In the name of Allah,
the beneficent,
the merciful

21st Iranian Inorganic Chemistry Conference

بیست و یکمین کنفرانس شیمی معدنی ایران

دانشگاه اراک - دانشکده علوم پایه - گروه شیمی

۶ تا ۷ شهریور ۱۳۹۸
28 to 29 Aug 2019

مهلت ارسال مقالات:
۱۵ فروردین
لغایت
۳۰ اردیبهشت

ارسال برای داوری:
۱ خرداد

اعلام نتایج داوری:
۳۰ خرداد

ثبت نام نهایی:
۱۵ تیر

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Book

Of

21st Iranian Inorganic Chemistry Conference

Arak University, 28-29 August 2019

Contents

Preface

As representatives of Iranian Chemical Society it is our great pleasure to invite you to participate in 21st Iranian Inorganic Chemistry Conference (IICC21), which will be held on August 28-29, 2019 at Arak University. Arak is the capital of Markazi Province and, as it is known, is Industrial Capital of IRAN. Arak hosts several industrial factories inside and within a few kilometers outside the city, including the factory of Machine Sazi Arak, Iranian Aluminium Company, Arak Petrochemical Company, HEPCO, AZAR AB IND'S Company, Ronass dye Company, and…. These factories produce nearly half of the needs of the country in steel, petrochemical, and locomotive industries.

The aim objective of IICC21 is to bring together leading academicians, researchers, scholars as well as industrial professionals from IRAN to exchange and share their experiences and research results about all aspects of inorganic chemistry science and discuss the practical challenges encountered and the solutions adopted. Also, IICC21 provides opportunities for the delegates to exchange new ideas and application experiences face to face, to establish research relations and to find global partners for future collaboration.

The conference will be held on Wednesday 28 until Thursday 29 August 2019 at faculty of science of Arak University and focuses on various topics in different areas of inorganic chemistry such as, nanotechnology, computational studies, synthesis and characterization of inorganic materials and also their applications.

The IICC21 is included 280 papers, 1 plenary lecture, 13 invited speakers and 9 short oral presentations. Also, there are many topics covered by 5 organized workshops as separate sessions. During recall, 350 papers were arrived. The papers were be reviewed by at least two independent peers for technical merit and content and in some cases, where the abstract were too far from the standard of the conference, we asked the authors to revise their abstracts. It should be noted that all accepted papers were considered as poster and organizing committee of conference, under authority of Iranian Chemical Society, invited the specialists and/or the known academic persons to have a significant lecture in the conference. The 2 short oral presentations are also considered for industrial professional members.

We wish to take this opportunity to express our thanks to the authors who made contribution to this IICC21. Also, we sincerely appreciate the Arak University authorities, the Faculty of Science, the Iranian Chemical Society, the executive and scientific committees and the chemistry students for their valuable supports, guidance and efforts in organizing the conference. Thank you very much for attending 21st Iranian Inorganic Chemistry Conference and we hope you find the sessions helpful and informative.

Dr. Hamid Khanmohammadi & Dr. Mojgan Zendehdel

Chairs of 21st Inorganic Chemistry Conference

Special Thanks to All Who Participated in Doing 21st Iranian Inorganic Chemistry Conference

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انجمن شیمی ایران	انجمن شیمی ایران Iranian Chemical Society
استانداری استان مرکزی	وزارت کشور استانداری استان مرکزی
سازمان صنعت، معدن و تجارت استان مرکزی	جمهوری اسلامی ایران وزارت صنعت، معدن و تجارت سازمان صنعت، معدن و تجارت استان مرکزی
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The Previous Iranian Inorganic Chemistry Conferences

1st	Isfahan	1990	Dr. Mehdi Amir Naser	Isfahan University of Technology
2nd	Tehran	1991	Dr.Yahya Farhangi	Alzahra University
3rd	Tabriz	1994	Dr. Ali Akbar Khandar	University of Tabriz
4th	Hamedan	1995	Dr. Seyed Javad Sabounchei	Bu-Ali Sina University
5th	Isfahan	1999	Dr. Mohamad Hosein Habibi	University of Esfahan
6th	Mashhad	2001	Dr. Mohamad Alizadeh	Ferdowsi University of Mashhad
7th	Zanjan	2002	Dr. Hasan Hoseini Monfared	University of Zanjan
8th	Tabriz	2004	Dr. Moayed Hoseini Sadr	Azarbaijan University of Tarbiat Moallem

