantum dots (CQDs, C-dots or CDs). Carbon quantum dots (CQDs) are of great importance in bioimaging, biosensors, catalysts, sensing of heavy metal elements as well as drug delivery. Also, these materials show intense blue photoluminescence (PL), which can be widely used in medical and other sciences.¹⁻² Phosphorus acid compounds are good candidates for synthesis of acidic catalysts due to their properties such as easy separation, high chemical stability and dramatic increase in the speed of chemical reactions.³ in this paper, nano-architectonic of hybrid carbon guantum dots (CQDs) with phosphorous acid tags was synthesized and fully characterized using various analysis techniques. We used carbon quantum dots (CQDs) with phosphorous acid tags in the preparation of new pyridines and 1,4-dihydropyridines compounds. Target molecules were synthesized by using an aldehydes derivative (1 mmol), pyrazole derivatives (1 mmol), pyrimidine-2,4,6(1H,3H,5H)-trione (1 mmol) and CQDs-N(CH₂PO₃H₂)₂ (10 mg) as catalyst under solvent-free conditions (Scheme 1).



Scheme 1: Preparation of new pyridines and 1,4-dihydropyridines using quantum dots (CQDs) with phosphorous acid tags.

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Synthesis and Catalytic Application of a Novel Magnetic Al-Based Metal–Organic Frameworks for the Preparation of Fused Nicotinonitrile Derivatives via a Cooperative vinylogous Anomeric Based Oxidation

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Abstract

Metal-Organic Frameworks (MOFs) are a bunch of new porous compounds that have expanded extensively over the last few years. These porous compounds are synthesized by bonding between metal ions and organic ligands.¹ Despite many years of synthesis and its various applications, magnetic particles retain their various applications and are expanding. Magnetite nanoparticles (Fe₃O₄) are used as suitable substrates for many catalysts.² Due to their magnetic properties, magnetic MOFs, using an external magnetic field, in addition to maintaining their previous properties, can be easily displaced and acquire a new feature.³ Herein, a novel nano-magnetic Fe₃O₄ based metal-organic frameworks were synthesized and characterized by various analyzes. This is a synthesized catalyst for the synthesis of a wide range of fused nicotinonitrile derivatives compounds as suitable drug candidates through a four-component reaction during densification between aldehyde derivatives, acetophenone derivatives, 3-oxo-3-phenylpropanenitrile or 3-(4-chlorophenyl)-3-oxopropanenitrile and ammonium acetate through a vinylogous anomeric based oxidation in mild and solvent-free conditions at 110 °C were used. One of the most important features of the method used in this paper is the easy separation of the catalyst using an external magnetic field due to the magnetic nature of the synthesized catalyst.



Scheme 1: Preparation of fused nicotinonitrile derivatives using AI-based metal-organic frameworks

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Synthesis of Pyrido[2,3-*d*]pyrimidine *via* Vinylogous Anomeric Based Oxidation Using [Zr-UiO-66-PDC]SO₃ as a Novel Metal Organic Framework

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Abstract

Acetonitrile (3-oxopropanonitrile or β -keto nitrile) materials tags are valuable intermediates because of their applications in the Stork enamine synthesis and Mannich-type reactions for the synthesis of dyes, biologicals and pharmaceuticals.¹ They have been applied as significant intermediates in various functional group transformations. The preparation and uses of acetonitrile, unlike traditional acetonitrile, have a short background. Acetonitrile is widely used as Michael acceptor in cycloaddition reactions, the Diels-Alder reaction, and the reaction to prepare various organic intermediates and also can be reduced to produce nitroalkanes. Therefore, being focused on enamines is one of the most fascinating developments in preparation of widely applied organic materials such as natural products as well as pyridine scaffolds.² The pyridine ring system are biological activity like as inhibiting HIV protease, antidepressant, anti-in ammatory, inhibiting acetylcholinesterase, treating hypotension or hypertension.³ Herein, we have prepared and [Zr-UiO-66-PDC]SO₃ and successfully tested it on the synthesis of pyrido[2,3-*d*]pyrimidine at 100 C under solvent-free conditions. (Scheme).



Scheme: Preparation of pyrido[2,3-*d*]pyrimidine derivatives using [Zr-UiO-66-PDC]SO₃ as mesoporous catalyst

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Synthesis of Highly Functionalized Pyrroles Using Magnetic Functionalized Graphene

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Abstract

Pyrroles are structural motifs which are found in a wide variety of natural products or pharmacologically active substances.¹ Although a number of methods for the construction of pyrroles have been established, the efficient synthesis of highly functionalized pyrroles remains challenging.

Graphene, a sp²-bonded two-dimensional carbon-based nanomaterial has attracted tremendous attentions due to its extraordinary properties such as a large theoretical specific surface area, superior mechanical strength, and high thermal/chemical stability.² Graphene-based catalysis is an ongoing research area, which opens new opportunities for graphene applications.³ However, the application of graphene as a catalyst is limited by the difficult separation and low recovery of the catalyst. This issue can be addressed by the development of magnetic graphene nanocomposites owing to easy separation by applying a magnetic field. In this study, a simple and efficient synthesis of highly functionalized pyrroles by a one-pot multi component strategy using aromatic amines, phenacyl bromide, and dialkyl acetylenedicarboxylate is reported. The reactions were performed in the presence of magnetic functionalized reduced graphene oxide as the catalyst and under environmentally-friendly solventless conditions (Scheme 1). Graphene oxide was prepared by the Hummers method according to the previously reported procedure.⁴ Reduced graphene oxide-supported nanoscale zerovalent iron (nZVI/rGO) composite was prepared by the reduction of Fe_SO₄.6H₂O and graphene oxide with NaBH₄ and was characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD), Raman spectroscopy, and Fourier-transform infrared spectroscopy (FTIR).

In order to identify suitable reaction conditions and determine the catalytic efficiency of nZVI/rGO, a threecomponent reaction between aniline (1 mmol), α -bromo acetophenone (1 mmol), and dimethyl acetylenedicarboxylate (1 mmol) as a model reaction was conducted under different operating conditions. To establish the generality of this method, the synthesis of various substituted pyrroles was investigated. A simple workup procedure, mild reaction conditions, a recyclable catalyst, and good yields (93–97%) make this methodology a valid contribution to the existing processes in the field of pyrrole derivatives.



Scheme 1. Catalytic synthesis of highly functionalized pyrroles using magnetic functionalized graphene. References

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A Phenanthro[9,10-d]imidazole Based Molecular Sensor for Detection of H⁺ Based on Photo-Induced Electron Transfer

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Abstract

A fluorophore-receptor system has been used to introduce a fluorescent chemosensor derived from phenanthro[9,10-d]imidazole. The sensor works based on photo induced electron transfer mechanism to detect H⁺ ions with a turn-on response. Upon excitation under neutral or basic condition, an electron transfer from the receptor to the fluorophore quenches the fluorescence emission but after bond formation with H⁺ ions under acidic conditions which the PET mechanism, a fluorescence enhancement is observed.



Scheme 1: The structure of the fluorescence pH sensor

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Electrochemical Dimerization of Trimipramine: Synthesis of New Dibenzazepine Derivative

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Abstract

Electroorganic reactions proceed generally smoothly with easy work-up and do not require the use of harsh conditions such as high temperatures and expensive reagents.¹ Trimipramine (TRI) (a dibenzazepine derivative) is tricyclic antidepressant drug (TCAs) referred to as monoamine re-uptake inhibitors because of it postulated principal mode of action and is used in the treatment of depressive disorders. Nitrogen-containing heterocycles have received much attention due essentially to a broad range of biological properties and a detailed history as significant medicinal pharmacophores. The dibenzazepine is among these heterocycles which exhibits a wide range of biological activities.² The electrochemical oxidation of TCAs occurs at the nitrogen atom in heterocyclic ring resulting in the formation of a radical which is similar to that for the oxidation of methyliminobibenzyl. Based on previous reports, dimerization is the main reaction of electro-oxidation of trimipramine.^{3, 4}

In this work, the electrochemical synthesis of a new dibenzazepine derivative was carried out *via* the electrochemical oxidation of trimipramine (TRI) in the presence of toluenesulfinic acid (TSA) as a nucleophile. The results indicate that the toluenesulfinic acid (TSA) participation in Michael addition reaction with the oxidized dimeric form of trimipramine via an ECEC electrochemical mechanisms. On the other hand the results indicate the existence of a catalytic (EC') electrochemical mechanism in parallel with ECEC electrochemical mechanism. The product has been characterized by IR, ^{1H} NMR, ¹³CNMR and MS methods.

This method provides a one-pot procedure for the synthesis of new dibenzazepine derivatives in good yields without using toxic reagents at a carbon electrode in an environmentally friendly manner.



Scheme 1: Electrochemical oxidation mechanism of trimipramine in the presence of TSA.

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A Green Approach for Synthesis New Dibenzodiazepine Derivative Based on The Electrochemical Oxidation of Clozapine in the Presence of 4,6-Dimethylpyrimidine-2-thiol

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Abstract

Electrochemical methods are widely applied to electrosynthesis, and mechanistic studies. In this case, due to the increase in the importance of green chemistry in organic synthesis, the development of more efficient and environmentally friendly processes for chemical transformations is desirable.¹

Dibenzoazepine derivatives are widely used among the tricyclic antidepressants. Clozapine (CLZ), is a dibenzodiazepine derivative with a typical antipsychotic drug. It bioactivated reactive intermediate of CLZ to be either a radical cation or the nitrenium ion.^{2, 3}

In this work, a new dibenzodiazepine derivative was synthesized in aqueous solutions via a green method using anodic oxidation clozapine in the presence of 4,6-Dimethylpyrimidine-2-thiol (DMPT) using a carbon anode. The results indicated that the generated nitrenium ion is then attacked by DMPT via the Michael addition type reaction to form new dibenzodiazepine derivatives. The overall reaction mechanism for anodic oxidation of clozapine in the presence of DMPT as nucleophiles is presented in Scheme 1. The results of this work show that, the reaction mechanism of electro-oxidation of CLZ in the presence of DMPT is an EEC mechanism. The product has been characterized by IR, ¹H NMR, ¹³C NMR and MS methods. The present method for the synthesis of dibenzodiazepine derivatives has several advantages over conventional methods and led to the development of a new strategy in accordance with the principles of green chemistry for the synthesis of some dibenzodiazepine derivatives.



Scheme 1: Proposed mechanism for the electrochemical oxidation of CLZ in the presence of DMPT.

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Computational Study of Steric Effects on Cyclopropylcarbene to Cyclobutene Rearrangement

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Abstract

The isomerization of cyclopropylcarbene (I) to cyclobutene (II) is typical of ring expansions of carbenes. The ring expansion reaction of (I) in its singlet ground state to (II) is initiated by an electrophilic attack of the empty p AO at the carbene site on the most electron-rich carbon atom of the three-membered ring.



In this report a DFT study is done on the substituted cyclopropylcarbene (I) to cyclobutene (II) rearrangement and is discussed steric effect on carbene center. Rearrangement of cyclopropylcarbene in singlet ground state have been studied using B3LYP/6-311G* method. Relative energies are estimated with 6-311 ++G**.

Table 1: Barrier Energy			Table 2: ΔE (E product – E reactant)			CC
substituent	Ea (Kcal/mol)		substituent	∆E (Kcal/mol)		
	endo	exo		endo	exo	
Н	16.1645	3.8048	Н	-66.1186	-63.8686	$C_2 - C_1$
Methyl	21.576	8.0988	Methyl	-65.4478	-60.3514	
Ethyl	21.3789	8.1069	Ethyl	-64.6021	-59.6844	Figure 1: TS of
iso propyl	20.5520	7.9676	iso propyl	-64.5613	-59.4543	Figure 1. 13 0
tert-Buthvl	16.6763	8.0504	tert-Buthyl	-71.7243	-61.5737	rearrangement
neo-Penthyl	22.3878	9.0708	neo-Penthyl	-61.6631	-56.3682	

There are two possible forms for substituted cyclopropylcarbene: endo and exo conformers. Two issues are concluded by surveying the barrier energy of some substitution (H \rightarrow neo-Penthyl), as follow:

- 1. When H is replaced by Methyl the barrier energy is maximum which is much more in the exo conformer than the endo one. (more than 2 times)
- There is no significant energy variation in barrier energy in both conformers (endo & exo) when the size of substitution increases (from Ethyl to neo-Penthyl) (Table1) but there is an exception about tert-Buthyl in which the barrier energy decreases and it increases again for neo-Penthyl. This is may be because of the high value of ∆E in this series of substitutions and bias to rearrangement. (Table2)

The rearrangement of (I) to (II) involves the formation of a bond between C4 and C1 and the breakage of a bond between C1 and C3. For this reaction path an electronic hypersurface was computed with the optimized B3LYP/6-311G* method, starting from either the exo or endo conformation. The total optimization of (I) in the singlet ground state reveals a geometry which is slight distorted so as to align the empty p AO at C4 with the bond C1-C3. In transition state the bond C1-C3 is paltry weakened, while the carbene center forms a weak bond with C1. (Figure1) **Conclusions**

The result of our investigation can be summarized as follows:

- 1. Rearrangement of cyclopropylcarbene to cyclobutene is initiated by an electrophilic attack of empty p AO at the carbene site C4 on the ring carbon C1 (or C2). In transition state, charge is transferred from C1 (or C2).
- 2. The transition state is stabilized by introduction of electron-releasing substituents at the ring carbon C1 (or C2) and at C3. This corresponds to the migration of the more electron-rich C-C bond.
- 3. The low-energy barrier (ease of rearrangement) depends on a three-center bonding between the atoms C1, C3, C4 and involves two electrons (of the C1-C3 bond).

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Preparation of Poly Ethersulfon Membrane Embedded by Chitosan Nanoparticles for Removal Sulphate

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Abstract

In this work, Different amounts of chitosan nanoparticles were embedded into the polyethersulfone (PES) membrane prepared by phase inversion precipitation method. Firstly, chitosan nanoparticles (CS-NPs) were synthesized using tripoly phosphate and transferred into the organic solvent via solvent exchange method.¹⁻² The membranes were employed for sulphate removal from water under various solution pHs (3.5, 7.0 and 9.0). Scanning electron microscopy and water contact angle and pure water flux measurements were employed to characterize the fabricated membranes. Addition of chitosan nanoparticles into the membrane matrix increased the water permeability from 15 for pristine membrane to 22 kg/m² h for modified membrane with 0.3 wt.% chitosan nanoparticles. However, the application of CS-NPs more than 0.6 wt.% led to membranes with a compact matrix and dense structure, thereby reducing water permeation even lower than PES. The complete sulphate removal (100%) was achieved at acidic pH due to protonation of amine groups of CS-NPs creating positive charge on the membrane surface.³



Fig. 1. Size distribution of chitosan nanoparticles in aquesous suspention of NPs optained by zetasizer

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One-pot and Green Synthesis of 4'-Aryl-2, 6-di (furan-2-yl) Pyridines under Ultrasound Irradiation

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Abstract

One-pot multicomponent coupling reactions (MCRs), where several organic moieties are coupled in one step, for carbon-carbon and carbon-heteroatom bond formation is an atractive synthetic strategy for the synthesis of small-molecule libraries with several derees of structural diversities.¹ sonochemistry can be used as a technique to improve chemical reactions under influence of ultrasound irradiation in which the sonic spectrum is used in the range of 20kHz to 100kHz.² In series of heteroaryl-substituted pyridine bases furylpyridines remain relaively little studied and difficult to obtain compounds; this is due to the limitations involved in the methods for their synthesis.³ The interest in furylpyridines is due to the fact that substances that have high and diverse biological activity are found among them.⁴

This study describes a simple and efficient synthesis of 4'-Aryl-2, 6-di (furan-2-yl) Pyridines have been prepared by one –pot reaction of 2-acetylfuran with aromatic aldehydes in the presence of aqueous ammonia and potassium hydroxide in ethanol. The reactions were performed under stirring at room temperature(A method) and ultrasound irradiation as the energy source(B method). The newly synthesized compounds were characterized by elemental analysis, NMR and MS spectroscopic data. In view of the literature survey on pyridine derivatives, encouraged us to synthesize (2,6-di-2-yl-4-Aryl-pyridine derivatives via two methods. In the both methods, reactants and their values were the same, only the conditions for the reaction were different. In the method A, reaction condition was under stirring at room temperature for 10h. And in the method B, reaction was under ultrasound irradiation for 45 min at 35 kHz and thermal condition (327k). In comparison, method B is convenient method than A for the synthesis of (2,6-di-2-yl-4-Aryl-pyridine derivatives (3a-h) in terms of yield, reaction time and condition.the highest percentage is related to 3h(A:39% , B:70%)



Scheme 1. Facile one-pot synthesis of 4'-aryl-2, 6-di (furan-2-yl) pyridine

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Synthesis of Two-Dimensional Triazine Polymers; How Organic Chemistry Help Us to Construct Giant New Materials

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Abstract

Two-dimensional triazine structures with great promises and unique physicochemical properties have emerged as new platforms for designing high performance materials during the past decade. The efficient synthesis of two-dimensional triazine structures with tailorable structures and properties is highly desired but has remained a long standing challenge. The harsh synthetic conditions and associated limited structural diversity together with unknown mechanisms hamper further development and large-scale synthesis of defined two-dimensional triazine structures.^{1,2}

Herein, we report on new strategies for the synthesis of two-dimensional triazine polymers at mild conditions. We have studied the mechanism of reactions in detail to find and control the parameters that affect the strcture of the final product. This help us to find the correlation between the strcture and properties of materials through which the desired compounds for special applications can be constructed. We have used coordination chemistry as well as aromaticity as two main factors to drive polymerization in certain topologies and orientations.^{3,4}

Taking advantage of such new strategies many new nano and micro-materials with defined structures can be synthesized. Figure (1) systematically summarizes the development in the synthesis of these two-dimensional polymers.



Figure 1: Schematic structure of the synthesis of 2D triazine polymers.

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Preparation of a Novel Hybrid Molecularly Imprinted Polymer for Solid Phase Extraction of Thiodicarb

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Abstract

Pesticides are a group of substances that have been extensively used in agriculture to control diseases and obtain high yields. Nevertheless, residues of these compounds may contaminate the air, water, soil, food chains and cause several problems to the humans and ecosystems. Therefore, the presence of residues of pesticides in natural waters and food is considered a public health concern. Thiodicarb (IUPAC: 3,7,9,13-tetramethyl-5,11-dioxa-2,8,14-trithia-4,7,9,12-tetra-azapentadeca-3,12-diene-6,10-dione) is acarbamate pesticide with a relatively narrow spectrum of activity closely related to its first metabolite, methomyl. It acts againstslugs (on ingestion) as well as lepidopterous pests, controllinglarvae at different stages as well as eggs in many instances. It isneurotoxic through the inhibition of cholinesterase causing paral-ysis followed by death. This pesticide is used in seed treatmentplants and for the control of various pests in cotton, soybeans,tomatoes, peanuts, corn and leafy vegetables, and other crops (1).

In this work, A novel molecularly imprinted polymer (MIP) as an artificial receptor for thiodicarb is prepared and used. A sol– gel process is used to prepare the hybrid MIP (2). For the organic part (gel) of the MIP, methacrylic acid (MAA), ethylene glycol dimethacrylate (EGDMA) and benzoylperoxide are used as functional monomer, cross-liker and initializer, respectively. As the inorganic part (sol) of the MIP, tetraethyl orthosilicate (TEOS) is used. The main parameters affecting the synthesis of the organic–inorganic hybrid MIP are investigated and optimized.