9th	Semnan	2006	Dr. Ali Amoozadeh	Semnan university
10th	Zahedan	2008	Dr. Mojgan Khorasani Motlagh	University of Sistan and Baluchestan
11th	Isfahan	2009	Dr. Mehdi Amir Nasr	Isfahan University of Technology
12th	Rasht	2010	Dr. Khalil Tabatabaeian	University of Guilan
13th	Kermanshah	2011	Dr. Ezat Rafiee	Razi University
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15th	Sabzevar	2013	Dr. Reza Tayebi	Hakim Sabzevari University
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We acknowledge also the collaboration of following academics, **Ph. D**, **M.Sc** and **B.Sc** students during the conference

Postdoctoral fellowship

Dr. Kh. Rezaiean

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Z. Faramarzi

Plenary

The Importance of the Periodic Table Elements in Science

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Abstract:

The discovery of the Periodic Table Elements by Mendeleev is one of the most significant achievements in science and a uniting scientific concept with extensive applications in various branches of science. The modern Periodic Table is the results of the efforts of many scientists, both chemists and physicists, before and after Mendeleev and one of the few scientific concepts that remained almost intact after 150 years. As the number of elements has gradually increased from 63 in the Mendeleev's time to the present118, the discovered elements over the years have been easily located in their right expected places in the Table. The Periodic Table provides extensive valuable information about chemical and physical properties of the elements as well as the variations of these properties at the minimum time. Therefore, the Periodic Table is considered as one of the most efficient, updated and unique tool enabling scientists to predict the appearance and properties of matter on Earth and in the Universe. Its wide application is not limited to basic science but also extend to advanced research studies. The Periodic Table has an important role in developing the science dealing with atomic and molecular structure, because for each well-known periodic trend or the observed exception to that trend, an advanced scientific interpretation is required. Moreover, the Periodic Table, unlike some other scientific concepts, is unlikely becoming obsolete in the future but rather it is getting more and more importance in chemistry and other scientific disciplines. The discovery of element 118 in recent years has completed the 7th raw of the Periodic Table but whether the Table can be extended to higher atomic number super heavy elements or not still remained as interesting scientific challenge.

References:

[1] P.Pyykkö, Chemical Review, 12 (2012) 371-384.

[2] R.Eichler, Journal of Nuclear Physics News, 29 (2019) 11-15.

[3] M.Jansen, Solid State Sciences, 7 (2015) 1464-1474.

Invited Speakers

How national and international collaborations can boost multidisciplinary research: Fabrication of organic light-emitting diodes (OLED) from novel complexes as a collaborative research

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Abstract:

Fast grow of technology for fabrication and commercialization of high-tech products demanding a collaboration of scientists in various filed for the development of advanced technology. In the present seminar, we will show how national and international collaboration can boost multidisciplinary research such as the fabrication of organic light-emitting diodes (OLED) from novel complexes. As an outcome of collaborative research between Department of Chemistry and Laser and Plasma Research Institute of Shahid Beheshti, and Institute für Anorganische Chemie of Düsseldorf University will be discussed, and a result of our recent work on the development of blue OLEDs technology as an example that outlined below will be presented.

In spite of vast study on the application of lanthanides complexes in the photonic devices, use of actinide complexes in the photonic device, specifically uranium complexes, is not investigated so far, to the best of our knowledge. In this context, three anthracene-9-carboxylic acid complexes of uranium have been synthesized and after characterization utilized for fabrications of OLED for the first time. Prepared uranium complexes showed emissions which made some of them suitable to fabricate rare blue OLEDs using vapor deposition method with and without orange pigment. The novel photoluminescent uranium complexes based on the anthracene-9-carboxylic acid ligand in the present study with stable blue emission may pave the path to accelerate the fabrication of low-cost and highly-efficient lighting sources based on OLED technology [1].

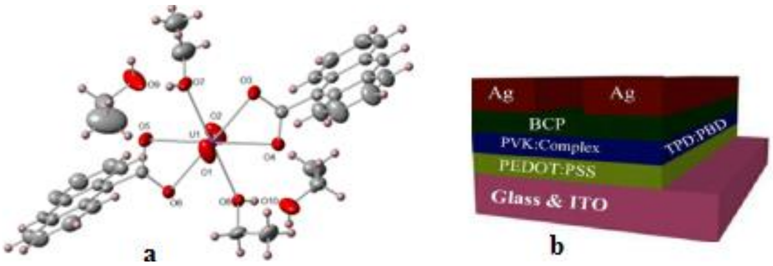

Fig.1 Crystal structure of precursor that used for fabrication of BOLED (a), structure of a fabricated BOLED device.

References:

[1] K. Darzinezhad, M. M. Amini E. Mohajerani, M. Armaghan, T. O. Knedel, A. Abareghi, Christoph Janiak, Dalton Trans., 48 (2019) 3695-3703.

Surface-grafted lanthanoid complexes of the Keggin-type heteropolyoxometallates: a hydrogen evolution reactivity, structural and computational investigation

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Abstract:

The hydrothermal syntheses of some inorganic–organic hybrids based on polyoxometallates, is surveyed. All compounds have been characterized using some physico–chemical approaches and single–crystal X–ray diffraction methods. Structural characterization by single–crystal X–ray diffraction reveals that these compounds consist of Keggin–type polyoxometallates, where a single $\{M_3O_{13}\}$ triad is decorated with a trinuclear Ln complex. Moreover, the decorated polyanions are involved in a series of intermolecular interactions, such as hydrogen bonds and anion–π interactions, resulting in three–dimensional supramolecular architectures. Density functional theory (DFT) studies were conducted to support these intermolecular interactions in the hybrids, and have been rationalized using molecular electrostatic potential (MEP) surface calculations. We reported the first examples of hydrogen evolution reactivity (HER) of lanthanide-functionalized Keggin-based polyoxotungstates under photochemical and electrochemical conditions.

References:

[1]. S. Derakhshanrad, M. Mirzaei, A. Najafi, C. Ritchie, A. Bauzá, A. Frontera, J. T. Mague, Acta Cryst., C74 (2018) 1300-1309.
[2]. M. Arab Fashapooyeh, M. Mirzaei, H. Eshtiagh-Hosseini, A. Rajagopal, M. Lechner, R. Liu and C. Streb, Chem. Commun., 54 (2018) 10427-10430.
[3]. S. Taleghani, M. Mirzaei, H. Eshtiagh-Hosseini, A. Frontera, Coord. Chem. Rev., 309 (2016) 84-106.
[4]. M.Mirzaei, H. Eshtiagh-Hosseini, M. Alipour, A. Bauza, J.T. Mague, M. Korabik and A. Frontera, Dalton Trans., 44 (2015) 8824-8832.
[5]. M. Mirzaei, H. Eshtiagh-Hosseini, M. Alipour, A. Frontera, Coord. Chem. Rev., 275C (2014) 1-18.
[6]. M. Mirzaei, H. Eshtiagh-Hosseini, N. Lotfian, A.R. Salimi, A. Bauzá, R. Van Deun, R. Decadt, M. Barceló-Oliver, A. Frontera, Dalton Trans., 43 (2014) 1906-1916.

Catalytic conversion of Venice lagoon brown marine algae for producing hydrogen-rich gas and valuable biochemical using algal biochar and Ni/SBA-15 nano catalyst

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Abstract:
Global warming and the widespread use of fossil fuels, such as petroleum, coal and natural gas, cause several environmental impacts which inspired many researchers to find alternative energy resources and more efficient technologies [1]. The energy derived from biomass in the form of bio-oil, biogas, and biochar has attracted great attention because of its obvious advantages such as being renewable, emitting relatively low carbon dioxide, and having a negligible amount of sulfur [2-4]. This study reports the conversion of *Sargassum* as a Venice lagoon brown macroalgae into gaseous, liquid and solid products via pyrolysis at different temperatures to determine its potential for bio-oil and hydrogen-rich gas production for further industrial utilization. Non-catalytic tests were performed to determine the optimum condition for bio-oil production. The highest portion of bio-oil was retrieved at 700 ℃. The catalytic test was performed using the algal biochar and Ni/SBA-15 at 700 ℃ as catalysts. Biochar catalyst exhibited excellent catalytic activity toward producing aromatic compounds via Diels-Alder-type reactions. However, Ni/SBA-15, because of interconnected pores provided easy passage for reactant and product during the catalytic pyrolysis process and resulted in an improvement in total gas yield and hydrogen-rich gas production. High specific surface area, large pore volume, highly ordered pore structure, and narrow pore size distribution make SBA-15 a promising catalyst support in pyrolysis of biomass.

References:

[1] P. Bartocci, G. Bidini, F. Asdrubali, C. Beatrice, F. Frusteri, F. Fantozzi, Renew Energy, 124 (2017) 1729.