The imprinting efficiency of the MIP is evaluated by comparing the adsorbed amount of thiodicarb by the MIP with that by the related non-imprinted polymer (NIP). This study revealed that the MIP possesses a remarkable affinity for thiodicarb. A limit of detection of 0.1 ng mL⁻¹ has been achieved. The linear range and relative standard deviation (RSD%) were 1–100 ng mL⁻¹ and 3 (n =3), respectively. The hybrid MIP provides fast, selective and convenient separation of thiodicarb from aqueous samples.

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Voltammetric Determination of Insecticide Thiodicarb Based on Molecular Imprinted Polymer

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Abstract

Several toxic organic compounds (herbicides, fungicides, acaricides, and insecticides) have been used in agriculture to control diseases and obtain high yields. Residues of these pesticides may enter the food chains through air, water and soil and cause numerous health problems to ecosystems and humans. They can produce bone marrow diseases, infertility, nerve disorders, and immunological and respiratory diseases.¹ Therefore, the presence of residues of pesticides in natural waters and in foods is of major concern for public health reasons.²

In this work, a novel molecularly imprinted electrochemical sensor (MIECS) was fabricated for detection of thiodicarb, which was based on Fe3O4 nanoparticles modified glassy carbon electrode. The thiodicarb molecularly imprinted polymers (MIPs) films were fabricated by electro-polymerization using Aniline(Ani) as functional monomers and thiodicarb as templates. The electro-polymerization was performed utilizing the cv procedure at a scan rate of 0.1 V/S among -0.3 and +0.9 V for 15 cycles. The trapped thiodicarb, was released from its binding sites by immersing in 1mol.L⁻¹ sulfuric acid for 1h. As a control, a NIPS was made and prepared in the similar way except for addition of template. The accuracy of MIP/Fe3O4/GCE formation was confirmed using the square wave voltammetry technique. Under the optimal conditions, the MIECS shown a linear range from 1.0×10^{-9} to 1.0×10^{-7} g/L of thiodicarb (R=0.9388) and the limit of detection was 7.6 ×10⁻¹⁰g/L. The calibration curve shows a 94.8% correlation of the data. Finally, the sensor has the advantages of good sensitivity, high stability, low cost, short response time and good repeatability.



SWV profile of the probe; (1) MIP probe; (2) electro-polymerized probe after template molecule removal (3) electro-polymerized probe after rebinding with 25ng/ml template and (4) electro-polymerized probe after rebinding with 12.5 ng/ml template . Analysis was done at potassium hexacyanoferrate solution (5mmol/l) made in KCI (0.1mol/l).

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Design of Novel Metal-Organic Frameworks [UiO-66]FeCl₄ as Catalyst: Application to the Synthesis of Dihydrobenzo[g]pyrimido[4,5-b]quinoline Derivatives

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Abstract

Nowadays, one of the porous materials as metal-organic frameworks (MOFs) is of great interest to scientists and research groups.¹ This crystalline material is including metal and organic compound as nuclei and ligand respectively. Metal-organic frameworks (MOFs) as multifunctional materials have been used suitable for storage and separation of gas, drug delivery, catalyst, proton conductivity and heavy metal adsorbent.²⁻³ Post modification and merge synthesis of metal-organic frameworks (MOFs) with acid groups and metal for the transportation of organic compounds, oxidation, and synthesis of biological compounds and effectiveness of the high-throughput approach.⁴ N-Heterocyclic scaffold compounds are invaluable candidates for the design and discovery of new biologically active compounds. Besides, it is very important to supply new and easy methods for the preparation of target compounds with unique feature. In this regard, 1,4-dihydropyridine structures containing uracil and henna (2-hydroxynaphthalene-1,4-dione) moieties are suitable candidates for biological and pharmacological researches.⁵⁻⁶ Therefore, in continuation of our investigations on development of preparation of metal-organic frameworks (MOFs) with sulfonic acid tags, we wish to preparing of novel [UiO-66]FeCl₄ as an efficient mesoporous catalyst for preparation of novel dihydrobenzo[g]pyrimido[4,5-b]quinoline-2,4,6,11(1H,3H)-tetraone derivatives by condensation reaction of 2-hydroxynaphthalene-1,4-dione, 6-amino-1,3-dimethylpyrimidine-2,4(1H,3H)dione and various aldehydes (mono and bis) under green conditions (Scheme 1).



Scheme 1: Preparation of dihydrobenzo[g]pyrimido[4,5-b]quinolines using [UiO-66]FeCl4.

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Heteropoly Acid Keggin Supported on Graphite Carbon Nitride Catalyst in The Synthesis of one-pot Three-Component 2-Amino-4-Hydrochromen as an Efficient and Reusable Catalyst

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Abstract

An efficient and environmentally benign procedure for the synthesis of 2-amino 4-hydro chromen derivatives has been developed by one-pot three-component reaction of aromatic aldehydes, malononitril and alpha-naphtol or beta-naphtol in the presence of a heterogeneous catalyst keggin heteropoly acid supported on graphite carbon nitride under room temperature and etanol solvent.

This new procedure has the notable advantages such as short reaction time, easy synthesis, high product yield and absence of any tedious work up or purification makes the procedure highly applicable.

Also, the catalyst can recovered by filter paper and reused for five consecutive reaction cycles with out significant loss of activity. The prepared catalyst was detected by FT-IR, DRS analysis and used in the synthesis of 2-amino-4-hydrochromic heterocyclic compounds.



Fig1: The general reaction of the synthesis of cyclic compounds pyran in the presence catalyst Keggin/g-C₃N₄

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Investigation of AIN Nanotubes as Carrier Systems for Nitrosamine Molecules

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Abstract

Nitrosamines are mutagen compounds and carcinogens that can damage DNA and induce tumors in humans and animals.¹ In recent years, the experimental and theoretical studies have been performed on evaluating the adsorption of nitrosamines with zeolites and nanotubes.^{2,3} In this work, the effect of the adsorption of nitrosamine (NA) on the electrical properties of (4,0) and (5,0) AIN nanotubes was investigated using the B3LYP/6-311++G (d) level of theory (Figure 1). The HOMO- LUMO gap, electronic chemical potential (μ), hardness (η), softness (S), the maximum amount of electronic charge (ΔN_{max}), and electrophilicity index (ω) for the monomers and complexes were calculated. It was found that the NA molecule can be chemically adsorbed by the AIN nanotubes. Also, the interaction energy of NA with AINNTs decreased with increasing the tube diameter. The results show that the interaction of NA with nanotubes cab be changes electronic properties of nanotubes. The energy gap and chemical hardness of nanotube decreased, whereas, the chemical softness, ΔN_{max} and electrophilicity index of the nanotube increased upon complexation. Also, the conductivity and reactivity of the nanotube reduced as the tube diameter increased. Based on the NBO results, in all complexes, charge transfer occurred from the NA to the nanotube. To investigate the interactions between the NA molecule and nanotubes, analysis of atoms in molecules was performed at B3LYP/6-311++G (d) level of theory. The AIM results revealed that, the O(N)...Al and H...N interactions are partially covalent in nature. It is predicted that, AIN nanotubes can be used as adsorption of NA molecules. It seems that the AINNTs could be a good candidate for adsorption of NA molecules. The results of this work were compared with the results of adsorption of NA molecule on BN nanotubes.⁴ It is expected that the AIN nanotubes can be used as sensor for detection of NA molecules.



Figure 1: The optimized structures for AINNT complexes

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Theoretical Study of the Reaction Between 3-Benzylidene-2,4-Pentanedione and Different Isocyanides

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Abstract

In recent years, the design of multicomponent reactions (MCRs) that preserve atom economy, conversion character, and simplicity in a one-pot operation has received considerable interest due to their ability to generate highly complex final products.^{1,2} Isocyanides undergo a formal [1+4] cycloaddition reaction with conjugated electrophilic heterocyclic five-membered ring systems.³⁻⁵The stepwise reaction mechanism of the [1+4] cycloaddition reaction between alkyl isocyanides with 3-Benzylidene-2,4-pentanedione both in the gas phase and in solvent was studied theoretically with B3LYP/ 6-311++G(d,p) method (Figure 1). The potential energy of all structures participated in the reaction path has been evaluated. Quantum mechanical calculations were made in order to study the potential energy surfaces, energetic, vibrational frequencies and topological properties of all structures in the reaction of alkyl isocyanides with 3-Benzylidene-2,4pentanedione in gas phase and in different solvents such as acetone and dichloromethane. The results show that, contrary to what was expected, in each reaction path, the second step of the reaction which contains an intermolecular proton transfer, recognized as rate-determining step. In dichloromethane and acetone solvents, no especial difference in the energy barrier of the first and the second step of the reaction was observed. All the structures in acetone solvent had been more stable compared to dichloromethane. Results show that the amount of change in potential energy surfaces in both acetone and dichloromethane solvents with different dielectric constants was approximately equal. The energy level of the most stable product in the presence of both solvents and in gas phase corresponds to P-a and the path a was determined as thermodynamically stable path. The least barrier height corresponds to the path band determined as a kinetically stable path. Results show that in going fromR1-a to R1-b or R1-c1 (R1-c2), increasing of the negative chargeof N28 and decreasing of the positive charge of C27 is the result of increasing electron donation of substituted groups of t-butyl or cyclohexyl. The high energy barrier of the two reaction steps well shows why the reaction doesn't proceed at room temperature.



Figure 1. The Reaction between alkyl isocyanides with 3-Benzylidene-2,4-pentanedione (R2). **References**

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Facile and Expeditious One-Pot Synthesis of Pyrroline Derivatives via Multicomponent Reaction

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Abstract

Multicomponent reactions (MCRs) have only recently been recognized as a major expansion of the synthetic chemist's toolbox.¹ These reactions are powerful tools for the generation of chemical libraries and they have attracted significant attention due to their broad applications in medicinal chemistry for the production of different structural scaffolds, and in combinatorial synthesis.² MCRs can be used to access various heterocycles and highly functionalized scaffolds.³ N-Substituted pyrrolines are an important class of heterocyclic compounds which exhibit neuritogenic activity⁴ and serve as useful synthetic intermediates.⁵ Arylglyoxals and β -enaminocarbonyls are among the most attractive precursors that are used to synthesize a variety of heterocyclic compounds.^{6,7} Therefore, continuing our interest in the synthesis of pyrroline derivatives, we decided to report the reaction of arylglyoxal monohydrates 1 with enaminoketones 2 and benzohydrazide 3 in acetonitrile in the presence of catalytic amounts of FeCl₃ at room temperature to provide a three-component facile and efficient route for the synthesis of the expected N- substituted 2-pyrroline derivatives 4 (Scheme 1). The products were isolated by column chromatography on silica gel (200-300 mesh) using petroleum ether and ethyl acetate. All compounds were characterized using the NMR and IR spectral and analytical data. The advantages of this method are readily available starting materials, neutral reaction conditions and high yield of products at ambient temperature.



Scheme 1: Reaction between arylglyoxal monohydrates, enaminoketones, and benzohydrazide.

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Synthesis of 5,6-Diaminouracils *via* Palladium Catalyzed Oxidative Coupling Reactions of Amines with 6-Aminouracils

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Abstract

Uracil is one of the five nucleobases and therefore an important component of nucleic acids.¹ Its chemistry and that of its derivatives *e.g.* 6-aminouracil are very rich, as these molecules can act as both nucleophiles and electrophiles. Uracils are widespread in natural products and are of interest because of their biological properties.² Uracil is an important component in helping enzymes to carry out different reactions and the making of polysaccharides. It has been found to be a common structural moiety of several bioactive compounds known for anti-inflammatory.³⁻⁴

In this work, we try to report a new, facile, and efficient pathway toward synthesis of asymmetric 5,6diaminouracils. Anilines was treated with 6-aminouracils **1** in presence of hydrochloric acid at $160^{\circ C}$ for 5h to give 6-N-aryluracils⁵, followed by addition of N-Bromosuccinimide and continuing of the reaction at room temperature in THF to give 5-bromo-6-N-aryluracils **2**. The reaction of compound **2** with alkylamins in the presence of palladium (II) acetate and sodium carbonate in DMF as solvent at $160^{\circ C}$ for 24h give asymmetric 5,6-diaminouracils **3**. All products are new compounds and their structures were characterized using the physical and spectral data.



Scheme 1: synthesis of asymmetric 5,6-diaminouracils 3

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Water Treatment and Desalination with Nano-Porous Graphene

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Abstract

Water is one of the most influential substances in human life. but water pollution, urbanization and it has pushed population growth to the brink of water scarcity. Various methods are used to sweeten the water, one of the most important of which is Reverse Osmosis

Traditional reverse osmosis membranes have low water permeability and thus require higher operation power for the Water purification process.¹

It is not economical to use this method due to the strong need for electricity and the economic aspect.² Graphene naturally repels water but when narrow pores are created, it accelerates its penetration.

This sparked ideas regarding the use of graphene for water filtration, especially once the technology for making these micro-pores has been achieved.

Graphene sheets are studied as a method of water filtration, because they are able to let water molecules pass but block the passage of contaminants and substances.³

This opens the door to the possibility of using seawater as a drinking water resource, in a fast and relatively simple way.

Nano graphene sheets are one of the most advanced methods recently. In this new membrane, graphene is modified by creating nanopores on the surface of the graphene. In this process, well-structured channels of pores can facilitate the water flow and thus make the flow fast.

For rejecting ions and other solute molecules, the pores use physical principals such as charge and hydrophobicity.

Graphene has many advantages over other membranes that are used for the purpose of water desalination. The first and most important advantage is that since it is one atom thick, its thickness can be neglected. On the contrary to its negligible thickness, graphene has high mechanical strength and these two attributes lead to low pressure requirements and faster water transport.⁴

In addition, The size of the pores must be very precis, The process of determining graphene holes should be done with control, If these pores are large, the push molecule and large salts will pass through it and if the pores are small, water molecules will not pass through.

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Investigation of Condensation Reaction of o-Phenylendiamines with 2-(Bis(methylthio)methylene)-1*H*-indene-1,3(2*H*)-dione for the Preparation of *N*-Containing Heterocycles

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Abstract:

Heterocycles have many applications for the development of science and technology.¹ Benzimidazoles² and Benzoxazoles³ are two classes of heterocyclic organic compounds that are of great importance in the field of medicine, pharmacy, and biological activities.⁴

Our previous studies are providing new methods for preparing a series of new heterocycle compounds containing nitrogen and oxygen, which while expanding the boundaries of knowledge in the field of heterocycles chemistry, can provide new synthetic tools for researchers in the field of chemistry, biology and pharmacy.

In this work we used the reaction of 2(-bis(methylthio)methylene)-5,5-dimethylcyclohexane-1,3-dione (1) with benzene-1,2-diamines to synthesize <math>2-(1H-benzo[d] imidazole-2(3H)-iliden)-5,5-dimethylcyclohexane-1,3-diones (2). Various derivatives of products (2) were prepared using different derivatives of*o*-phenylenediamines. The reactions were done in ethanol at room temperature and the products were obtained in good to excellent yields. One pot, easy work-up, practical simplicity and no extraction and chromatographic purification steps are of the most advantages of this method. All products are new compounds, and their structures were characterized using the physical and spectral data.



Scheme 1: Synthesis of 2-(1H-benzo[d] imidazole-2(3H)-iliden)-5,5-Dimethylcyclohexane-1,3-diones

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Synthesis of New Schiff Base Benzothiazole Derivative

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Abstract

Schiff bases are important chelating agents which offer great versatility in the design of useful, interesting and commercial ligand system.¹⁻² Schiff bases and their metal complexes have been used in quantitative analysis, photometric analysis, fluorometry, as potentiometric sensors, in solvent extraction, as solid phase extraction sorbent, in high-performance liquid chromatography, in antimicrobial studies, as plant growth regulators, as insecticides, as a catalyst, in antifertility and enzymatic activity, as dyes, polymer and other miscellaneous applications.³ Synthesized compounds containing a thiazole moiety have been used for the treatment of allergies, hypertension, inflammation, human immunodeficiency virus (HIV) infections, and schizophrenia. Thiazoles also exhibit other biological activities, such as antibacterial, antitumor, analgesic, anticonvulsant, antimelanogenesis, antipsychotic, and antioxidant. Also, thiazoles can act as cyclin-dependent kinase (CDK) inhibitors and β -glucuronidase inhibitors. New 2,5-disubstituted hydrazinyl-thiazoles with 2-hydroxynaphthalen-1-yl 1 for first time was synthesized via the reaction of 2-hydroxy-1-naphtaldehyde 2, thiosemicarbazide 3, and 4-methoxy phenacyl bromide 5 in the presence of AcOH in EtOH under reflux conditions (Scheme 1). A literature survey indicated that hydrazone-thiazoles are generally synthesized in a two-step procedure. In other efforts, one-pot synthesis report for 1 was also completed.⁴



Scheme 1: Synthesis of 2,5-disubstituted hydrazinyl-thiazoles with 2-hydroxynaphthalen-1-yl

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A New and Practical Method for the Synthesis 5'-Amino-4'-nitro-3*H*-spiro[isobenzofuran-1,2'-pyrrole]-3,3'(1'*H*)-diones

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Abstract

Substituted phthalides (isobenzofuran-1(3*H*)-ones) represent an important class of natural products that possess significant biological properties.¹ In particular, 3-substituted phthalides are vital heterocyclic motifs in many bioactive compounds such as isocoumarins, anthraquinones, anthracyclines, and several alkaloids.² Their notable characteristics include antibacterial, anticonvulsant, anti-HIV, antiasthmatic, antitumor, antiplatelet activities, anesthesia prolongation, and PGF_{2α} inhibitory properties.³ Furthermore, the chemistry of isobenzofurans is of great importance, because they are 10π electron systems with a quinoid nature, which makes them attractive as unique building units for oligomeric and polymeric π-conjugated compounds.⁴⁻⁵

In continuation of our programs to develop more efficient processes for the synthesis of biologically potentially important oxygen- and nitrogen-containing heterocycles⁶, Herein, we try to report and a new and efficient method for the synthesis of 5'-amino-4'-nitro-3*H*-spiro [isobenzofuran-1,2'-pyrrole]-3,3'(1'*H*)-diones **2** by the oxidation of 2-amino-3*a*,8*b*-dihydroxy-3-nitro-3*a*,8*b*-dihydroindeno[1,2-*b*]pyrrol-4(1*H*)-ones **1** with lead acetate in acetic acid as solvent at room temperature (Scheme 1).



Scheme 1. Synthesis of 5'-amino-4'-nitro-3H-spiro[isobenzofuran-1,2'-pyrrole]-3,3'(1'H)-diones

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Synthesis of Novel Di indolyl Terpyridines in the Presence of Ammonium Acetate as a Catalytically Active Reagent *via* Cooperative Vinylogous Anomeric Based Oxidation

<u>Morteza Torabi</u>, Meysam Yarie, Mohammad Ali Zolfigol* Corresponding Author E-mail: Torabimorteza74@yahoo.com

Department of Organic Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan **Abstract**

Pyridine scaffolds as the most important families of nitrogen-containing heterocycles, have wide spread applications in natural products, pharmaceuticals, supramolecular chemistry, molecular machines, catalytic applications and functional materials.¹⁻³ These systems, due to privileged characteristics in medicinal chemistry have a tremendous application such as antiasthmatic, preventing or inducing apoptosis, antidepressant and inhibiting HIV protease.⁴⁻⁵ Recently, terpyridines as the preeminent subset of pyridine derivatives have found extraordinary application in modern chemistry. Undoubtedly, these compounds are the most important category in coordination chemistry.⁶⁻⁷ There are many applications for terpyridine families such as cancer therapy⁸, self-healing materials⁹, catalytic applications, chemical probes and chemical sensors. In this study, ammonium acetate was used as a catalytically active reagent for the synthesis of novel di indolyl terpyridines via cooperative vinylogous anomeric based oxidation (Scheme 1).



Solvent-free, 100 °C, 35-70 min, 60-83 %

Scheme 1: Synthesis of novel di indolyl terpyridines in the presence of ammonium acetate as a catalytically active reagent.

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Synthesis of New Series of Pyridines Hybrids Using A New Porous Polymer *via* Cooperative Vinylogous Anomeric-Based Oxidation

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Abstract

Design and investigation of new pyridine hybrids with less toxicity and higher selectivity can be a suitable and attractive topic for any medical chemist. On the other hand, pyridine hybrids are in the hearth of medical chemistry that have a good response as anticancer, antihypertensive, antidepressant, antifungal and antibacterial agents. Furthermore, pyridine family traces are found in many fields of chemistry including catalytic application, supramolecular chemistry, molecular machines and chemical sensors.¹⁻⁶ Sulfonamides as the main domains of organosulfur compounds, have a pivotal role in the areas of medicinal chemistry. Undoubtedly, the importance of sulfa drugs is obvious to any chemist. Then, design and synthesis of sulfonamides deserves more attention.⁷⁻⁹ Applications of triazole families was extensively studied as precursors in pharmaceutical and biological systems. There are unique application for triazoles such as antimicrobial, antiinflammatory, antitumor, inhibitors and antimalarial agents. Here, we studied the catalytic application of a porous polymer for the the synthesis of pyridines with sulfonamide, triazole and indole sections *via* cooperative vinylogous anomeric-based oxidation.



Scheme 1: Catalytic synthesis of hybrid pyridine.

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The Catalytic Role of Triphenylarsine in the (Z)-*N*-vinyl Heterocyclic Compound: An Experimental Mechanistic Study

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Abstract

In this scrutiny the kinetics and mechanism of the reaction between dimethyl acetylendicarboxcylate (DMAD) and phthalimide (N-H heterocyclic compound) in methanol environment with triphenylarsine (TPA) as a catalyst using UV/vis spectrophotometry. The effect of temperature, solvent and dialkyl acetylendicarboxcylate on the rate of reaction was investigated. The reaction followed second-order kinetics and the partial order of DMAD and phthalimide is one and one, respectively. Also, step2 of the reaction mechanism was recognized as a rate-determining step (RDS). In contrast, previous research was performed with triphenylphosphine (TPP) as a reactant (not catalyst) instead of TPA, so partial orders in related to DMAD, TPP and different cases of acids were 1, 1 and zero, respectively, in addition step1 was RDS. In recent work, TPA acted as a strong nucleophile, so in accordance with the experimental data was identified as a fast step. In fact, with a change from TPP towards TPA in the reaction environment and subsequently its reactivity, the behavior of the kinetics and mechanism of reaction also differed. From the temperature, concentration and solvent studies, the activation energy and the related activation parameters (Ea, Δ H‡, Δ S ‡ and Δ G‡) were calculated.



Figure 1: Condensation of acetylenic esters and phthalimide in the presence of triphenylarsine.

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Synthesis of Substituted Pyridines in the Presence of Novel Magnetic Nanoparticles

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Abstract

The high activity of catalysts and their reusability are two important factors in the modern catalytic processes. In this respect, magnetic nanoparticles (MNPs) have been emerged as one of the most useful heterogeneous catalysts due to their numerous applications in the chemical processes as well as organic synthesis. They are robust, inexpensive and recyclable by an external magnet for several runs without considerable loss of their selectivity and activity.¹⁻²

Pyridines have a key role in the biological behavior of several natural molecules and also, they are responsible for the pharmaceutical activity of various influential drugs.³ In addition, pyridine derivatives represent numerous capabilities in diverse areas such as catalysis, coordination chemistry, polymer science, materials and surfaces engineering and agrochemistry.⁴

In this exploration, we reported the synthesis and catalytic performance of novel magnetic nanoparticles for the preparation of linked-pyridine systems under solvent-free conditions (Figure 1).



Figure 1: Synthesis of substituted pyridines in the presence of pseudopolymeric magnetic nanoparticles

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A New Method for the Synthesis of Azocine Derivatives Using One-Pot Addition-Oxidation of Acenaphthoquinone and 2-Nitroethene-1,1-diamines

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Abstract

Medium ring heterocycles are abundant in natural products. Particularly, eight-membered heterocycles containing one nitrogen atom are the interest of chemists in such well-known targets. Azocine derivatives are a common precersors, which may be used to make a wide diversity of compounds that they are found in a variety of natural and synthetic products.¹ Many natural chemicals such as apparicine magallanesine and manzamine A², contain the eight-membered heterocycles having nitrogen- in their complicated structures.

In continuation of our ongoing programs for the synthesis of *N*-containing heterocycles³, herein, we try to report a clean and green method for the synthesis of new azocine derivatives **4** *via* addition reaction of 2-nitroethene-1,1-diamine derivatives **1** with acenaphthoquinone **2** in acetic acid at 50 °C followed by oxidative cleavages of the corresponding vicinal diols **3** using periodic acid (Scheme 1). Various azocine derivatives were synthesized and their structures were thoroughly characterized using their physical and spectral data. The protocol's key advantages include good yields, a simplified synthesis technique, lack of a need for any time-consuming work-up or column chromatography, no need for catalysis and mild reaction conditions.

General Procedure

A mixture of 2-nitroethene-1,1-diamine derivatives **1** (1 mmol) and acenaphthoquinone **2** (1 mmol) in acetic acid (3 mL) was stirred at 50 °C. The progress of the reaction was monitored by thin layer chromatography. All reactions were completed in about 6-8 h. The reaction mixture was then cooled to room temperature, H_5IO_6 (1 mmol) added and stirring was continued for additional 2 hours. Filtration of the reaction mixture and washing of the precipitates with distilled water (2× 3 mL) yielded pure azocine derivatives **4** (Scheme1).



Scheme 1. Synthesis of azocine derivatives 4 *via* addition reaction of 2-nitroethene-1,1-diamines 1 and acenaphthoquinone 2 followed by oxidative cleavages of the corresponding vicinal diols 3.

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Facile Synthesis of 3,4-Dihydropyrimidin-2-thiones by Ring Forming Multicomponent Reactions

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Abstract

Multicomponent reactions (MCRs) are of increasing importance in organic and medicinal chemistry because the strategies of MCR offer significant advantages over conventional linear-type syntheses.¹ Compared with conventional methods of organic synthesis, MCRs have the advantages of high selectivity, good yields, milder reaction conditions, and simple work-up procedures, among others. Thus, a vast number of diverse compounds can be obtained in parallel synthesis.² MCRs play an important role in the generation of multi functionalized products, including 3,4-dihydropyrimidin-2-thiones (DHPMs).³ These compounds exhibit widespread biological applications such as antihypertensive, antiviral, antitumor, antibacterial, α -1a-antagonism, antioxidant, and anti-inflammatory actions.⁴ Therefore, there is a considerable demand for efficient synthetic strategies for producing these compounds.

This research focuse on ring-forming multicomponent reactions for synthesizing substituted DHPMs. The reaction of arylglyoxal monohydrates **1** with enaminoketones **2** and ammonium thiocyanate **3** in dichloromethane in the presence of catalytic amounts of FeCl₃ at room temperature provided a threecomponent facile and efficient route for the synthesis of the expected products **4** (Scheme 1). The products were separated by column chromatography (silica gel, *n*-hexane-ethyl acetate, 5:1). All compounds were characterized using the NMR and IR spectral and analytical data. The advantages of this method are readily available starting materials, neutral reaction conditions, and high yield of products at ambient temperature.



$$Ar^2 = C_6H_5$$
, 4-CH₃C₆H₄, 4-CH₃OC₆H₄, 4-ClC₆H₄

Scheme 1: One-pot domino synthesis of 3,4-dihydropyrimidin-2-thiones

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Co(II) complex immobilized on graphene oxide: As a catalyst for the oxidation of thiols to disulfides

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Abstract

Oxidation of thiols to disulfides is an important transformation from synthetic, biological, and industrial viewpoints. In addition, disulfides find extensive applications as protecting groups in the synthesis of pharmaceutical, bioactive compounds and as vulcanizing agents for rubbers.¹ Recently, graphene oxide (GO) with unique properties² and interesting two-dimensional structures³ have emerged as ideal supports for a variety of catalytic species. Besides the availability of surface functionalization, their two-dimensional structures not only allow excellent dispersion of the catalytic species but also facilitate mass transfer in the reaction processes. Reactive species can readily access the active sites with limited mass transfer resistance. Therefore, the remarkable catalytic performance of graphene or GO-supported catalysts has been observed. Herein, we developed an in situ strategy of synthesis and immobilization of a copper complex onto GO support. It was found that the immobilized copper complex [Cu(TSC)@GO], not only showed superior catalytic activity for the oxidation of thiols but also exhibited outstanding stability even after intensive reuse, which displays its potential for practical applications(Scheme 1).



Scheme 1 Oxidation of thiols to a disulfide.

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Functionalized Graphene Oxide Supported Copper (I) Complex as Effective and Recyclable Catalyst for Synthesis of Triazoles

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Abstract

Triazoles have gained interest over the past few years following the introduction of the "click chemistry" concept. 1,2,3-Triazoles are typical five-membered nitrogen heterocyclic compounds.¹ Advancement in the field of heterogeneous catalysis has introduced retrievable catalysts which offer immense surface area, excellent activity, selectivity, non-toxic nature, recyclability, and chemical stability. Among several types of solid materials, graphene oxide has attracted tremendous attention in the development of composite materials and catalysts, due to their remarkable physical, chemical and electrical characteristics, including a very high specific surface area.² In the present report, we have synthesized and characterized a retrievable, easily generated, chemically stable, and environmentally friendly copper-based catalyst for the synthesis 1,2,3-triazoles (Scheme 1). The obtained heterogeneous catalyst was thoroughly characterized by various techniques. This catalyst was then used for the efficient synthesis of 1,2,3-triazoles giving access to these products in excellent yields. Further, this protocol involves low loading of copper and undergoes no leaching. Additionally, superb catalytic activity, effortless catalytic recovery, and recyclability of the catalyst up to five consecutive runs without significant loss of activity.



Scheme 1. Synthesis of 1,2,3-triazoles

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Synthesis of New Pyridines Containing Sulfonate and Sulfonamide Groups in the Presence of Novel Nanomagnetic Hydrogen Bond Catalyst

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Abstract

The development of environmentally firendly catalytic systems is one of the main goals of green chemistry.¹⁻² To this end, designing of nanomagnetic catalysts due to their high catalytic performance and easy recovering and reusing capability³ provide great help to achieve the goals of green chemistry.⁴⁻⁵

Many types of natural products, such as hormones, vitamins, and even necessary antibiotics for life, have heterocyclic skeletons.⁶

Pyridine, a heterocyclic compound, is used as a medicine for treatment of diseases such as depression.⁷⁻⁸

In this study, with the support of the anomeric effect, synthesis of new pyridines sulfonate and sulfonamide sections in the presence of novel nanomagnetic hydrogen bond catalyst is reported (Scheme 1).



Scheme 1: Catalytic synthesis of pyridine derivatives in the presence of novel nanomagnetic hydrogen bond catalyst.

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Synthesis of New Pyridines Incorporated with 1,2,3-Triazole by the Cooperative Vinylogous Anomeric-Based Oxidation in the Presence of a Nanomagnetic Catalyst

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Abstract

Substituted pyridines are common in many biologically active compounds, among them, 3-cyano-2-hydroxypyridines have been an essential part of molecular structures for the design and construction of a variety of biologically active compounds.¹ Recently multicomponent reactions (MCRs) have received great attention from researchers for the synthesis of new heterocyclic compounds due to the wide range of their potential biological and pharmaceutical activities and industrial applications.² On the other hand, magnetic nanocatalysts are easy to separate from reaction media, thus have been used for various purposes.³ Herein, we represent the synthesis of novel pyridines incorporated with 1,2,3-triazole *via* a green one-pot four-component reaction of arylaldehydes, ethyl cyanoacetate, 1-(5-methyl-1-(4-nitrophenyl)-4,5-dihydro-1H-1,2,3-triazole-4-yl)ethenone, and ammonium acetate using a recyclable magnetic nano-sized catalyst





Scheme 1: General procedure for the synthesis of novel pyridines incorporated with 1,2,3-triazole in the presence of Fe₃O₄@SiO₂@ULCA as catalyst.

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Magnetic Nanoparticles Bearing Urea Moiety: A Novel Efficient Catalyst for the Synthesis of 2-Amino-3-cyano pyridines *via* Vinylogous Anomeric-Based Oxidation

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Abstract

2-amino-3-cyano pyridines are a very prominent series of the heterocyclic component as they represent the exceptional pharmacological role.¹ On the other hand, multicomponent reactions (MCRs) are becoming important instruments in the new synthesis chemistry due to their efficiency, economic benefits, green synthesis and ease of formation of various new compounds in one-pot reactions, which operated effective characters in developing the green chemistry and complex structures.² In recent years, the use of magnetic nanocatalysts has become attractive due to separation and reusability.³

In this context, we report the synthesis of 2-amino-3-cyano pyridines *via* a one-pot four-component reaction of arylaldehydes, malononitrile, ammonium acetate and (methyl ethyl ketone or methyl isobutyl ketone) by use of a highly efficient magnetic catalyst, the reaction proceeds with high yield under solvent-free conditions then the catalyst could be separated from the reaction mixture by use of an external magnet (Scheme 1).



Scheme 1: Synthesis of new 2-amino-3-cyano pyridines using a novel magnetically separable catalyst

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Synthesis of α-Ariloxy Alcohols Using [Zr-UiO-66]CO₂H as A Novel Metal Organic Framework

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Abstract

Epoxides are important starting materials and useful synthetic intermediates in organic synthesis. Also, the conversion of an alkene to an epoxide is a part of a more extensive molecular transformation. Since epoxide ring-opening is usually stereospecific, such reactions can be used to establish stereochemical relationships between adjacent substituents.¹ For this purpose, a wide range of mono or 1,2-disubstituted products, have been synthesized *via* the addition of various nucleophiles to epoxides and different promoters and conditions have been proposed.² Ring-opening of epoxides with phenol or thiophenols has a considerable role in pharmaceutical manufacture because of their remarkable efficiency in the preparation of natural products, organic products and bioactive compounds such as guaifenesin, mephenesin, chlorophenesin, propranolol and naftopidil.³ Herein, we have prepared and [Zr-UiO-66]CO₂H and successfully tested it on the synthesis of α -ariloxy alcohols at 110 °C under solvent-free conditions (Scheme).



Y=Ar, R, CH₂OR

Scheme: Preparation of *α*-ariloxy alcohols using [Zr-UiO-66]CO₂H as a novel metal organic framework

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Synthesis of A Novel Calix[4]Arene Appended Aminochalcone

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Abstract

In this study, we have synthesized novel calix[4]arene N-chalconeamid derivatives by the reaction of N-acylated aminochalcone with calix[4]arene **1**. Indeed, by controlling the reaction conditions, we could produce di-substituted and mono-substituted calix[4]arene individually. The structure of the calix[4]arene derivatives were characterized by ¹HNMR and ¹³CNMR.



Scheme 1 Synthesis rout of novel calix[4]arene N-chalconeamid derivatives 2,3.

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Synthesis of Bis(aminopyrimidine) Derivatives Using Graphene Immobilized Cobalt Ferrite (CoFe₂O₄@CS@GO) as Catalyst

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Abstract

Pyrimidine derivatives are a group of compounds containing naturally fused uracils due to their wide range of pharmacological activities such as antiviral¹, anti-cancer², and antibacterial³ have a special place in synthetic and pharmaceutical chemistry. In this study, graphene oxide immobilized on chitosan contains cobalt ferrite (CoFe₂O₄@CS@GO) as a new recyclable magnetic nanocatalyst was used in the synthesis of bis(aminopyrimidine) derivatives by the reaction of aromatic aldehydes and 6-aminouracil in ethanol with good to excellent yields under reflux conditions (Scheme 1). The CoFe₂O₄@CS@GO catalyst can be easily recovered by magnetic separation and used several times without significantly reducing its catalytic activity. The catalyst was characterized by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), thermal gravimetric analysis (TGA), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDs), and vibrating sample magnetometer (VSM).The high efficiency of the products and easy separation of the nanocatalyst from the products with an external permanent magnet are some advantages of this method. Products were identified by the comparison of their physical properties and spectra data, with those reported for authentic samples.



Scheme 1: Synthesis of bis(aminopyrimidine) derivatives using CoFe2O4@CS@GO

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Design and Synthesis of Amino Acid Prodrug of Methotrexate for Enhanced Brain Delivery

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Abstract

Methotrexate (MTX), a selective anticancer drug, has a weak permeability of the blood brain barrier (BBB), which makes it unable to treat brain tumors.¹ Therefore, the poor permeability of methotrexate against the blood brain barrier limits its administration for treating brain cancer.²⁻³ To use phenylalanine as a carrier, a derivative of methotrexate with structural phenylalanine properties, with the aim of enhancing drug delivery to the brain, was synthesized. MTX was reacted with phenylalanine by amide bonding. Purities of the final compound was determined by an analytical HPLC. Using the NMR spectroscopy analysis, its chemical structure was confirmed and examined.



Scheme 1: Synthesis steps of phenylalanine-methotrexate prodrug. Reagents and conditions: (i) Anhydrous DMF, DCC, Ethyl Acetate, stir at 0 °C for 2 h, MTX stir at room temp. for 24 h; (ii) TFA, Anhydrous DMF, stir at room temp., 3 h.

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ZnFe₂O₄@L-Arginine–Ni Nanoparticles: A novel, Efficient and Recyclable Catalyst for the Synthesis of Tetrazole and Oxidation of Sulfides Derivatives

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Abstract

In this work, a green method was suggested for the synthesis of ZnFe₂O₄ magnetic nanoparticles (MNPs) as a novel heterogeneous catalytic support in order to immobilize the homogeneous complexes.¹ In this case, the study aims at immobilizing L-Arginine-Ni complex on the surface of ZnFe₂O₄ MNPs. L-Arginine-Ni was immobilized on ZnFe₂O₄ MNPs surface by a simple, fast, and convenient route. The structure and composition of the prepared ZnFe₂O₄@L-Arginine-Ni MNPs were completely characterized by XRD, EDX, ICP, SEM, X-ray mapping and TGA and VSM techniques. Besides, it was applied as a green nanocatalyst for 5-substituted 1H-tetrazole derivatives and Oxidation of sulfides reactions under green conditions. The ZnFe₂O₄@L-Arginine–Ni MNPs offer several advantages i.e. simple synthesis method under green conditions, thermal and chemical stability during organic reactions, short reaction times, high yields of the products, excellent selectivity and easy work-up procedure.² Moreover, the recycled nanocatalyst was reused for at least five cycles with no significant loss of its activity. Hot filtration test indicated heterogeneous catalysis for both of the mentioned reactions. This work is useful for the development and application of the magnetically recoverable Ni nanocatalyst on the basis of green chemistry principles.







Scheme 2. ZnFe₂O₄@L-Arginine-Ni MNPs catalyzed the oxidation of sulfides to sulfoxides

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M. Hähsler *et al.*, Magnetic Properties and Mössbauer Spectroscopy of Fe3O4/CoFe2O4 *Nanorods, Inorg. Chem.* **2020**, *vol.* 59, no. 6, pp. 3677–3685, doi: 10.1021/acs.inorgchem.9b03267.