[2] X. Hu, J. Xu, M. Wu, J. Xing, W. Bi, K. Wang, et al, J Anal Appl Pyrolysis, 127 (2017) 196202.

[3] G. Yildiz, F. Ronsse, R. Venderbosch, R. Duren, SAR.Kersten, W. Prins, Appl Catal B Environ, 168 (2015) 20311.

[4] T. Kan, V. Strezov, TJ. Evans, Renew Sustain Energy Rev, 57 (2016) 112640.

Assembly of Platinum or Palladium-Based Nanostructures and Metal-Organic Framework at liquid/liquid Interface

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Abstract:

Recently, the interface between two immiscible electrolyte solutions has been investigated as it suggests a simple, easy and non-cost experiment to handle system for the assembly of nano objects [1]. The drop in the total free energy of the system brought about by the reduction in the liquid/liquid surface area is the most common explanation for the nanoparticles assembly [1]. Platinum is a noble and expensive metal with high catalytic activity and stability that has many technological applications especially as electrocatalyst in fuel cell or water splitting reaction. Also, platinum (II) complexes have been known as anticancer drugs and are used in the chemotherapeutic regimes of cancer patients. Catalytic efficiency and selectivity of platinum are highly dependent on the size and shape of the platinum materials. Therefore, the synthesis of platinum nanoparticles with small size and special shape can contribute to the lowering of Pt usage, enabling much-needed cost reduction [2]. The method used to assembly of metal nanoparticles at the oil–water interface involves dissolving organometallic precursor in organic layer and injecting appropriate reducing reagent in the aqueous layer. Herein, we present our attempts for synthesis of different organoplatinum complexes [3,4], platinum or palladium-based nanostructures for application in direct methanol fuel cell [5], C-C coupling reactions [6], reduction of *p*-nitrophenol [7] or as the cocatalyst for photocatalytic water splitting [8] and assembly of Zeolitic Imidazolate Framework (ZIF-8) at oil/water interface.

References:

[1] S. G. Booth, R. A. W. Dryfe, J. Phys. Chem. C, 119 (2015) 23295-23309.
[2] S. J. Hoseini, M. Rashidi, M. Bahrami, J. Mater. Chem., 21 (2011) 16170- 16176.
[3] S. J. Hoseini, R. Hashemi Fath, M. A. Fard, A. Behnia, R. J. Puddephatt, Inorg. Chem. 57 (2018) 8951-8955.
[4] P. Hamidizadeh, S. M. Nabavizadeh, S. J. Hoseini, Dalton Trans., 48 (2019) 3422- 3432.
[5] S. J. Hoseini, N. Mousavi, M. Roushani, L. Mosadeghi, M. Bahrami, M. Rashidi, Dalton Trans., 42 (2013) 12364-12369.
[6] S. J. Hoseini, M. Dehghani, H. Nasrabadi, Catal. Sci. Technol., 4 (2014) 1078-1083.
[7] A. Zare Asadabadi, S. J. Hoseini, M. Bahrami, S. M. Nabavizadeh, New J. Chem., 43 (2019) 6513.
[8] P. Fatahi, A. Roy, M. Bahrami, S. J. Hoseini, ACS Appl. Energy Mater., 1 (2018) 5318-5327.

Metal-Organic Polyhedra as Molecular Nanoparticles

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Abstract:

Ultra-small inorganic nanoparticles (i. e. size below 10 nm) are important because they fill the gap between the molecular and the nanoscale regimes.1 On this scale, nanoparticles can merge properties of both regimes, such as solubility in different media with high reactivity and unique physicochemical and pharmacokinetic properties. However, their practical application demands chemical functionalization of their external surface, as it enables their stabilization and protection, tuning of their hydrophilic/hydrophobic character, and introduction of new functional molecules in to them (e.g. to modulate interactions between the nanoparticles and Biosystems). Thus, inorganic ultra-small nanoparticles are inherently polydisperse by virtue of the core or the external functionalization. This limitation makes it impossible to utilize a variety of methods that would provide molecular-level information regarding their composition and structure, which ultimately dictates the performance of the ultra-small nanoparticle.