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Stabilized Ascorbic Acid on Ferrite Nanoparticles, A Green Catalyst, Efficient and Useful in the Synthesis of Quinazoline and Chromeno[2,3-d] pyrimidin-8-amine Derivatives

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Abstract

In the present study, ZnFe₂O₃ nanoparticles were prepared in a simple and versatile way. Then, a new green catalyst with ascorbic acid immobilization was synthesized on ZnFe₂O₃ nanoparticles.^{1,2} The activity of this nanostructured compound was investigated for the synthesis of chromeno[2,3-*d*] pyrimidine-8-amine and quinazolinone derivatives. The catalyst prepared by Fourier transform infrared spectroscopy (FT -IR), scanning electron microscopy (SEM), energy scattering X-ray spectroscopy (EDS), X-ray diffraction (XRD), thermal gravity analysis (TGA) and size Vibration magnetometer (VSM) sampling was examined and identified.^{3,4} This metal-organic catalyst was recovered from the reaction mixture using an external magnetic field and reused for five continuous cycles without significant change in its catalytic activity.



Scheme 1. Synthesis of chromeno[2,3-d]pyrimidin-8-amines catalyzed by ZnFe₂O₄@SiO₂-ascorbic acid



Scheme 2. Synthesis of quinazoline catalyzed by ZnFe₂O₄@SiO₂-ascorbic acid

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Greener One-Pot Synthesis of Dithiocarbamate Derivatives in Deep Eutectic Solvent

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Abstract

One of the ultimate goals and challenges in chemistry is developing highly efficient transformations to prepare biologically active and functional materials from small and commercial compounds with potential application in the pharmaceutical or agrochemical industries.¹

lonic liquids were the first potentially promising alternative to organic solvents for biotransformation; due to their nonvolatility, thermal stability, and high solvation properties. Recently, a new generation of green solvents, namely deep eutectic solvents (DESs), has emerged as an environmentally-benign media alternative to hazardous organic solvents in various applications. DESs are liquid systems formed from a eutectic mixture and, due to the similar common properties of ionic liquids (ILs) serve as a low-cost alternative to ILs. DESs can be prepared in a pure state by combining hydrogen bond donors and hydrogen bond acceptors by simply mixing two or more cheap and biodegradable components.²

Based on our continuous interest in establishing green solvents for organic transformations, we recently developed the deep eutectic solvent as a green solvent and catalyst in organic synthesis. This paper reports green and efficient multicomponent domino reactions of ketones, aldehydes, amine, and carbon disulfide in urea-choline chloride-based DESs under catalyst/ solvent-free conditions. DES very efficiently catalyzes the tandem Knoevenagel condensation and Michael constructing multisubstituted dithiocarbamates in good to excellent yield (Scheme 1).



Scheme 1. one-pot synthesis of dithiocarbamate in DES, DES: urea-choline-chloride (2:1)

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Highly Efficient Synthesis of Rhodamine Derivatives in Water

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Abstract

Recent years have witnessed a significant drive to increase the efficiency of organic transformations while lowering the number of waste materials. Solvents play a central role in these efforts: solvents are often the largest sources of wastes in chemical syntheses and processes. Eliminating solvents can dramatically reduce the amount of waste and volatile organic compounds in the industrial revolution. Recent endeavors have focused on limiting organic solvents and replacing them with new, environmentally benign media. In these contexts, room temperature ionic liquids, water, and polyethylene glycol have attracted considerable attention as novel reaction media over the last decade.¹

Rhodamine, thiazolidine-2,4-diones, and pseudothiohydantoins have become an exciting class of heterocyclic compounds since various glitazones and epalrestat were introduced into clinical use for clinical use the treatment of type II diabetes mellitus and diabetic complications, respectively. Chemical modifications of these heterocycles constantly result in compounds with a broad spectrum of pharmacological activities. 5-Arylidenerhodanines are frequently potent hits in high throughput screening against various prokaryotic and eukaryotic targets. Synthesis of substituted rhodanine, based on high throughput screening hits, often leads to potent and selective modulators of targeted enzymes or receptors, which exert their pharmacological activities through different mechanisms.²

During our investigation aimed at improving the greener parameter of organic processes, we evaluated the possibility of performing these organic transformations by using water as green solvent or under solvent-free conditions to develop environmentally benign reactions.³ We report a practical and straightforward synthesis of rhodamines promoted by water under mild reaction conditions (Scheme 1).



R= Alkyl and Aryl

Scheme 1. General scheme

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Synthesis of 7-Hydroxybenzo[c]pyrrolo [4,3,2-*mn*]acridin-5(6*H*)-ones from 2-Aminonaphthalene-1,4-diones and Isatins

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Abstract

Cancer is one of the most dreaded diseases of mankind and it is the principal cause of mortality worldwide. Fortunately, Isatin (indoline-2,3-diones) exhibits anticancer activities by inhibiting tyrosine kinase or caspase.¹ Acridine occurs in a large number of natural products and attracts much attention due to its widely biological activities.² Acridine derivatives exhibit many biological activities and due to their importance in human health care and many other applications, significant effort has been devoted to the synthesis of these valuable compounds.³ It was also found that pyrroloacridines and pyrroloacridones are attractive antitumor anthelmintic and antifungal organic molecules. Some of them may be useful to develop chemotherapy antitumor drugs since they can bind to DNA and inhibit the growth of cancerous cells.⁴

A mixture of 2-aminonaphthalene-1,4-dione **1** (1 mmol), isatins **2** (1 mmol) and 5-methyl-2-phenyl-2,4dihydro-3*H*-pyrazol-3-one **3** (1 mmol) as catalyst in ethanol (3 mL) was stirred under reflux for about 4 hours. The reaction mixture was filtered and the filtrate was washed with hot ethanol (10mL) to give the desired pure product **4** (Scheme 1). All products are new compounds, and their structures were characterized using the physical and spectral data.



Scheme 1: Synthesis of 7-hydroxybenzo[c]pyrrolo[4,3,2-mn]acridin-5(6H)-one

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One-Pot Three-Components Synthesis of Pyrroloacridine Derivatives from the Reaction of Dimedone, Amines, and Isatins using Copper (II) Acetate as Catalyst

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Abstract

Nitrogen-containing heterocyclic compounds, especially with the core-acridine skeleton, are very promising and noteworthy targets because of their remarkable array of bioactivity profiles such as anti-helmintic and antitumor activities.¹ Pyrroloacridone derivatives are of interest owing to their various pharmacological and biological activities.² Derivatives of pyrroloacridine exhibit promising biological activities such as anthelmintic and anticancer activity.³ Some of these compounds inhibit the growth of cancerous cells *via* binding to DNA, whereupon they offer potential lead frameworks for developing novel anticancer drugs.⁴

In continuation of our previous works on the synthesis of N-containing heterocycles⁵, herein, we try to report a new one-pot three-component procedure for the synthesis of pyrroloacridine derivatives. The reactions were carried out based on the reaction of aromatic amines, isatins, and dimedone in ethanol, under reflux conditions, and in the presence of copper (II) acetate as catalyst. The reactions were completed in 1h and the products were easily obtained by simple filtration of reaction mixture and recrystallization of crude products from ethanol.



Scheme 1: Copper (II) Acetate catalyzed one-pot three-components synthesis of 2-arylpyrroloacridin-1(2*H*)-ones

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Application of CuO Nanoparticle, Polypyrrole and CuO-Polypyrrole Nanocomposite in CHF Enhancement

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Abstract

In recent years, using nanofluids (resulting from the dispersion of nanoparticles or nanocomposites in the base fluid) as thermodynamic liquids has increased. The first phase in nanocomposites (a combination of several materials, at least one of them is in the dimensions of 1 to 100 nanometers), which is the base of the nanocomposite, is usually made of polymer, metal or ceramic and the second phase is nanometerscale particles that are distributed in the first phase. Conductive polymers are used as the first phase of nanocomposites for reasons such as high conductivity, low cost, ease of fabrication and low density (which makes nanocomposites more stable in fluid).¹ Boiling is one of the many chemical engineering processes. Boiling in static conditions and closed chamber is called pool boiling. One way to increase the efficiency of pool boiling systems is to apply a change to the fluid used and replace it with nanofluid, which can transfer more heat flux in certain dimensions.² In this study, copper oxide nanoparticle, polypyrrole and copper oxide-polypyrrole nanocomposite were synthesized and their characteristic were analyzed by TEM and FTIR. Then samples containing 0.015 and 0.03% by weight of the synthesized materials in the water-based fluid were made. These samples have been used to measure the critical heat flux (CHF) and to evaluate the stability. The results of examination of these samples showed that at the same concentration, the sample containing polypyrrole has more stability and lower thermal conductivity than other samples. Copper oxide/water nanofluid has a higher thermal conductivity and less stability than other samples and copper oxide-polypyrrole/water nanofluid has an optimal thermal conductivity and stability. Also by increasing concentration of nanoparticles in nanofluid, CHF increase.

	DW	CuO/DW		ppy/DW		CuO-ppy/DW	
		0.015 wt%	0.03 wt%	0.015 wt%	0.03 wt%	0.015 wt%	0.03 wt%
Stability	-	Less than one hour	Less than one hour	Stable (15 day)	Stable (15 day)	Stable (15 day)	Stable (15 day)
CHF (MW/m ²)	1.14	5.94	6.9	2.01	2.88	4.83	5.76

Table 1: Result of CHF and stability measurement of nanofluids

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Lipase Immobilized on the Magnetic Cross-Linked Chitosan Hybrid Polymer and Investigation of Catalytic Activity in Henry Reaction

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Abstract

In this work, we immobilized the lipase from Aspergillus oryzae enzyme on the magnetic chitosan crosslinked hybride network and investigated its efficiency in Henry reaction. The oxidation of chitosan polymer was performed to afford chitosan dialdehyde and used as a cross-linking agent for the content connection of chitosan chains. The hybrid polymer was stabilized and also provided aldehyde functional groups for futher modification. The magnetization process was carried out through the reaction of CS-CSOX polymer with iron oxide nanoparticles. Lipase enzyme was covalently immobilized on the magnetic Fe3O4@CS-CSOX biopolymer through imine bond formation between amine groups of the enzyme with the extant aldehyde functional groups of polymeric hybrid. After the synthesis of biosupport based on the enzyme, its catalytic activity was examined in Henry reaction. This bionanocomposite has shown the high activity in reaction 4-nitrobenzaldehyde with nitromethane or nitroethane (Scheme 1).



Scheme 1: The catalytic activity of bionanocomposite in Henry reaction

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Synthesis of Benzothiazole Compounds and their Derivatives from Vinamidinum Salts

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Abstract

Benzothaizole is a fused benzoheterocyle which is present in many naturally occurring products and responsible for the medicinal, applications of natural product.¹ Thiazole and its derivatives have been of great scientific exploitation and interest as these are accompanied with almost all the biological and pharmacological activities, like antibacterial, antiprotozoal, antimalarial, anticancer, treat allergies.² And anticancer drugs.³

A mixture of (Z)-N-(2-argio-3-(dimethylamino)allylidene)-N-methylmethanaminium **1**, 2-hydrazineylidene-3methyl-2,3-dihydrobenzo[d]thiazole **2** and triethylamine as a base in acetonitrile was stirred at 80 °C for about 12 hours 3-methyl-2-(((1E,2Z)-3-(2-((E)-3-methylbenzo[d]thiazol-2(3H)-ylidene)hydrazineyl)-2phenylallylidene) hydrazineylidene)-2,3-dihydrobenzo[d]thiazole **3** were easily obtained by filtration of the reaction mixture and recrystallization of crude products from boiling ethanol and water (Scheme 1). All products are new compounds, and their structures were characterized using the physical and spectral data.



Scheme 1: (Z)-3-methyl-2-(((1E,2E)-3-(2-((Z)-3-methylbenzo[d]thiazol-2(3H)-ylidene)hydrazineyl)-2-phenylallylidene)hydrazineylidene)-2,3-dihydrobenzo[d]thiazole

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Synthensis of 2-Aryl-3-((benzothiazole)-2-ylidene)-2-propenol from Vinamidinium Salts

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Abstract

Heterocyclic chemistry has become one of the most important fields of research in pharmaceutical industry due to their many fold applications.¹ Benzothiazoles and benzotriazoles are extensively applied in various consumer products and industrial application that they are employed as vulcanization additives in rubber and corrosion inhibitors.² Synthesis of benzothiazole derivatives is necessary since benzothiazole is of major interest in medicinal chemistry due to its wide range of biological activities. This is why many effective and attractive methods were developed for the synthesis of benzothiazole derivatives.³ Besides, the application of these molecules was ascer- tained by testing their anticancer potential because of a great de- mand of new anticancer drugs.⁴

A mixture of (Z)-N-(2-argio-3-(dimethylamino)allylidene)-N-methylmethanaminium **1**, 2-hydrazineylidene-3methyl-2,3-dihydrobenzo[d]thiazole **2** and triethylamin as a base in acetonitrile was stirred at 80 °C for about 12 hours. Products 2-Aryl-3-((benzothiazole)-2-ylidene)-2-propenol **3** were easily obtained by filtration of the reaction mixture and recrystallization of crude products from boiling ethanol and water (Scheme 1). All products are new compounds, and their structures were characterized using the physical and spectral data.



Scheme 1: 2-Aryl-3-((benzothiazole)-2-ylidene)-2-propenol

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Preparation of Magnetic NiCuFe₂O₄ NPs and its Application as A Reusable Nanocatalyst for the Synthesis of Xanthene Derivatives

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Abstract

Xanthenes are pharmaceutically useful oxygen heterocycles that have a significant position in the field of medicinal and material chemistry. They are known to show a wide range of biological properties such as; antibacterial¹, anticancer², anti-inflammatory³, antiviral agents⁴, and photosensitizers in photodynamic therapy for the treatment of localized tumors.

Ferrite spinels may also include a mixture of two divalent metal ions, in which the ratio of these divalent metal ions may vary, which are called mixed ferrite. The cation's combination of mixed ferrite significantly influences the surface properties of ferrospinels making them catalytically active. Due to the small size of metal nanoparticles, their catalytic activity increases sharply. One of the most important factors for the design and preparation of catalysts is their recoverability. Catalysts with easy recovery capability and no decrease in reaction yield after recovery are very economically desirable. The multimetallic catalysts are a major type of heterogeneous catalysts due to their superior catalytic activity compared to single metal catalysis components.

In this research, we hope to report preparation of magnetic NiCuFe₂O₄ NPs and using as reusable nanocatalyst for synthesis of xanthenes from the reaction of 2-naphthol with aldehydes under reflux conditions (Scheme 1). The catalyst was characterized by FT-IR, XRD, SEM, EDX and VSM techniques. The obtained products were identified by IR and ¹H NMR spectra.



Scheme 1. Synthesis of Xanthene derivatives using NiCuFe₂O₄ nanocatalyst

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Synthesis of Tetrahydrobenzo[b]pyran Derivatives in the Presence of Glydi(pyridin)-Mn Schiff-Base Immobilized on Fe₃O₄ MNPs

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Abstract

In recent years, the improvement of nanotechnology led to an increasing insist for multifunctional materials owing to simplicity in operation, remarkable recyclability, high surface area of catalysts and ecofriendly nature.¹ In this regard, solid catalysts and magnetic composite nanoparticles are interesting for industrial and biomedical applications and, especially, in catalysis studies as a magnetically separable catalyst.²

Oxygen containing heterocycles have an important role in organic and bio-organic Chemistry. The synthesis of these compounds is now very important and various methods for the synthesis of these compounds have been reported. The role of catalysts in the production of these compounds is undoubtedly important. So far, various catalysts have been used in the synthesis of these compounds, the most efficient of which are solid acid catalyst.³

In the development of greener and sustainable processes for the organic synthesis, di(pyridin)-Mn Schiff-Base complex supported on Fe₃O₄ magnetic nanoparticles (Fe₃O₄@Gly-di(pyridin)-Mn Schiff-Base) was prepared by simple procedure and applied as catalyst for the preparation of Tetrahydrobenzo[b]pyran derivatives using expensive, green and available materials in ethanol at reflux conditions (Scheme. 1). In addition, the magnetic and heterogeneous nature Allows easy separation of the catalyst from the reaction mixtures by a magnet and decantation and the catalyst could be reused at least 5 catalytic cycles for both of the mentioned reactions without obvious drop of initial activity.



Scheme 1: Fe₃O₄@Gly-di(pyridin)-Mn Schiff-Base catalyzed the synthesis of Tetrahydrobenzo[b]pyran derivatives in ethanol at reflux conditions.

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Application of MIL-100(Cr)/NHEtN(CH₂PO₃H₂)₂ as Mesoporous Catalyst in the Synthesis of Spiro Derivatives

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Abstract

Nowadays, Multi component reaction as an efficient synthetic route has been used for the synthesis of a wide range of organic molecules.¹ Target molecules may be produced via its rational design and applying a suitable multi component method. Spiro compounds as drug candidates are target molecules for pharmaceutical investigations. To the best of our knowledge, some pharmaceutical properties have been reported for spiro compounds such as spasmolitic, anticoagulant, anticancer, antimicrobial and anti naphylactic activities.² Metal–organic frameworks (MOFs) have been considered as a new category of nanoporous material. They have been used for various purposes such as storage and separation of gas, catalysts, and heavy-metal adsorption.³ In this work, we have prepared and characterized MIL-100(Cr)/NHEtN(CH₂PO₃H₂)₂, as a mesoporous catalyst. The described MIL-100(Cr)/NHEtN(CH₂PO₃H₂)₂, used for synthesis of spiro compounds via one-pot condensation of acenaphthylene-1,2-dione, 3-methyl-1-phenyl-1*H*-pyrazol-5-amine and 3-(1-methyl-1*H* indol-3-yl)-3-oxopropanenitrile under CH₃CN reflux (Scheme 1).



Scheme 1: Preparation of spiro compounds using MIL-100(Cr)/NHEtN(CH₂PO₃H₂)₂

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Synthesis of Poly-Functionalized Pyridine Derivatives in the Presence of a Novel Phosphonium-Based Ionic Liquid Catalyst Under Green Conditions

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Abstract

Recently, some specific efforts have been made to design organic reactions to afford hetroatom-containing molecules, among which the synthesis of pyridine-containing molecules – e.g. poly-functionalized pyridines an bis-functionalized pyridines – has been extensively investigated due to their biological and pharmaceutical activities.¹ One of the most recent approaches to synthesize these important products is the multicomponent synthesis in which the raction mechanisen contains at last one anomeric process, coming from Nitrogen to generate the aromatic ring via an oxidation process.² These techniques have been used to modify the antiquated synthetic methods.

lonic liquids (ILs) with unique properties have gained increasing attention in modernchemistry. During the last two decades, a large number of ILs has been reported in the literature, among them phosphoniumbased ionic liquids have drawn great attention due to their potential applications in many fields especially in the catalytic synthesis of various organic and bioorganic molecules via organic transformations.³ Herein, we want to desig a novel phosphonium-based ionic liquid catalyst, which was synthesized used as catalyst in the synthesis of bis-functionalized pyridine derivatives *via* a pedso-four-component reaction (Scheme1). Resulting experimental data suggest that the plausible mechanism proceeds *via* a cooperative vinylogous anomeric-based oxidation mechanism.



Scheme 1: Phosphonium based ionic liquid catalyzed the synthesis of poly-functionalized pyridine derivatives at 90 °C under solvent-free comditions.

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Synthesis of Imidazole by Metal Ferrites as Nanomagnetic Catalyst (CoCuFe₂O₄)

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Abstract

Imidazoles are a major of five membered heterocyclic compounds which have a wide range of biological and physical activities.¹They are also the active nucleic of therapy in many biological and pharmaceutical molecules that have been used in recent years to synthesize various compounds and various drug.² The best reported way for the preparation of 1,2,4,5-tetra substituted imidazoles is to use Benzil, primary amines ,aryl aldehydes and ammuniom acetate in the presence of acid catalysts³ under reflux conditions (Figure 1). To develop a non-toxic, inexpensive ,environmentally friendly and efficient catalyst for the synthesis of 1,2,4,5-tatra substituted imidazoles. Tri-transition metal ferriets nano crystals prepared by solgel method and used as an acid catalyst. In this research for the production of nano composite (CoCuFe₂O₄), we report a sol-gel method using ultrasonic and thermal to fabricate a tri-metal catalyst significantly. Which with different analyzes such as FT-IR, XRD, SEM, VSM, Melting point (M.P) and methods IR, H-NMR were identified.



Figure 1: Synthesis of substituted imidazoles by CoCuFe₂O₄ nanocoposite.

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Thermal Pyrolysis of Linseed Waste for the Production of Biochar

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Abstract

Pyrolysis is a thermochemical decomposition process that degrades the organic biopolymers that make up a biomass through a series of complex reactions in an oxygen-free environment, mainly caused by nitrogen gas. Pyrolysis includes solid, liquid and gaseous products.¹

Biofuel is a dark brown organic liquid that has received much attention in the pyrolysis process. This product is of strategic importance because as a liquid product is similar to petroleum oil.

Biochar is a solid product of the pyrolysis process and a polycyclic aromatic carbon obtained by combining or condensing benzene rings during the pyrolysis process. Land reclamation, soil fertility improvement, pollution remediation, agricultural waste recycling, use as a catalyst, use to remove water pollutants and suitable substances to eliminate pollutants in exhaust gases is one of the applications of it.²

The purpose of this study is to produce biochar from linseed oil waste by thermal pyrolysis. The pyrolysis process was performed in the temperature range of 350-550 °C and particle size with mesh number 30-100 under the nitrogen gas flow rate of 125 cm³/min and the heating rate of 20°C/min in a tubular reactor. All experiments were designed using the response surface method.

Figure 1 shows the simultaneous effect of temperature and particle size on biochar yield. High temperatures increase yield, but it cannot be increased by any measure. Primary biomass decomposition at high temperatures as well as secondary thermal decomposition of biochar leads to reduced biochar yield. However, at very high temperatures, due to the reduction of organic matter and compounds and the secondary decomposition of volatile compounds, the yield increases. But particle size has no effect on yield and can be ignored.³ As a result, temperature is the most effective parameter on the biochar yield produced by pyrolysis of linseed waste.



Figure 1: Response surface 2D plot and contour plot of Biochar yield

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Catalytic Application of Urea-Benzoic Acid Functionalized Magnetic Nanoparticles for the Synthesis of 2-Aminothiophene Derivatives

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Department of Organic Chemistry, Faculty of Chemistry, Bu-Ali Sina University, Hamedan **Abstract**

Heterogeneous catalysis due to unique perspective in the areas of chemistry increasingly have been considered by researchers. On the other hand, magnetic nanoparticles (MNPs) as a preeminent subset of heterogeneous catalyst are a useful strategy in many of catalytic reactions.¹⁻³ MNPs, with high surface area, durability, low toxicity, designability in modification and decoration and easy synthetic procedure are suitable for catalytic processes.⁴⁻⁵ One of the main applications of MNPs is in multi-component reactions. This strategy with excellent selectivity, efficiency, high atom economy, ideal synthetic routs for complex molecules and simplicity is a foreceful methods for the synthesis of biological and pharmaceuticals compounds.⁶⁻⁹ 2-Aminothiophene scaffolds derived from Gewald reaction have been attracted the great attention of many researchers.¹⁰⁻¹² These compounds have pivotal role as intermediates of organic synthesis and have many applications in medicinal chemistry, agrochemicals, dyes, and biologically active products.¹³⁻¹⁵ Therefore, we focused on the synthesis of 2-aminothiophene derivatives in the presence of urea-benzoic acid functionalized magnetic nanoparticles namely $Fe_3O_4@SiO_2@ULB$ as efficient and green heterogeneous catalyst.



R= H, 4-Cl, 4-OH, 3-OH, 4-NO₂, 3-NO₂ 4-OMe, 3-OMe

Scheme 1: Synthesis of 2-aminothiophene derivatives using Fe₃O₄@SiO₂@ULB as heterogeneous catalyst. **References**

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Synthesis of New Iariat Crown Macrocycles Containing Two Triazole Rings

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Abstract

Lariat ethers are compounds with a macrocyclic ring and a side arm which bears a donor group.^{1,2} It has been designed as cation complexing agents which exhibit complexation behavior similar to crown ethers, but with a three-dimensional binding character. Lariat ethers can be divided into two categories depending upon the nature of the secondary binding site: that with a pendent neutral side arm, and lariat ethers with a pendent proton-ionizable arm. Non-ionizable lariat ethers may exhibit an enhanced cation complexation and selectivity when compared to crown ethers without side arms.

In continuation of our interest to develop the synthesis of new macrocycles and lariat ether,³ I report herein, a simple and efficient method for the synthesis of new macrocycles **3a-b** and lariat **macrocyles 4a-b**. The synthetic strategy includes the cyclocondensation between bis aminotriazoles and the appropriate bisaldehydes, to give the corresponding Schiff bases. (Scheme 1)



Scheme 1: Synthesis of lariat crown macrocycles

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One-Pot Synthesis of 1,3-Thiazolidin-4-one Using Tannic Acid as Catalyst

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Abstract

4-thiazolidinones derivatives are an important class of compounds in medicinal chemistry. The 4-thiazolidinone ring system is a core structure in various synthetic pharmaceutical compounds, displaying a broad spectrum of biological activities.^{1,2}

In continuation of our interst to develop the synthesis of thiazolidinone 3, herein, I report a novel and facile synthesis of 1,3-thiazolidin-4-one in good yields (Scheme 1). In a one-pot procedure, compounds **4a–h** were obtained in the course of a three component reaction with aromatic aldehyde **1a-e**, aromatic amine **2a-c** and mercaptoacetic acid **3** using tannic acid at an ambient temperature under solvent free condition. In conclusion the notable advantages of our work are as follows: (1) the reaction is performed under mild condition and more important is under solvent-free condition. (2) good yields of cyclization products without any byproduct. (3) simple of purification.



Scheme 1: Synthesis of 1,3-thiazolidin-4-ones

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Determination the amount of Glyphosate as herbicide to control tall weed

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Abstract

Background and purpose: Glyphosate is an herbicide from the group of phosphonic acid (isopropylamine salt) which is used to control tall weeds. Glyphosate toxin is considered a common and safe toxin by proponents of transgenic crops. Recent studies, show that the use of these products causes gene mutations and causes many problems. Therefore, identifying and determining the amount of this toxin is very important.1

Analysis of herbicide residues in food and cereals is difficult due to matrix complexity and low concentration. Since the glyphosate herbicide lacks chromoform groups, we will not be able to directly analyze this herbicide with a HPLC device with a UV-Vis detector and it is a critical derivation step before the first analysis of Phenyl isothiocyanate (PITC) derivative was used to derivate glyphosate.

In this work, for the first time, an electric membrane combined with HPLC was performed to measure this herbicide in aqueous samples. Electromembrane extraction has been used in the past few years to extract basic, acidic, and metal ions, but so far this technique has not been used to extract glyphosate. Therefore, in this project, the electromembrane extraction method was used to preconcentrate phenoxy acid herbicides in environmental samples. Also in this first use, agarose gel was used as the green membrane and no other organic solvent was used for extraction.^{2,3}

The results showed that using this method, the glyphosate herbicide can be determined at concentrations of 1.5 µg /mL and the relative standard deviation obtained was less than 5.8%, which indicates suitable reproducibility for the proposed extraction method. Since the facilities and costs required to perform this electromembrane analysis are economically viable, it can have a very good future for development and wide application.

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Synthesis and Characterization of A New Diferrocenylaminoborane

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Abstract

In the search for new materials with useful electronic and magnetic properties, diferrocenylboranes (Fc₂BR, Fc=Ferrocene) are of great interest because the three-coordinate boron atom provides a free p orbital for conjugative interaction with the cyclopentadienyl π -systems. The degree of electronic communication between the boron atom and cyclopentadienyl rings can be fine-tuned by modifying the π -donor ability of the substituent on the boron atom, thereby offering a way for the rational design of novel materials with potentially useful electronic properties. The synthesis of bromo-diferrocenylborane **1** was reported for the first time in 2004 by Wagner and et al.^{1,2} Preparation of its derivatives is provided because the active boron atom can act in the reaction with organic bases as an electron acceptor (as Lewis acid) due to its empty p-orbital.³ In the present study, compound 1 was synthesized in our laboratory and reacted with aniline in the presence of NEt₃. The acidic proton of the resulting diferrocenyl-N-phenylaminoborane **2** was eliminated with ¹BuLi. The reaction of deprotonated diferrocenyl(N-methyl-N-phenyl)-aminoborane **3**. All reactions were carried out under argon atmosphere (Scheme 1).



Scheme 1: Synthesis of new diferrocenyl(N-methyl-N-phenyl)aminoborane 3

The compound **3** was characterized via ¹¹B- and ¹H-NMR spectroscopy. The observed peaks in ¹¹B-NMR spectra at 45.7 and 41.9 ppm were attributed to <u>B</u>-NH and <u>B</u>-NCH₃ for compounds **2** and **3**, respectively.

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A Novel Ferrocene-Based Azine Derivative

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Abstract

Ferrocenylcomplexes display pharmacological and medicinal activities as antimicrobial agents against different microbes.¹ Schiff-bases, compounds having an azomethine (RR'C=NR") linkage, are an essential class of organic compounds as chelating ligands. The presence of nitrogen and oxygen donor atoms in such compounds make them structurally similar to the neutral biological systems and are utilized in elucidating the mechanism of transformation of racemization reactions. Schiff-bases having a ferrocene moiety have drawn substantial consideration due to superior anticancer and free-radical scavenging properties.² Accordingly, the importance of ferrocene schiff-bases was our motivation for trying to prepare new ferrocene-based hydrazone Schiff-base as a ligand for the preparation of metal complexes.

The reaction between ferrocenecarboxaldehyd **1** and hydrazine (H₂N-NH₂) resulted in the formation of ferrocenyl hydrazone **2**. The synthesis of Schiff-base **2** was confirmed by disappearing of the aldehyde proton peak and also observation of two singlets at δ =6.21 and 7.48 ppm related to <u>H</u>C=N and N<u>H</u>₂, respectively in the ¹H-NMR spectrum. The condensation reaction of Schiff-base **2** with 1,1'-ferrocenedicarboxaldehyde **3** in a mole ratio of 2:1 (scheme 1) led to the synthesis of a novel ferrocenebased azine derivative **4**, which can be used as an attractive novel bis-Schiff-base or "azine-ligand" (>C=N-N=C<) to synthesis of new metal complexes and investigation of their properties and applications. In the ¹H-NMR spectrum of the new schiff base **4**, there is no trace of the peak related to N<u>H</u>₂. The peak of <u>H</u>C=N was observed at δ =8.52 ppm. Furthermore, the spectrum indicated a singal for two identical Cp-H₅ rings at δ =4.27 ppm. Two other singlets were observed at δ =4.49 and 4.74 ppm attributed to Cp-H₄ rings.



Scheme 1: Synthesis of a novel ferrocene-based azine derivative 4

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Graphene Quantum Dots/Carboxymethyl Starch as a Biocompatible Platform for the Synthesis of Zn-MOF

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Abstract

Today's metal-organic framework (MOFs) as newly introduced porous inorganic-organic hybrid materials has been received more interest in drug delivery, gas storage, catalysts, etc.¹ Up to now various systems have been introduced as a platform for MOFs synthesis, which hydrogels are one of them. Hydrogels are defined as three-dimensional cross-linked polymer networks having a large number of functional groups.² The incorporation of MOFs into hydrogel matrixes can promote their practical application in various fields as well as can inhibit their aggregation.³ By considering these, herein, we have developed a simple strategy to fabricate novel photoluminescent carboxymethyl starch microspheres containing MOFs which was named Zn-MOF@CMS/GQDs. For this, at first, graphene quantum dots were prepared from the pyrolysis of citric acid. In the following, the mixture of GQDs and CMS was crosslinked employing sodium trimetaphosphate (STMP) as a biocompatible chemical crosslinker. Eventually, Zn-MOF was in situ synthesized employing zinc sulfate and glutamic acid within CMS/GQDs matrix. Fourier transform infrared (FT-IR), and X-ray diffraction (XRD) analysis revealed successful synthesis of the Zn-MOF@CMS/GQDs synthesis. Then the fluorescent feature of the Zn-MOF@CMS/GQDs was confirmed employing photoluminescence analysis.



Scheme 1: The schematic route for the preparation of CMS/GQDs

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Fabrication of Photoluminescent and Bio-Based Metal-Organic Framework as a Platform for 5-Fluorouracil Delivery

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Abstract

The chemotherapeutic effect usually is associated with severe toxic side effects on the normal tissues, because of its non-specificity.¹ Nowadays, different types of functional nanomaterials have been introduced as novel drug carriers for obtaining the new system with controlled drug release performance.² Recently, much more attention has been devoted toward the use of metal-organic frameworks (MOFs) for drug delivery applications. Additionally, the MOFs could be synthesized in the presence of other nanoparticles to obtain a new system with new beneficial features, graphene quantum dots (GQDs) are one of them.³ In this work, for the first time, the GQDs/Cd-MOF bio-nanohybrids were prepared via two-step proedure. At first, GQDs were synthesized through the direct pyrolysis of citric acid. Then the bio-based MOFs were fabricated from the phenylalanine in the presence of as-synthesized GQDs. After detailed characterization of GQDs/Cd-MOF about 67% of the 5-fluorouracil was prepared on GQDs/Cd-MOF. Finally, the 5-Fu release profile was assessed as in vitro.



Scheme 1: The schematic route for the preparation of GQDs/Cd-MOF

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Modification of Salep Biopolymer and Its Utilization in Removal of Heavy Metals from Water

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Abstract

Salep is a polysaccharide extracted from natural terrestrial orchids. This product has a lot of applications in the food industry and pharmacy industry.¹ Polysaccharide-based hydrogel have specific properties to be known as unique adsorbents. The nature and the density of the hydrophilic groups of hydrogels effect the absorbency of them.² In this study Hydrogel of salep is synthesized and inorder to improve its properties sulfate groups are replaced on this polysacaride. Sulfonation of salep was performed according to the method of Gamzazade et al.³The sulfating reagent was prepared by adding HCISO₃ to DMF, then one gram of salep was added to this reagent and the reaction was mixed well, then neutralized and dried to obtain modified polymer. During the next step, salep sulfate was dissolved with H₂O at stable temperature (70 $^{\circ}$ C), then Acrylic Acid monomer and MBA cross-linker were added to it and after 15 min. APS initiator was added. The resulted gel product was dewatered by ethanol and the dried gel were milled used for test.

The structure of salep sulfate was investigated by means of 1H NMR and FTIR spectroscopy. In the 1H NMR Spectrum, the signals of the parent salep at 4.013 and 4.159 ppm are are shifted to low field at 4.064 and 4.262 ppm after sulfonation which indicates that the hydroxyl groups are sulfated. The FTIR spectra showed a band at 814 cm⁻¹ for S– O stretching from the sulfated glucosidic units and absorption bands at 1618, 1445, and 1414 cm⁻¹ verifying the formation of graft copolymer product, the SS-g-PAA hydrogel.

The swelling degree of the hydrogel was measured in distilled water at consecutive time intervals. The high equilibrium water absorbency was obtained when the sulfate content of salep sulfate is high.

The influence of the sulfate content on adsorption of hydrogels for heavy metal ions, Co(II), Cu(II), and Zn(II) from water, at pH = 7 was studied and the heavy metal ion concentration was measured by atomic absorption spectroscopy. It is observed that the adsorption capacities of SS-g-PAA hydrogels are more than salep-graft-polyacrylic acid (S-g-PAA) hydrogel. The decreasing adsorption capacity with sulfate content increasing evidently may be attributed to steric effect beyond a certain point and a dense complex formation on the surface of the hydrogel which prevent the diffusion of metal ions into the hydrogel. This phenomenon further suggests that the adsorption capacity of salep sulfate-based hydrogels not only depends on sulfate group but also on the other group with different affinity, such as –COOH and – OH group which have interaction or synergistic action for heavy metal ions adsorption.



Figure 1: Preparation of Salep Sulfates

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Nanoparticles in COVID-19 Vaccines: Applications, Chemistry and Methodes

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Abstract

Coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), is a global pandemic which has induced unprecedented ramifications, severely affecting our society due to the long incubation time, unpredictably high prevalence and lack of effective vaccines.Vaccination represents the best line of defense against infectious diseases and is crucial in curtailing pandemic spread of emerging pathogens to which a population has limited immunity. In recent years, mRNA vaccines have been proposed as the new frontier in vaccination, owing to their facile and rapid development while providing a safer alternative to traditional vaccine technologies such as live or attenuated viruses. Recent breakthroughs in mRNA vaccination have been through formulation with lipid nanoparticles (LNPs), which provide both protection and enhanced delivery of mRNA vaccines in vivo. In this study, the application and chemistry of nanoparticle technology in various types of mRNA-based COVID-19 vaccines have been investigated.

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Synthesis of Thermosensitive Two-Dimensional Polymers

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Abstract

The recent discovery of graphene has caused a surge of interest in the research and development of 2D materials and opened up a new pathways to low dimensional nanostrcutures.¹⁻³ Two-dimensional polymers are fascinating research targets, due to their interesting properties. A 2D polymer is a covalently linked network of monomers with periodic bonding in two orthogonal directions. These polymers have been classified in three categories: layered crystals, multilayer and monolayer⁵ films on surfaces, and free-standing sheets. Two-dimensional polymers also often have pores of a certain size and shape, high specific surface areas, and a good free volume that can have different functions. They can be used as membranes for filtration, molecular recognition and sensing, catalysis, optoelectronic devices and many other applications that leverage specific molecular organization, including gas storage, sensing, energy conversion and storage, and electrocatalysis.²⁻⁴ In the study, we have synthesized a two-dimensional polymer by a template assisted strategy. (Scheme 1) A porous two-dimensional template was synthesized by cupper-catalyzed click-chemistry and used as a cage for the initiators by which a new thermosensitive polymer was synthesized inside the template. The physicochemical properties of the synthesized two-dimensional polymer were studied by microscopy and spectroscopy as well as thermal analysis methods. The obtained polymer due to its high porosity and thermosensitivity can be used as a template for loading water-insoluble drugs and their controlled release upon manipulation of temperature.



Scheme 1: Schematic representation of the synthesis of thermosensitive two-dimensional polymer

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Investigation of Mechanical and Antibacterial Properties of the PVA/AG/2D-tr Hydrogels

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Abstract

Hydrogels are a promising class of scaffold materials in tissue engineering witch are cross-linked polymers suitable for various applications, but main limitation of hydrogels is their poor mechanical strength. Much effort has been made to improve the mechanical properties of hydrogels.¹⁻⁵ In this study, the novel hydrogels were fabricated with a mixture of a poly (vinyl alcohol)/agarose (PVA/AG) dual-network hydrogel and the different concentrations of triazin-based two-dimensional sheets by a freeze/thaw method.(Scheme 1) The mechanical and antibacterial property of these fabricated hydrogels can be modulated by the different concentration of triazin-based two-dimensional sheets. The mechanical and antibactrial properties of the PVA/AG/2D-tr Hydrogels were significantly improved. Compared to pure PVA/AG dual-network hydrogels, an increase in compressive strength and improved tensile strength was obtained by adding triazin-based two-dimensional sheets, which suggests a good physical crosslinking between PVA/AG dual-network hydrogel and triazin-based two-dimensional sheets.