Herein, we propose the use of metal-organic polyhedral molecules (MOPs)2 assembled from metal ions and organic ligands, which size is comprised between 1 – 5 nm, as new nanoscopic platforms or "molecular nanioarticles" (Figure 1). MOPs present reactive groups of different nature decorating their structure that can be reacted stoichiometrically to functionalize their structure and add new functionalities such as chirality and being soluble in a broad range of solvents. Specifically, we take advantage of the hybrid nature of MOPs to post-synthetically modify their composition through coordination and/or covalent chemistry. This new strategy provides structurally well-defined nanoscopic platforms for delivery, sorption and catalytic applications.

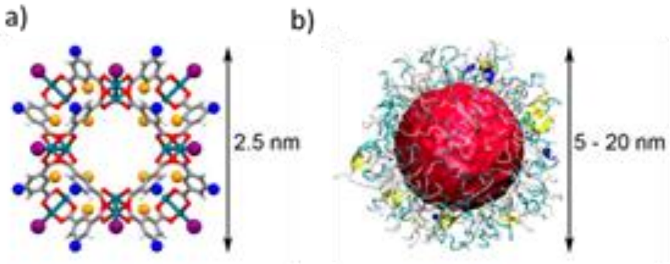

Figure 1. (a) Schematic representation of a MOP highlighting its well-defined reactive sites: the covalent inner and outer part (orange and blue) and the axial position of the metal ions (purple). (b) Illustration of a inorganic nanoparticle functionalized through surface chemistry.

References:

[1] R. Jin, C. Zeng, M. Zhou, Y. Chen, Chem. Rev., 116 (2016) 10346.

[2] Tranchemontagne, D. J. Ni, Z.; O'Keeffe, M.; Yaghi, O. M. Polyhedra. Angew. Chem. Int. Ed. 47 (2008) 5136.

[3] Carné-Sánchez, A.; Craig, G. A.; Larpent, P.; Hirose, T.; Higuchi, M.; Kitagawa, S.; Matsuda, K.; Urayama, K.; Furukawa, S. Nat. Commun, 9 (2018) 2506.

[4] Carné-Sánchez, A., Albalad, A., Grancha, T., Imaz, I., Juanhuix, J., Larpent, P., Furukawa, S., Maspoch, D. J. Am. Chem. Soc.141 (2019) 4094.

Application of nanocomposites derived from the transition metals in catalytic processes

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Abstract:

A broad variety of transition metal compounds and composites have been used by our research group as highly active catalysts for various transformation reactions in homogeneous, heterogeneous and heterogenized homogenous catalysis. The followings are some examples. We successfully synthesized a quadruple Pd-rGO/CNT/$CaFe_2O_4$ nanocomposite as an effectiveness photocatalyst for the Heck–Mizoroki coupling reaction at room temperature under irradiation of visible light [1]. A new SnS_2-$BiFeO_3$/rGO nanocomposite has been prepared for the increased visible-light-responsive photodegradation of organic dyes such as cationic methylene blue (MB) and anionic methyl orange (MO). It was found that the optimized photocatalyst showed high visible-light photocatalytic performance toward the degradation of organic dyes in water with high stability [2]. 5,10,15,20-Tetrakis(4-benzoate) porphyrinato manganese(III) acetate (Mn(TCPP)OAc) was intercalated into Mg–Al LDH using the co-precipitation method. The catalytic activity of the composite was studied in the epoxidation of olefins for the design of new catalytic materials [3].

References:

[1] M. Bagherzadeh, R. Kaveh, H. Mahmoudi, J. Mat. Chem. A, 2019, DOI: 10.1039/C9TA02882J
[2] M. Bagherzadeh, R. Kaveh J. Photochem. Photobio. A: Chem.,359 (2018) 11–22.
[3] M. Bagherzadeh, E. Mesbahi, Appl. Organometal. Chem., 33 (2018) 1-8.

Template strategies with MOFs

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Abstract:

Metal-organic frameworks or MOFs are porous compounds with special properties like controllability in terms of composition and structure coupled with high porosity. These kind of porous materials have enticed a great deal of attention in various fields including energy storage and conversion, ion exchange, separation, sensor, drug delivery, molecular recognition, and catalysis. Also, MOFs have been considered as flexible precursors for synthesis of different nano-materials and novel multifunctional nanocomposites/hybrids with preferable functional characteristics compared to their initial components. Hence, development of different strategies for size and shape controlling of MOFs is very important for obtaining ordered MOFs and their derived materials/hybrids.