Scheme 1: Schematic of the reaction process for the preparation of the PVA/AG/2D-tr hydrogels

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Comparison of the Mechanism of CO Substitution Reaction in Iron Complexes

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Abstract

In this investigation, density functional theory calculations were used to compare the CO substitutions reaction of the Cp (Cp=C5H5) and indenyl (Indenyl=C7H9) ligands in the complexes (η 5-C5H5) Fe (CO)2(η 1-C5H5) (I), (η 5-C5H5) Fe (CO)2(η 1-indenyl) (II), (η 5-indenyl) Fe (CO)2(η 3-indenyl) (III) . ¹⁻² The reaction energy for CO substitutions by η^1 -Cp giving Fe (η^5 -Cp)₂ is exergonic while that by (η^1 -indenyl) giving Fe(η 5-indenyl)₂ and Fe (η 5-C5H5) (η^1 -indenyl) are thermoneutral.³ Our calculations show that he activation energy barrier in the first and second CO substitution reactions in complexes II and III is higher than in complex I which indicate that the pair of π - bonded electron in the η 3-indenyl ligand has less nucleonyl properties than the η 3- cyclopentadieneanil ligand.⁴⁻⁵ (Figure 1) In addition, calculations show that the monocarbonyl complexes are stable in the exo form and the CO substitution by endo η 3-indenyl form never happens.



Figure 1: Isomer endo and exo show ligand for complexe(I)

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Synthesis of Redox-Responsive Shell Cross-Linked Nanocarriers from 6-Arm Star Copolymer

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Abstract

Shell cross-linked micelles have attracted a lot of interest duo to stabilizing the core-shell micelle morphology and eliminating the distortion or destruction of the assemblies under dilution or mechanical shear forces and also shell cross-linked micelles are possibly valuable nanosized delivery vehicles for the delivery of different actives such as drugs, fragrances, pesticides.¹ The special morphology endows star polymers with great stability and functions. Preparation of s-PCL-g-(PDMAEMA-b-PAA)-SS based on poly (ε-Caprolactone) (PCL), poly (2-(dimethylamino) ethyl methacrylate) (PDMAEMA) which is known as a kind of hydrophilic, pH cationic polymer, were designed and synthesized by combination of ring opening polymerization (ROP) using dipentaerythritol as an initiators and continuous activators regenerated by atom transfer radical polymerization (ATRP)(Figure 1). The molecular weights and chemical structure of the copolymer were confirmed by gel permeation chromatography (GPC), H-NMR and FT-IR spectroscopy. GPC traces of s-PCL-g-(PDMAEMA-b-PAA) showed a monomodal symmetric distribution indicating a well-controlled process of polymerization and expected composition and structure was achieved. The thermogravimetric analysis (TGA) experiment approved successful cross linking by cystamine reagent and thermal stability of cross linked polymer in contrast to uncross linked one. Also pH responsive behaviour and size distribution of micelles were characterized by dynamic light scattering (DLS) analysis.²



Figure 1: the synthesis rout of micelles

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Design, Fabrication, and Stability Analysis of a New Cobalt Modified Electrode in Organic Transformations

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Abstract

Employing new modified electrodes as heterogeneous catalysts has various advantages for fine chemical synthesis. They can unquestionably display a high specific surface area to volume ratio, which heightens the contact between reactants and catalyst support and consequently increases the catalytic activity and easily separate out of the reaction mixture.¹ In this regard, Cobalt-based materials can offer very promising features as catalyst supports due to their worthy features such as high surface area, porosity, and stability, which raise the efficiency of them upon reaction completion.²⁻⁵

Very recently, we have designed and synthesized new cobalt electrodes for the synthesis of aldehydes using advanced oxidation processes (figure 1).



Figure 1: Green Synthesis of Aldehydes

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Design, Fabrication, and Stability Analysis of a New Zink Modified Electrode in Coupling Reactions

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Abstract

The C-S bond formation methods leading to the synthesis of aryl sulfides are among the most important ways in organic synthesis.¹ Various biologically active compounds certainly include aryl sulfides moieties with broad-spectrum therapeutic actions for the treatment of some disorders including Alzheimer, Parkinson, HIV, inflammatory and immune diseases.² Furthermore, aryl sulfides could quickly change into other useful building blocks such as sulfonium, sulfones, or sulfoxides.³ Both Pd(II) salts and Pd(0) systems have been applied in C-S bond formation chemistry.⁴ Firstly, Migita reported the Pd-catalyzed thiation of aryl halides using Pd[PPh3]4 as the catalyst.⁵ After that, Buchwald and several groups were exposed to aryl sulfide synthesis in different techniques.⁶ Very recently, we have designed and synthesized new Zink electrode as electro-catalyst for the C-S bond formation using a new and green protocol (figure 1).



Scheme 1: Green Synthesis of unsymmetrical aryl sulfides

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Synthesis of a New Schiff Base Compound and Its Effect on the Inhibition Efficiency for mild steel in Hydrochloric Acid

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Abstract

In this study, the 2-(2-mercaptophenylnitrilomethyl-idyne)-phenol as a New schiff base compound was synthesised from the reaction of 2-aminothiophenol with salicylaldehyde in methanol in the refluxed condition nearly for 1.5h, then purified and characterized (scheme). The newly synthesized compound was used as a corrosion inhibitor for mild steel in 0.1 M sulphuric acid media and its inhibitive effect was investigated by applying potentiodynamic polarization and electrochemical impedance spectroscopy techniques. The experimental results showed that this compound sluggish the kinetics of hydrogen evolution reaction and reduces the anodic dissolution. The corrosion current density increases by increase in temperature but in the presence of this compound the corrosion current density is lower. The inhibition efficiency decreases from 85% to 73% in solution containing 400 ppm inhibitor by increase in temperature from 25 °C to 55 °C. Thermodynamic adsorption parameters show that the inhibitor adsorption mechanism is combination of physical and chemical interactions.



Scheme: 2-aminothiophenol and salicylaldehyde reaction in methanol to produce Schiff base.

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Synthesis of Molecular Imprinted Polymer to Prepare Graphene Composite and its Application in Methylene Bule Sensing

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Abstract

Molecular imprinted polymers (MIPs), as a class of smart polymers, containing a large number of molecular recognition cavities were designed for the selective recognition and separation of target molecules, due to its low cost, outstanding selectivity, and high stability. These polymers are prepared by using target molecule with a functional monomer used as a reactant agent in presence of cross-linking agent and initiator. Then, strong acid is used to leach out the target molecule from the imprinted polymer to form selective template cavities. The morphology of the prepared polymer particles can be controlled by varying the experimental conditions such as solvent volume, temperature and stirring speed of polymerization solution, specially the cross-linker/monomer feed ratio. A new MIP was synthesized to prepare MIP/Graphene composite and its application in sensitive and selective detection of methylene blue (MB) dye. A thermal polymerization technique was used to prepare MB imprinted nanobeads. For this purpose, MB as imprint molecule, oxine as π stacking agent to interact with MB, 2-methoxyethanol as porogen solvent, EGDMA (Ethylene glycol dimethaacrylate) as cross linker agent , styrene as monomer, and AIBN (2,2'-azobisisobutyronitrile) as initiator, were used to preparation of MIP. After polymerization, the obtained MIP nanoparticles, were used to leaching process. The experimental results showed that the increasing of the cross-linker/monomer feed ratio from 1 to 8 produce MIP nanoparticle from micro to nano sized. Finally, a homogenized MIP/Graphene mixture was prepared by dispersing in deionized water and dropped on the glassy carbon electrode surface and left to dry in air before being used. The MIP/Graphene modified electrode was successfully applied in electrochemical sensing of MB by voltammeric technique in optimum condition.



Scheme: Preparation of MIP/Graphene Nanocomposite

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A New Strategy for Synthesis of Enantiopure Spirocyclopropyloxindoles Through via Asymmetric [3+2] Cycloaddition Reaction

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Abstract

As a subset of the spirocyclic oxindole family, cyclopropyl spirooxindoles constitute a privileged molecular architecture and are prominent in among of natural products and bioactive compounds.¹ The enantioselective synthesis of these scaffolds is difficult because they have a highly hindered spirocyclic quaternary carbon center. Specifically, the asymmetric synthesis of spirooxindole containing a cyclopropane ring remains a challenging task in the current organic synthesis.² In the present study, a new strategy has been established for the preparation of important class of spiro-cyclopropane oxindole scaffold via the catalyst-free asymmetric [3+2] cycloaddition reaction of readily accessible 3- diazooxindoles and chiral cinnamoyl-sultam dipolarophiles. Highly enantioenriched 3,3'-Spiro-cyclopropane oxindoles were generated in broad range with three contiguous stereogenic centers and a highly hindered spirocyclic quaternary carbon center by utilizing chiral auxiliary controlled method.(Schem1)



Schem1. Asymmetric synthesis of spiro-cyclopropyloxindole derivatives

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Organocatalytic Synthesis of Spiro-pyrrolidine-3,3'-oxindoles via A Three-Component Asymmetric 1,3-Dipolar Cycloaddition Reaction

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Abstract:

The spiro-pyrrolidine-3,3'-oxindole unit has been seen as a privileged structure in organic synthesis and pharmaceutical research¹, because it is found as a core in lots of natural products that often exhibit excellent biological activities. The structural diversity and complexity of these compounds have been inspired chemists to develop numerous efficient synthetic strategies to construct these scaffolds.² Herein, We have introduced a highly stereoselective 1,3-dipolar cycloaddition reaction of imino esters with (E)-2-oxoindolin-3-ylideneacetyl sultam derivatives using readily available H-bond donor thiourea catalysts. This method provides facile access to a wide range of chiral spiro[pyrrolidine-3,3'-oxindoles] in high yield and with excellent enantio- and diastereoselectivity under mild conditions. In most cases, the use of these catalysts led to increased stereospecificity of the reaction and accordingly, the highly enantioenriched products were generated. In addition, the absolute configuration of these cycloadducts with four contiguous stereogenic centers was directly determined by X-ray structure analysis. (Schem1)



Schem1. Asymmetric synthesis of spiro-pyrrolidine-3,3'-oxindole derivatives

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Three-Component Synthesis of Some Novel 8-Caffeinyl Dithiocarbamate Derivatives as Potential Chemotherapeutic Agents

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Abstract

Caffeine is a xanthine alkaloid found in the seeds, leaves and fruit of some plants. Mainly, the coffee beans, tea leaves, cocoa beans and kola nut are the most known natural sources of caffeine. Caffeine is most commonly consumed worldwide by humans in infusion extracted from the seeds of the coffee plant and the leaves.¹ Caffeine, the naturally occurring methylxanthine, is of an unquestionable interest as a leading compound for the development of new derivatives with enhanced activities and/or lower toxicities. It modulates drugs used for curing lung, liver, uterine cervix and breast cancer and enhances gastric secretion and urine production, reduces the risk of developing gallstone disease and also reduces asthma.² The studies have shown that C8-caffeinyl derivatives are adenosine receptor antagonists³, acetylcholinesterase inhibitors⁴ and monoamine oxidase inhibitors, and that within this group the 8-thiocaffeine analogues belong to a pharmacologically important subclass.⁵⁻⁸

Chemical reactions that use more than two different starting materials and yield the single product in a one-pot procedure are usually called multi component reactions. The specific advantages of MCRs technology acquires a new tool to create the chemical input for medicinal chemistry to match the space of biological targets with relevant chemistry.⁹ In terms of biological activity of C8-caffeinyl derivatives, hereby we have explained the synthesized and characterization of a new series of structurally diverse 8-caffeinyl dithiocarbamates through three-component reaction in good to excellent yields.



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A Novel Bromine-Catalyzed, One-Pot Synthesis of 2-(Alkylthio)benzothiazole From Phenyl Isothiocyanate and Alkylthiols

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Abstract

Heterocycles bearing nitrogen, sulphur and thiazole moieties constitute the core structure are an attractive therapeutic approach for most types of human cancers.^{1,2}

several analogues containing benzothiazole ring system exhibit significant antitumour, antimicrobial, antidiabetic, anti-inflammatory, anticonvulsant, antiviral,antioxidant, antitubercular, antimalarial, antiasthmatic, anthelmintic, photosensitizing, diuretic, analgesic and other activities.^{1,2} For example SKLB-163, a novel benzothiazole-2-thiol derivative, showed it had potent anti-proliferative activity on various human cancer cells.³

In this work, the reaction of Phenyl isothiocyanate with different derivatives of alkyl thiols in the presence of a bromine catalyst was studied for the first time (Scheme 1).

The important feature of this method is the use of bromine as the Lewis acid catalyst, which is an available, and very efficient reagent for the one pot synthesis of 2-(Alkylthio)benzothiazole in good to excellent yields.



Scheme 1: Synthesis of 2-(Alkylthio)benzothiazole from Phenyl isothiocyanate and alkylthiols

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BTMA-Br₃ Promoted One Pot Synthesis of 2-(Alkylthio)benzothiazole from Phenyl Isothiocyanate and Alkylthiols

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Abstract

Thioethers including a benzothiazole moiety are a significant class of heterocyclic due to the inherent reactivity of the thiazole ring, and there are many industrial, biological and pharmaceutical applications.¹⁻³

several analogues containing benzothiazole ring system exhibit significant antitumour, antimicrobial, antidiabetic, anti-inflammatory, anticonvulsant, antiviral, antioxidant, antitubercular, antimalarial, antiasthmatic, anthelmintic, photosensitizing, diuretic, analgesic and other activities.¹⁻³

In this work, the reaction of Phenyl isothiocyanate with different derivatives of alkyl thiols in the presence of a bromine catalyst was studied for the first time (Scheme 1).

The important feature of this method is the use of benzyltrimethylammonium tribromide as the Lewis acid catalyst, which is a very efficient reagent for the one pot synthesis of 2-(Alkylthio)benzothiazole in good to excellent yields.

Since bromine is volatile and highly toxic by inhalation, we use of benzyltrimethylammonium tribromide instead of adding bromine directly, it is produced in the reaction mixture (Scheme 2).



Scheme 1: Synthesis of 2-(Alkylthio)benzothiazole from Phenyl isothiocyanate and alkylthiols

Scheme 2: In situ generation of bromine

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Spectroscopy Study on Sulfobutyl Ether Beta Cyclodextrin (SBE-β-CD) Inclusion Complex with Vitamin E (VE)

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Abstract

Sulfobutyl ether beta-cyclodextrin (SBE-β-CD) is a versatile derivative of the parent beta-cyclodextrin(β-CD). The ability to solubilize poorly soluble drugs is higher than parent β -CD due to the presence of hydrophobic butyl moiety. SBE-β-CD can be applied for use in formulation of various drug delivery systems incorporating a variety of guest molecules ranging from small molecules to large compounds, peptides and proteins. An optimised inclusion complex can be an efficient strategy to increase the solubility of poorly soluble compounds and provide stability to a large number of active pharmaceutical ingredients.¹ Vitamin E (VE) is an important natural antioxidant, and its most common and biologically active form is α -tocopherol. While pure Vitamin E is insoluble in water, Vitamin E/SBE- β CD-IC has displayed fast-dissolving behavior.² This study aimed to characterize inclusion complexes of vitamin E with SBE- β -cyclodextrin. The SBE- β -CD -vitamin E inclusion complexes were prepared by freeze-drying (FD) method and SBE- β -CD-vitamin E inclusion complexes. The AL-type diagram of the phase solubility studies of vitamin E exhibited the formed inclusion complexes with the 1:1 molar ratio. The vitamin E-SBE-β-CD were characterized using UV-Vis absorption, FT-IR, 1HNMR and SEM. These results supported a successful formation of the inclusion and the preliminary structure of host-guest inclusions was constructed. Therefore, SBE- β -CD can be used as a solubility and stability enhancer for VE through inclusion complexation.



Figure 1: FTIR spectra of 1) SBE-βCD/Vitamin E-IC, 2) pure Vitamin E, and 3) SBE-βCD in full range (4000–500 cm⁻¹)

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Wettability and Morphological Characterization of Electrospun Chitosan/PVA/Tannic Acid Nanofibers

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Abstract

Tannic acid (TA), as a naturally derived polyphenol with relatively high molecular weight, possesses several favorable features such as antioxidant activity, biocompatibility, hemostatic and antibacterial properties that make it attractive for several applications.¹

The chitosan-based solutions (CS/PVA and CS/PVA-TA) were electrospun using a double nozzle electrospinning apparatus. Electrospinning of polymer solutions was carried out at a voltage of 25 kV, a spinning distance of 17 cm, a volume flow rate of 0.6 mL/h, and a rotating drum speed of 150 rpm at room temperature. The size and morphologies of electrospun nanofibers were evaluated by field-emission scanning electron microscopy. The wettability of nanofibers was also investigated using a water contact angle measurement device (CAG-20, Jikan Co., Iran).

Morphological study through FESEM confirmed the fabrication of almost uniform nanofibers with no agglomeration and bead-like structures (Figure 1). Modification of CS/PVA nanofiber with TA leads to the increase of the average fiber diameter by \sim 5%. This phenomenon could be attributed to the large number of hydroxyl groups of TA, forming hydrogen bonds with CS and PVA; thus, the viscosity of polymer solution was increased with the addition of TA, which lead to the slight increase of average diameter values.

The water contact angle of fabricated nanofibers is shown as an inset image in Figure 1. As can be seen, all nanofibers exhibit high wettability with hydrophilic properties. The contact angle of CS/PVA nanofibers was found to be 45.3°. For CS/PVA-T nanofibers, the contact angle (37.7°) was lower than that of CS/PVA nanofibers, which is attributed to a large number of hydrophilic hydroxyl groups of the TA molecules. A similar result has been reported, indicating that incorporation of TA leads to decreasing the contact angle of electrospun nanofibers.² The addition of TA as a crosslinking agent of CS had the same effect.³



Figure 1: FESEM images and water contact angles of (a) CS/PVA, and (b) CS/PVA-TA nanofibers.

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Green Synthesis of AgNPs on the Surface of Modified Chitosan using Salvia Ieriifolia as a Catalyst for the Reduction of Methylene Blue

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Abstract

In the present study, an eco-friendly and facile method for green synthesis of silver nanoparticles (AgNPs) on the surface of modified chitosan by vanilin has been developed using extract of *Salvia leriifolia* plant. AgNPs were decorated on chitosan after it had been functionalized with vanilin. Then, the catalyst was characterized and The reduction process of methylene blue (MB) with NaBH4 was used as a model reaction to evaluate the catalytic activity of synthesized AgNPs. MB is a thiazine dye, also known as methylthioninium chloride, that has a wide range of applications in chemical sciences and biochemistry, as well as as a stain and a pharmaceutical.¹⁻³ When MB is oxidized, it is blue, but when it is reduced, it becomes colorless leucomethylene blue. In the utter lack of the AgNPs catalyst, the UV-Vis absorption spectra of MB reduction with NaBH4 are shown in Fig. 1a. The studying showed that partial reduction of MO occurred within 2h in the presence of NaBH₄ alone. In contrast, upon addition of AgNPs (in the presence of NaBH₄), complete reduction was achieved within 90 s. The kinetic data obtained for the reduction of MB was fitted to first-order rate equations.⁴ The catalytic efficiency of Ag nanocatalyst toward the degradation of the MB studied herein is shown in Figs. 1(b). The calculated rate constants for the reduction of MB was -0.0225 and also the catalyst exhibited high efficiency after 5th run.



Figure 1. a) Time dependent UV-Vis absorption spectra of MB In the presence of catalyst and NaBH₄; (b) Rate constant versus time in the catalyst and NaBH₄.

Acknowledgements

We thank the University of Jiroft, Faculty Research Committee for supporting this investigation.

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An Eco-Friendly Approach for Synthesis of Fe₃O₄ Nanoparticles: Making of an Efficient Vehicle for Diagnostic and Therapeutic Potential

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Abstract

In the present study, Fe₃O₄ magnetic nanoparticles (MNPs) are one of the most extensively investigated inorganic nanomaterials for biomedical applications due to their special superparamagnetic ability and outstanding biocompatibility¹. In magnetic resonance imaging (MRI), MNPs are commonly utilized as contrast agents for disease diagnosis. Combining multiple imaging modalities is currently being viewed as a new trend in disease diagnosis and therapy, with the potential to raise disease diagnosis accuracy while also providing novel therapeutic strategies. New contrast agents for multifunctional imaging are therefore desperately needed. Fe₃O₄ MNPs are being considered as a good candidate for use in the development of a multifunctional platform for disease diagnostics and therapy². We report successful eco-friendly syntheses of Fe₃O₄ nanoparticles with a size of 25.7 nm via a low-temperature route (Figure 1). According to EDAX's detailed analysis, the generated samples include 62.6% wt of Fe and 39.4% wt of O.



Figure 1. a) EDAX spectrum of synthesized Fe₃O₄ nanoparticles; (b) Scanning electron microscopy (SEM) images of the as-synthesized Fe₃O₄ nanoparticles at 500 nm scale bar.

Acknowledgements

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Synthesis and Characterization of Amine-Modified Mesoporous MCM-41 Nanoparticles

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Abstract

Nanomaterials have an effective role in the biomedical fields due to their diverse potential applications, such as increasing the therapeutic effects of anticancer drugs, bioavailability, biodegradability and biocompatibility.¹ Among all nanosystems, mesoporous silica nanoparticles are widely used in the field of targeted cancer treatment. The mesoporous M41S molecular sieves called MCMs (Mobil's Composition of Matter) include lamellar MCM-50, cubic MCM-48 and hexagonal MCM-41.² MCM-41 is a silica derivative that has several outstanding properties such as a highly ordered porous system indicating pore diameters changing within 2–10 nm range, large pore volumes, high BET surface areas, great sorption capacity, biocompatibility, non-toxicity, extraordinary thermal stability and numerous surface silanol groups.³

Nanoparticles of mesoporous MCM-41 silica were synthesized, functionalized by hexamethylenetetramine (HMT) and characterized by diverse analysis techniques. The XRD pattern of the MCM-41 demonstrated a hexagonal crystalline structure for the MCM-41 with a two-dimensional network. The peak located at 20=2.26° was attributed to the presence of pores in the MCM-41 structure. This peak moved to lower angles while the MCM-41 was functionalized with HMT. Additionally, the two peaks positioned at 3.91 and 4.45° were observed as a broad peak in the XRD diagrams of the HMT-functionalized MCM-41 compounds. Such changes verified that the HMT molecules were entered within the pores and somewhat occupied them. The pore size, pore volume and surface area of pure MCM-41 were obtained equal to 32.54 Å, 0.89 cm³/g and 996.84 m²/g but they were noticeably decreased for the HMT-functionalized MCM-41 materials approving the HMT molecules were bound onto the surfaces and pores of such samples.



Scheme 1: The schematic structures of MCM-41 and MCM-41/HMT samples.

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A Molecular Docking Study of Flavonoids and their Glycosides as P-glycoprotein Inhibitors

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Abstract

Chemotherapy is widely used for the treatment of cancer, but its efficiency is being compromised because of the development of drug resistance due to the overexpression of drug efflux pumps such as P-glycoprotein (P-gp) ¹. Although P-glycoprotein inhibitors, such as verapamil and cyclosporine A, could increase the efficiency of chemotherapeutic agents, the application of these compounds is currently limited due to undesirable pharmacokinetic interactions and side effects.

Flavonoids constitute one of the largest groups of plant secondary metabolites representing a wide variety of biological activities. In addition to the known anti-cancer properties of flavonoids, they have also been introduced as the third generation of P-glycoprotein inhibitors². Unlike first-generation inhibitors of Pgp such as verapamil, flavonoids do not show unfavorable side effects.

In order to create a model, simulating the inhibition of P-gp by flavonoids as well as their glycosides, in this work a molecular docking study using AutoDock 4.2 software was used. The 3D structure of a P-gp model provided by homology modeling and critical residues in the enzyme binding site were determined based on crystallographic data presented in Protein Data Bank (PDB). Analyzing the docking results revealed an effective inhibition of P-glycoprotein by flavonoids as well as correlated glycosides according to their corresponding binding energies.

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Synthesis of Thiophenol-Formaldehyde Resin and some Carbon Allotropes and Evaluation of Their Supercapacitor Performance

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Abstract

Today, to meet the growing needs of society to demand more energy in the world and with increasing environmental pollution due to the widespread use of fossil fuels, requires the development of storage systems and energy conversion devices with high performance and low cost and co- We are so environmentally friendly.¹ Among the various energy storage devices such as batteries, supercapacitors and solar cells, etc., supercapacitors have been in the spotlight for reasons such as high density power, long life and fast discharge of charge.² In this project, polymerthiophenol-formaldehyde was synthesized to investigate the effect of its supercapacitor performance. The effect of the presence of azobisobutyronitrile AIBN as a porosity agent on the supercapacitor performance of pure TPFR polymer was also studied. The results were successfully confirmed by three-electrode cyclic voltammetric (CV) electrochemical test using nuclear magnetic resonance spectroscopy (NMR) and infrared (IR) spectroscopy.



Scheme 1. Synthesis of thiophenol-formaldehyde resin

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Biography of Presenting Author

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Sonocatalyst Efficiency of Fe₃O₄- Graphene/Poly Aniline Nanocomposite for Methyl Red Degradation From Aqueous Solution

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Abstract

In recent decades, because of the advancement in nanotechnology, advanced oxidation processes (AOPs), especially sonocatalysis have been shown to be a promising alternative in water treatment and environmental remediation. In this research, an attempt has been made to investigate and establish a physicochemical mechanism for the catalytic activity of Fe_3O_4 - Graphene/Poly Aniline nanocomposite in AOPs by the removal of organic dyes as model contaminants. Fe_3O_4 - Graphene/Poly Aniline nanocomposite showed brilliant sonocatalytic activity for the removal of methyl red as an anionic dye. The removal efficiency of Fe_3O_4 - Graphene/Poly Aniline nanocomposite was estimated via analysing the variation in the absorbance of dye under a UV-Vis spectrophotometer. The effect of various operating factors on the catalytic activity of Fe_3O_4 - Graphene/Poly Aniline nanocomposite, such as the amount of catalyst dosage, pH of the solution, and the initial pollutant concentration, was thoroughly studied. From Figure 1, the DR% decreases as the initial reactant concentration increases. The maximum degradation of methyl red by Fe_3O_4 - Graphene/Poly Aniline nanocomposite was found at an initial concentration of 20 mg L⁻¹, pH 3, catalyst's dosage 500 mg L⁻¹, and contact time equal to 20 min.



Figure 1. Influence of dye concentration on degradation rate of methyl red via Fe₃O₄- Graphene/Poly Aniline nanocomposite.

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Preparation and Characterization of Fe₃O₄- Graphene/Poly Aniline Nanocomposite

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Abstract

Considering the limited availability of water resources in the world, the problem of water pollution is one of the most serious *problems* in today's' *world*. In this regard, Fe₃O₄-Graphene/Poly Aniline nanocomposite with high adsorption capacity has been synthesized. In the present study the synthesis and structure characterization of a novel nanocomposite based on Graphene and Fe₃O₄/Poly Aniline nanostructure has been reported. Characterization of Fe₃O₄- Graphene/Poly Aniline nanocomposite was carried out by various instruments, including SEM, EDX, FT-IR and XRD. The X-ray diffraction pattern of the nanocomposite is shown in Fig. 1. Fe₃O₄- Graphene/Poly Aniline nanocomposite shows six characteristic peaks near to 30. 5° (220), 35. 6° (311), 43. 5° (400), 53. 8° (422), 57. 2° (511) and 63. 4° (440), which are consistent with the standard data for magnetite¹⁻³. These crystalline entities show the typical pattern of Fe₃O₄, and there was no other phase such as Fe₂O₃ or Fe(OH)₃, which were the usual co-products in chemical reverse coprecipitation process. The peak positions of Fe₃O₄ nanoparticles are unchanged after encapsulation by poly Aniline, which illustrated that the crystalline structure of Fe₃O₄ nanoparticles was not changed during the preparation procedure of Fe₃O₄/ poly Aniline.



Fig. 1: XRD pattern of Fe₃O₄- Graphene/Poly Aniline nanocomposite.

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Preparation and Characterization of Sulfobutyl Ether Beta-Cyclodextrin Binary Inclusion Complexes of Curcumin

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Abstract

The low solubility Curcumin (CUR) is a natural polyphenol with antioxidative, anti-inflammatory, and anticancer properties and it's therapeutic. Relatively low water solubility and low bioavailability of curcumin reduce its potential in food industry applications. In this work, the inclusion of a new solution CUR complex was prepared with cyclodextrin sulfobutyl ether (SBE- β -CD) and using different preparation techniques and characterized by fourier transform infrared (FTIR), nuclear magnetic resonance(HNMR), phase solubility method. The phase-solubility diagrams indicate an enhancement of the CUR solubility in the presence of β -CD, as well as its derivatives, SBE- β -CD in different extents, related to the type of cyclodextrin. The content, solubility, dissolution, and stability of the complexes were evaluated and compared with curcumin and their physical mixture.

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Sulfobutylether-β-cyclodextrin Complexes Loaded Alginate/Chitosan Nanoparticles as a Potential Approach for Indomethacin Drug Delivery

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Abstract

The low solubility and the irritant and harmful effects of oral indomethacin on the gastro-intestinal mucosa have limited its therapeutic potential.¹ The aim of this study is first; to enhance the solubility, stability and bioavailability of indomethacin (IND) through complexation using sulfobutylether- β -cyclodextrin (SBE- β -CD). Second; to prepare IND/SBE- β -CD/chitosan nanoparticles by the ionic gelation of chitosan with tripolyphosphate, to control the drug release and finally; to coat the nanoparticles with alginate to avoid drug release at acidic pH condition of stomach whereas, in intestinal pH can offer controlled release of the drug and thus reduce its gastrointestinal side effects.^{2,3} The formation of inclusion complexes was characterized by Fourier transform spectroscopy (FTIR), ultraviolet-visible (UV-Vis) and nuclear magnetic resonance (NMR) spectroscopies. The solubility of IND increase with increasing the SBE- β -CD concentration in A_L-type system.The influence of different process variables on particle size, zeta potential, drug content, in vitro release was investigated. In vitro release of IND from its SBE- β -CD complex alone as well as from the alginate coated IND/SBE- β -CD loaded chitosan nanoparticles were compared at pH 1.6 and pH 7.

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The Highly Efficient Capture of Cationic Dyes with Fe/Ni-Based Metal-Organic Frameworks

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Abstract

In this work, effective mixed-metal organic frameworks Fe-Ni MOF were synthesized via most favored and cost-effective solvothermal method for the removal of brilliant green (BG) and Methylene blue (MB) cationic dyes from aqueous solutions. XRD, FTIR, FESEM, EDS, BET, and TGA analytical techniques were used to investigate and confirm the structural characteristics of the Fe-Ni MOF adsorbent. The effect of the contact time, adsorbent dosage, and initial dye concentration, and pH on the removal efficiency of BG and MB cationic dyes were examined. Also, The isotherm and kinetic parameters of BG and MB removal on Fe-Ni MOF catalyst from aqueous solutions were checked out. The results showed that Fe-Ni MOF displayed the best adsorption capacity for BG and MB at the optimal experimental conditions, which was ascribed to its high porosity and higher pore volume. In addition to the synergistic effects of metallic ions in Fe-Ni MOFs which are intermediate acids, can lead to substantial dye removal performance. Also, The isotherm and kinetic parameters of BG and MB dye removal on Fe-Ni MOFs were well-fitted by the Freundlich and pseudo-second-order models. These findings suggest that the adsorption process takes place on a multilayer surface.

Furthermore, the Fe-Ni MOFs adsorbent had a stable adsorption capability after regeneration. The good adsorption efficiency of Fe-Ni MOFs catalyst makes it a potential adsorbent for the removal of cationic dyes from aqueous solutions.



Graphic abstract: Schematic synthesis of Fe-Ni MOF adsorbent and its application in removing cationic dyes.

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Spectroscopy Study on Sulfobutyl Ether Beta Cyclodextrin (SBE-β-CD) Inclusion Complex with Fenofibrate Cholesterol Lowering Drug

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Abstract

The present work is a study in order to enhaused a improved oral bioavailability of the poorly water-soluble fenofibrate(FNB) cholesterol lowering drug. For this purpose the physicochemical characterization of fenofibrate/SBE- β -CD binary systems was carried out by fourier transform infrared (FTIR), ultraviolet-visible (UV-Vis) and nuclear magnetic resonance (NMR) (Fig.1) spectroscopies. Phase solubility analysis and in vitro release studies revealed enhancement in the solubility of fenofibrate. The effect of freeze drying on the cyclodextrin complexation was also evaluated. Phase solubility studies revealed 1:1 M complexation of fenofibrate with SBE- β -CD. The dissolution study revealed that the drug dissolution rate was improved by the presence of SBE- β -CD as compared to pure drug. It is concluded that fenofibrate/SBE- β -CD complexation results in an increase in the solubility and dissolution rate of the drug, suggesting a possible enhancement of its oral bioavailability.



Figure 1: ¹ HNMR spectra of 1) SBE- β CD. 2)Fenofibrate. and 3) fenofibrate/SBE- β -CD complex

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A Facile One-Pot Five-Component Synthesis of Novel 1,2,3-Triazole-Linked dicyanoanilline and Photophysical Studies

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Abstract

Multicomponent reactions (MCR) involving domino processes, with at least three different simple substrates, has emerged as a powerful strategy in synthesis in recent decades.¹ The MCR approach allows molecular complexity to be created by the facile formation of several new covalent bonds in a one-pot transformation quite closely approaching the concept of an ideal synthesis.²

Dicyanoanilines are useful intermediates and act as building blocks for cyclophanes, large molecular cavities, and host–guest complexes.³ According to this, and based on our pervious experiences,⁴ we decided to link dicyanoanilines to triazole compounds to enhance their usual properties.

An efficient one-pot synthesis of novel dicyanoanilline linked to triazol analogues is reported here. The synthesis take place by the combination of various cyclic ketones with malononitrile and 4-(prop-2-yn-1-yloxy)benzaldehyde derivatives in a *t*-BuOH/NaOH_{aq} medium (Scheme 1). The whole reaction was carried out under ambient temperature and mild conditions. Due to the presence of A-D-A fragment in the structure of dicyanoanillines, they are known for exposing optical activities. Thus, the products were studied for their photophysical properties, exhibiting improved fluorescence properties.



Scheme 1: Descriptive synthesis of triazole anchored dicyanoanilines.

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Efficient One Pot Three Component Route for the Synthesis Novel Dicyanoanilines Under Ultrasonic Condition

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Abstract

Substituted 2,6-dicyanoanilines are important compounds studied as the intermediates in diverse fields such as optical materials, dyes, textile printing, heat resistant polymers, chiral stationary phases in chromatography and so on.¹ Substituted 2,6-dicyanoanilines constitute an important group of useful compounds with acceptor-donor-acceptor (A-D-A) systems having various applications. Many of the compounds with A-D-A systems including substituted 2,6-dicyanoanilines exhibit strong fluorescence² and have been studied as substrates for non-linear optical materials.³

In the present work, an eco-friendly three-component synthesis of novel 2,6 dicyanoanillines with malononitrile and 4-(prop-2-yn-1-yloxy) benzaldehyde derivatives in aqueous sodium hydroxide under ultrasonic irradiation is described. Reactions are completed after a few minutes, the work-up is convenient, and the only reaction product was obtained by recrystallization in ethanol. This facile approach reduces the reaction time and the energy consumption and increases the yield and selectivity of the process.



Scheme 1: Description synthesis of dicyanoanilines.

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Tandem Oxidative Amidation of Benzylic Alcohols Catalyzed by Dopamine/Cu(II) Immobilized on ZnFe₂O₄ Nanoparticles

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Abstract

Amide as multifunctional groups in organic chemistry has been received special attention in recent decades. Numerous methods were reported to synthesize amide, but their use was limited due to problems such as high cost, the creation high amount of chemical wastes, low efficiency, and the use of dangerous or toxic reagents. In this study, amide was prepared by tandem oxidative amidation of benzyl alcohols in the presence of amine hydrochloride salt as a fast, efficient, and cheap method. To prepare the catalyst, $ZnFe_2O_4$ nanoparticles were synthesized by co-precipitation method and functionalized by dopamine/Cu(II).¹ This surface modification was performed via tetraethyl orthosilicate and (3-chloropropyl)trimethoxysilane. The reaction was carried out within 4 hours in the presence of amine hydrochloride (1.0 mmol), benzyl alcohols (1.5 mmol), catalyst (20 mg), CH₃CN (3 mL), CaCO₃ (1.1 equiv), TBHP (70 wt % in H₂O, 4 equiv) at 80 °C under N₂ atmosphere.² In this conditions, a variety of amide derivatives with an efficiency of 70-90% were synthesized. In addition, the synthesized catalyst can be easily separated from the reaction medium by an external magnet and can be reused for 5 consecutive runs without a significant reduction in reaction efficiency.



Scheme 1: Graphical illustration of tandem oxidative amidation of benzylic alcohols

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Preparation and Characterization of Graphitic Carbon Nitride (g-C₃N₄) Nanosheets Modified by Copper as an Efficient Catalyst for the Tandem Oxidative Amidation of Benzylic Alcohols

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Abstract

The design and synthesis of safe, inexpensive, recyclable, and efficient catalysts for chemical reactions is an important goal in the synthesis of organic compounds. Amides are one of the most important functional groups that can play a key role in various industrial and scientific research fields such as polymers, drugs, chemical raw materials, biomolecules, and natural products. Various protocols have been used to synthesize amides, but the risks and negative effects of these methods such as difficult reaction conditions, the use of hazardous substances, and the low level of atom efficiency, lead to creating novel methods. In this study, copper-modified g-C₃N₄ nanosheets were used as an efficient catalyst for one-pot tandem oxidative amidation of benzyl alcohols. In order to fabricate the catalyst, bulk $g-C_3N_4$ was prepared by using melamine as cheap raw ingredients.¹ Subsequently, g-C₃N₄ nanosheets were prepared during the exfoliation process and modified by copper (II) acetate. The conversion of substituted benzyl alcohols to various amides were efficiently performed with synthesized catalyst via a one-pot direct oxidative amidation reaction and the desired amides were obtained with high to moderate yields. The reaction was carried out within 3 hours in the presence of amine hydrochloride salts (1.0 mmol), benzyl alcohols (1.5 mmol), catalyst (20 mg), CH₃CN (3 mL), CaCO₃ (1.1 equiv), TBHP (70 wt % in H₂O, 4 equiv) at 80 °C under N₂ atmosphere.² Notably, the one-pot tandem reaction has several outstanding advantages including facile synthetic method, excellent activity, and simple workup. In addition, it should be noted that the synthesized catalyst can be reused for 5 consecutive runs without a significant reduction in reaction efficiency.



Scheme 1: Graphical illustration of tandem oxidative amidation of benzylic alcohols

Reference

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Metal-free N, S-doped biographene in Green Synthesis of [1]benzopyranopyrido[d]pyrimidines

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Abstract

The multicomponent reactions are well-known strategies in macrocyclization, peptide cyclization, and diversity oriented derivatization of complex fused heterocyclic.¹⁻²

We have reported here an operationally simple and green synthesis of 7-(4-chlorophenyl)-9,11-dimethyl-6H-[1]benzopyrano[3',4':5,6]pyrido[2,3-d]pyrimidine-6,8,10(9H,11H)-trione via cyclocondensation reaction of 4-hydroxycoumarin, aromatic aldehydes, and 6-amino-1,-3-dimethyluracil catalyzed by a bioinspired porous N,S-doped graphene catalyst.

The N,S-doped graphene was synthesized from natural gum and characterized by FT-IR, XRD, SEM, XPS, Raman, and TGA analysis. The structures of target compounds were also confirmed by IR, ¹H NMR, and ¹³C NMR spectroscopic data and also by elemental analyses. High yields of products, short reaction times, the use of green solvent and reusable catalyst, and easy work-up are the main advantages of this protocol.



Scheme 1: Synthesis of 7-(4-chlorophenyl)-9,11-dimethyl-6H-[1]benzopyrano[30,40:5,6]pyrido[2,3-d]pyrimidine-6,8,10(9H,11H)-trione

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Bioporous SiO2/ZnO Nanocomposites as Efficient Catalyst in Synthesis of Chromeno-Pyrido[d]pyrimidine Derivatives

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Abstract

Compounds containing [1]benzopyran (chromene) framework are well-known natural and non-natural pharmacological agents and additionally, they possess diverse biological activities such as antibacterial, antineoplastic, antimicrobial, and anti-HIV.¹⁻²

Here, the synthesis of efficient heterogenous catalysts for the environmentally friendly and economic synthesis of 9,11-dimethyl-7-aryl-6H-chromeno[3',4':5,6]pyrido[2,3-d]pyrimidine-6,8,10(9H,11H)triones was reported via cyclocondensation reactions between 4-aminocoumarin, 1,3-dimethylbarbituric acid, and aromatic aldehydes. Bioporous SiO₂ were synthesized from natural grasses, then ZnO nanoparticles stabilized on the surface of porous silica through hydroxyl functional groups and characterized by FTIR, XRD, SEM/EDX, and BET/BJH methods. The structures of chromene compounds were fully confirmed via IR, ¹H NMR and ¹³C NMR spectroscopic studies, and also from elemental analyses. High yields of products, the use of a green solvent, the easy work-up procedure, the short reaction times, and the easily separable catalyst are the main advantages of this protocol.



Scheme 1: Synthesis of 9,11-dimethyl-7-aryl-6H-chromeno[3',4':5,6]pyrido[2,3-d]pyrimidine-6,8,10(9H,11H)triones

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Drug and Physicochemical Properties of 4-cyclopentyl-7,7-dimethyl-2-phenyl-1,2,4,7,8,9-hexahydro-3H-pyrazolo[3,4-b]quinoline-3,5(6H)-dione

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Abstract

Antimicrobial drugs, structurally diverse molecules, can be natural products, semisynthetic derivatives of natural compounds, or chemically synthesized compounds. The development of antimicrobials in general, first of all antibiotics, but also antivirals and antimalarials, revolutionized medicine in many ways, and as such is one of the greatest successes of modern medicine. Unfortunately, time with these drugs is rapidly running out. Occurrence and global spread of resistance of bacteria, fungi, viruses, and protozoan parasites to available antimicrobial medicines threaten to send humanity back to pre-antimicrobial era. Therefore, there is an urgent need not just to develop novel antimicrobials but also to introduce into practice novel therapeutic options to fight against both drug-sensitive and drug-resistant pathogens.

Quinine, quinoline alkaloid isolated from the bark of the Cinchona tree in 1820, used in the treatment of malaria played a historical role in the development of quinoline alkaloids as therapeutics. These quinoline based compounds have been isolated and identified from natural sources (plants, animals, and microorganisms), and many studies have documented their antitumor, antimalarial, antibacterial, antifungal, antiviral, antiparasitic and insecticidal, anti-inflammatory, antiplatelet and other activities. In this study 4-cyclopentyl-7,7-dimethyl-2-phenyl-1,2,4,7,8,9-hexahydro-3H-pyrazolo[3,4-b]quinoline 3,5(6H) dione has been investigated as drug by density functional theory. All calculations were accomplished using the B3LYP/6-311G exchange-correlation function. Fig 1 demonstrated the structure of drug. The drug behaviour of 4-cyclopentyl-7,7-dimethyl-2-phenyl-1,2,4,7,8,9-hexahydro-3H-pyrazolo[3,4-b]quinoline 3,5(6H) dione is studied by caculating the physicochemical properties such as η , χ , μ , α , ρ , ω , σ and logp. All resulted data showed good and valuable properties for 4-cyclopentyl-7,7-dimethyl-2-phenyl-1,2,4,7,8,9-hexahydro-3H-pyrazolo[3,4-b]quinoline 1,2,4,7,8,9-hexahydro-3H-pyrazolo[3,4-b]quinoline 3,5(6H) dione as drug.



Figure 1: Structure of 4-cyclopentyl-7,7-dimethyl-2-phenyl-1,2,4,7,8,9-hexahydro-3H-pyrazolo[3,4-b]quinoline 3,5(6H) dione.

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In Silico Study of PFKFB3 Inhibitors as Anti-Cancer Compounds

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Abstract

PFKFB3 is a gene that encodes the 6-phosphofructo-2-kinase/fructose-2,6-biphosphatase 3 enzyme in humans is one of 4 tissue-specific PFKFB isoenzymes. PFKFB3 converts fructose-6-phosphate to fructose-2,6-bisP (F2,6BP). F2,6BP is a potent allosteric activator of 6-phosphofructokinase-1 (PFK-1), stimulating glycolysis. Energy and biomass production in cancer cell is largely supported by aerobic glycolysis in what is called the Warburg effect and other Cancer Connections of PFKFB3 like in Hypoxia Signaling Pathway, Cell Cycle and Apoptosis and Circadian Clock.¹ Many small molecule inhibitors of PFKFB3 are currently in development and Inhibition of PFKFB3 is being analyzed as a potential anti-cancer therapy.^{2,3}

We employed virtual screening tools to search for PFKFB3 inhibitors to accelerate the drug discovery process.⁴ The hit compounds from reference ligand pharmacophore search were subsequently docked into the active site of PFKFB3 Structure and ranked by their binding energy.⁵ Finally, In silico ADME studies were performed on top 10 compounds to probe for adoption with the standard ranges.⁶



Scheme 1: Insilico study of PFKFB3 inhibitors

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Nef-isocyanide Reaction in Synthesis of Functionalized Thiazolidines

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Abstract

Isocyanides have played a significant role in the successful development of classical multicomponent reactions, such as the Passerini 3-component and Ugi 4-component reactions, and have also been used in the synthesis of a wide range of heterocyclic systems.^{1,2} The reaction of isocyanides with acyl chlorides gives α -ketoimidoyl chlorides (Nef-isocyanide adducts), which can be trapped by various nucleophiles for the synthesis of N-heterocyclic compounds.³ The thiazolidine derivatives with regard to their notable medicinal and pharmaceutical properties are a very important structural motif in medicinal chemistry. These compounds posses diverse biological activities including anticancer, antimicrobial anticancer, antimicrobial, antitumor, antidiabetic, antiparasitic, anti-inflammatory, antitubercular, antifungal, antiviral, anti-HIV, cytotoxicity, antitrypanosomal, antinociceptive and anti-hypernociceptive compounds.⁴

we here report an efficient one-pot method for the direct synthesis of ethyl 5-(alkylimino)-4-hydroxy-2-(arylimino)-3-alkylthiazolidine-4-carboxylates from the reaction of ethyl 3-chloro-3-(alkylimino)-2oxopropanoate (obtained from alkyl isocyanides and ethyl 2-chloro-2-oxoacetate) and 1-alkyl-3arylthioureas (prepared from primary alkylamines and aryl isothiocyanates) in dry MeCN at room temperature. The structures were corroborated spectroscopically (IR, 1H-, 13C- NMR, and EI-MS). Various features of these transformations will be presented and discussed (Scheme 1).



Scheme 1: synthesis of ethyl 5-(alkylimino)-4-hydroxy-2-(arylimino)-3-alkylthiazolidine-4-carboxylates

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Synthesis of Unsaturated Polyester by Transesterification of Castor oil-derived Methyl ester

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Abstract

Castor oil, as a renewable resource, has several reactive sites, including double bonds, hydroxyl and ester groups, and acts as a platform chemical for the synthesis of various highly valuable materials.^{1,2} Biopolymers such as oligomeric polyesters of castor oil derivatives can be produced chemically or biotechnologically for use in food, cosmetics, lubricants and other industrial applications.^{3,4}

In this work, methyl ricinoleate (biodiesel) was derived from castor oil via transesterification with methanol in the presence of an alkaline catalyst. After separation and purification, methyl ricinoleate was reacted with 1,4-butanediol in xylene in the presence of tin catalyst. The polymerization was stopped by cooling the reaction mixture and the the product was washed with hot water to remove the catalyst and any unreacted 1,4-butanediol. Water and xylene were distilled off and the unsaturated polyester was obtained. The overall synthetic procedure is illustrated in Figure 1.

The effect of various parameters of the reaction including residence time, castor oil to methanol molar ratio, catalyst concentration, and reaction temperature on the yield of transesterification and polymerization was investigated. The optimum operating conditionsobtained in the present work are 1:9 molar ratio of oil to methanol, 60 °C reaction temperature, 1 wt% catalyst concentration and 45 min reaction time for first step and 120 °C reaction temperature, 1.5 wt% catalyst concentration for the second step.



Figure 1: Synthesis of unsaturated polyester from castor oil-derived methyl ester.

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Preparation of a Polyhydroxystearic Acid by Self-condensation Method

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Abstract

Polyesters based on polyhydroxystearicacid are biopolymers attracted much attention due to their biodegradability, biocompatibility, and relatively high thermal oxidative and hydrolytic stability.^{1,2} Polymers based on hydroxystearic acid and its derivatives are used in the production of elastomers, foams, coatings and adhesives.^{3,4}

Herein, hydroxystearicacid was polymerized by self-polycondensation in the presence of 1 wt% paratoluene sulphonic acid (PTS) as catalyst and xylene as a solvent. The reaction was performed for 6 h. The progrees of the reaction was monitored by determination of acid value of the reaction mixture. When carboxylic acid groups reach to a minumum value, the esterification was completed and the product was washed with water and distilled under vacuum to remove xylene. The resulting product was characterized by FT-IR and NMR spectroscopy and gel permeation chromatography (GPC). The polymerization conditions were optimized to to achieve the polyester polyol with desired properties. The results showed that polyhydroxystearicacid with 2060 g/mol was synthesized.



Figure 1: Synthesis of polyhydroxystearic acid.

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Ring-opening Polymerization of Tetrahydrofuran

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Abstract

The ring-opening polymerization is a useful method to prepare polymers and copolymers with controlled microstructure, chain length and functionality that are otherwise difficult to obtain by conventional polymerization methods.^{1,2} This method is usually used for the production of high performance polymeric materials and engineering plastics. Poly(tetramethylene ether glycol) (PTMG), also called poly(tetrahydrofuran), is a colorless waxy polymer that is widely used as a soft segment for the production of thermoplastic elastomers and as an intermediate for the synthesis of elastic fibers, polyurethanes, and polyesters.^{3,4} Due to its unique physical and chemical properties and its use in advanced applications, it is very demanding to design efficient methods for the synthesis of PTMG.

In this study a catalytic prodecure has been developed for the synthesis of PTMG by ring opening polymerization of THF.Herein,a heteropolyacid (H₃PW₁₂O₄₀) and acetic anhydride as a co-catalyst are used to control the molecular weight of the resulting polymer. The heteropolyacid has high acid strength and forms stable polyanions and in combination with acetic anhydride can activate THF ring. The activated THF rings are opened and polymerized to form the acetate-terminated polymer. Polymerization was terminated and the acetate end-groups are hydrolyzed with the addition of NaOH aqueous solution. The overall synthetic procedure is shown in Figure 1. The resulting product was characterized by gel permeation chromatography (GPC) and ¹H NMR, ¹³C NMR and FT-IR spectroscopy.

 $(CH_{3}CO)_{2}O + H_{3}PW_{12}O_{40} = [CH_{3}CO]^{+} [H_{2}PW_{12}O_{40}]^{-} + CH_{3}COOH$



Figure 1: Synthesis of PTMG by ring opening polymerization of THF.

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Synthesis of Azelaic Acid by Oxidative Cleavge of Oleic Acid

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Abstract

Azelaic acid is a biologically active dicarboxylic acid found in whole grains, wheat, rye and barley.¹ Due to its anti oxidative, anti inflammatory and bactericidal properties, azelaic acid is used as a pharmacological ingredient especially for the treatment of skin disorders like acne.² It is also used for the synthesis of polyesters, polyamides, placticizers and lubricants.³ The azelaic acid market is growing yearly and predicted to reach USD 160 million by 2023. Azelaic acid is usually produced by the ozonolysis of oleic acid.⁴ Pelargonic acid is also produced as the by-product of the reaction. However, alternative methods are highly demanding due to the toxicity of ozone gas, safety risks, the need to specific equipments and high energy consumption of ozonolysis.

Herein, the synthesis of azelaic acid is performed by oxidative cleavage of oleic acid using hydrogen peroxide aqueous solution (30 wt%) in the presence of tungstophosphoric heteropolyacid as a catalyst and benzyl triethyl ammonium chloride as a phase transfer catalyst. The effect of the reaction temperature, catalyst concentration, hydrogen peroxide/oleic acid molar ratio on the yield of the reaction was also studied. The conversion attained at optimum conditionwas 96% in 5 hours. Azelaic acid and pelargonic acid as the products of oxidative cleavage were obtained in high yield. The schematic illustration of the reaction is shown in Figure 1.



Figure 1: Synthesis of azelaic acid and pelargonic acid by oxidative cleavage of oleic acid.

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Nano-Pistachio Hull-OSO3H: Synthesis, Characterization and Application as an Efective and Novel Nanocatalyst for One-Pot Synthesis of Dihydropyrano [3, 2-*b*] Chromene Dione Derivatives

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Abstract

In this work, the novel pistachio hull-OSO₃H catalyst was synthesized via preparing pistachio hull as a support followed by treatment with chlorosulfonic acid (CISO₃H) and identifed by Fourier transform infrared spectroscopy (FT-IR), feld emission scanning electron microscopy (FE-SEM), X-ray difraction spectroscopy (EDX), Thermogravimetric analysis (TG) and X-ray powder difraction (XRD). The size of the pistachio hull-OSO₃H nanocatalyst was shown by a scanning electron microscope below 100 nm. The catalytic activity of the solid acid catalyst has been successfully examined in a one-pot, three-component condensation reaction of aromatic aldehydes, dimedone and kojic acid under solvent-free condition to furnish dihydropyrano [3,2-*b*] chromen dione derivatives. The proposed approach has some advantages as excellent yields, mild reaction conditions, short reaction times, use of agricultural waste and eco-friendly nature.



Figure 1: Synthesis of dihydropyrano[3,2-*b*]chromene dione derivatives in the presence of nano-pistachio hull-OSO₃H as a catalyst

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Preparation and Characterization of Novel Nano-cellulose-OSO₃H Prepared from the Almond Shell as a Catalyst and Its Application in Synthesis of 2-Amino-3-Phenylsulfonyl-4-Aryl-4*H*-Benzo[*h*]Chromen Derivatives

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Abstract

The novel nano-cellulose-OSO₃H prepared from the almond shell was synthesized via preparing mesoporous almond shell as an efficient support followed by treatment with chlorosulfonic acid (CISO₃H). This catalyst was characterized by FT-IR, FE-SEM, TEM, EDX, BET, TGA and XRD methods.

Through SEM device, the size of the cellulose-OSO3H nanocatalyst revealed <30 nm. The catalytic activity of the solid acid catalyst has been successfully investigated in a one-pot three-component condensation reaction. In these procedures, aromatic aldehydes, α -naphthol and (phenylsulfonyl)acetonitrile were applied under solvent-free condition producing 2-amino-3-phenylsulfonyl-4-aryl-4*H*-benzo[*h*]chromen derivatives with high yields.

cellulose-OH

 $\frac{\text{CISO}_{3}\text{H}}{\longrightarrow} \text{cellulose-OSO}_{3}\text{H} + \text{HCI}$

Chloroform, 0°C

Figure 1: Preparation of nano-cellulose-OSO₃H catalyst

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Highly Efficient Synthesis of Silica-Coated Magnetic Nanoparticles Modified with Iminodiacetic Acid Applied to synthesis of 1,2,3-Triazoles

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Abstract

Great efforts have been made to discover new catalysts to facilitate synthesis of organic fine chemicals. In this research, a new silica-coated magnetic nanoparticles functionalized by iminodiacetic acid (Fe₃O₄@SiO₂@IDA) was prepared by the sol-gel method. The structure of nanoparticles was fully characterized by using X-ray diffraction, scanning electron microscopy, energy-dispersive X-ray spectroscopy, Fourier transform infrared spectroscopy and thermogravimetry analysis. The results revealed that the nanoparticles have spherical morphology and an average size of around 40 nm. The analysis also illustrated that the copper nanoparticles had been successfully loaded on the nitrogen-rich carbon support with a uniform distribution. The inductively coupled plasma analysis showed that about 0.22 mmol g^{-1} of Cu was loaded on the Fe₃O₄@SiO₂@IDA support. Application of Fe₃O₄@SiO₂@IDA-Cu as a magnetically recyclable nanocatalyst for synthesis of 1,4-disubstituted-1,2,3-triazole derivatives through an azide-alkyne [3 + 2] cycloaddition reaction was also investigated. Mild reaction conditions, excellent yields (65-90 %), environment-friendly synthesis and easily prepared starting materials are the key features of the present method. The catalyst is easily removed from the reaction media using an external magnetic field and can be re-used at least 5 times without any considerable loss of its catalytic activity.



Scheme 1: Schematic of triazoles derivatives synthesis by using of Fe₃O₄@SiO₂@IDA-Cu

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Highly Efficient Synthesis of Silica-Coated Magnetic Nanoparticles Modified with Dipicolylamine Applied to Suzuki-Miyaura Reaction

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Abstract

Aryl halides and especially (iodide and bromid) were catalyzed by a benzonoid aromatic ring in a Suzukimyaro coupling reaction in the absence of organic solvents and toxic phosphine ligands by a magnetic nanocatalyst. Great efforts have been made to discover new catalysts to facilitate synthesis of organic fine chemicals. In this research, a new silica-coated magnetic nanoparticles functionalized by dipicolylamine (Fe₃O₄@SiO₂@DPA) was prepared by the sol-gel method. The structure of nanoparticles has been completely identified using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FT-IR) and thermal gravimetric analysis (TGA). The results revealed that the nanoparticles have spherical morphology and an average size of around 26-36 nm. By analyzing the nanocatalyst ICP analysis ,the concentration of pd in the substrate (Fe₃O₄@SiO₂@DPA-Pd) was reported to be 1.1 % by weight (Fe₃O₄@SiO₂@DPA-Pd) EDX analysis (Fe₃O₄@SiO₂@DPA-Pd) nanocatalyst confirm the presence of iron as well as palladium and silica in the nanocatalyst structure. Application of (Fe₃O₄@SiO₂@DPA-Pd) as a magnetically recyclable nanocatalyst for synthesis Aryl halides derivatives through Suzuki-Myaro reaction . Mild reaction conditions, excellent yields (68-95 %), environment-friendly synthesis and easily prepared starting materials are the key features of the present method. The catalyst is easily removed from the reaction media using an external magnetic field and can be re-used at least 5 times without any considerable loss of its catalytic.



Scheme 1: Schematic of Biaryl derivatives synthesis by using of (Fe₃O₄@SiO₂@DPA-Pd)

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