While synthesis of MOFs is hard to be pmalaced in a determined area with traditional methods, it is possible to use pre-patterned solid matter in desired positions. Application of solid substances as metal ion source has a kinetic role in regulating the coordination behavior of desired MOFs [1]. Even though this is a simple procedure, structures with well-determined shapes are mostly acquired under strict conditions and their shapes can be completely lost. Using templates is a far more versatile method which offers the possibility to achieve a more diverse morphology in MOFs. Furthermore, regular MOFs have been synthesized using soft or hard templates in which the hierarchical MOFs and MOF core–shell heterostructures can also be obtained with appropriate control of parameters such as morphology and size.

MOFs have been widely applied as suitable precursors to construct inorganic nanomaterials like metal oxides with certain benefits including simplicity in terms of the processes involved as well as the required equipments, relationship between target product structures and raw materials, usefulness for phase controlling of the final products, greater control upon procedure conditions, purity, particle crystal structure, and particle size, reduced the possible interparticle collisions, being cost effective, in addition to the possibility for large-scale construction [2].

References:

[1] M.Y. Masoomi, A. Morsali, Coord. Chem. Rev. 256 (2012) 2921-2943.
[2] M. Eddaoudi, J. Kim, N. Rosi, D. Vodak, J. Wachter, M. O'keeffe, O.M. Yaghi, Science 295 (2002) 469-472.

Synthesis and application of chiral functionalized quantum dots

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Abstract:

Recent progresses in design and preparation of new chiral materials resulted in the development of molecular recognition methods [1]. Chiral receptors can discriminate between left- and right-handed enantiomers of target analytes resulting in the chiral recognition. This discrimination takes place if the analyte species can interact differently with the chiral receptor sites. A measurable difference in the interaction between the chiral receptor sites and analyte species is necessary for chiral recognition. Chiral colloidal quantum dots (QDs) have been appeared as new nanomaterials with extensive potential applications [2]. Functionalization of QDs with desired chiral groups is a promising method for tailoring tunable chiral QDs with potential uses in chemical or biological applications. The QDs core with appropriate optical absorption or emission properties may be designed and prepared separately and then functionalized with appropriate chiral ligands. Chiral amino acids containing thiol groups such as cysteine are appropriate capping groups and their use have provided new pathways for the preparation of chiral QDs [3]. In spite of the importance of chiral QDs in chiral analysis, there are few reports on their preparation and utilization in practical chiral recognition and analysis of chiral species [4]. Moreover, the selective interaction of different enantiomers of chiral QDs with chiral molecules has not been well-described. Here, the design and characterization of optically active chiral QDs is described with functionalization of achiral QDs with chiral l- and d-cysteine groups. According to the results of fluorescence spectroscopy, the prepared chiral functionalized QDs exhibited selective interaction with chiral analytes. Thus, the chiral recognition of analytes is possible by their enantioselective interaction with the functionalized chiral QDs. Some of the chiral analytes quenched the fluorescence intensity of the functionalized chiral QDs more efficient than the other.

References

[1] Y. Xia, et al., Nanoscale, 3 (2011) 1374-1382.

[2] B.P. Bloom, et al., J. Am. Chem. Soc.139 (2017) 9038-9043.

[3] P. Liu, et al., *J. Phys. Chem. C*. 113 (2009) 7670-7676.

[4] M.V. Mukhina, et al., *Sci. Rep*. 6 (2016) 24177.

Borosilicates: synthesis, properties and applications

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Abstract:
Borosilicate zeolites are synthesized via isomorphous substitution of Al by B in the framework of zeolites. The first attempts for the incorporation of boron into the framework of zeolites were not successful; the crystallization of borosilicate zeolite did not take place or the substitution of Al by B was negligible. The successful replacement of Al by B in the framework of zeolites was reported only after the discovery of high silica zeolites [1]. Because of differences between the chemical properties of Al and B, borosilicate zeolites exhibit different properties in comparison with aluminosilicate counterparts. For instance, the borosilicate zeolites have intrinsically weak acidity and thus they are not considered as useful catalysts in acid catalysis processes. However, they find their applications as efficient catalysts in reactions requiring low acidity and as precursors for the preparation of other metallosilicates by post-synthesis method [2].

In recent years, we have studied the synthesis of ZSM-5 type borosilicate zeolites using different methods (including hydrothermal and dry gel conversion methods) that here we mainly focus on the hydrothermal synthesis. According to our findings, the synthesis condition such as gel composition, pH, crystallization time and temperature can influence the morphology, particle size, boron content and crystallization degree of the synthesized zeolites [3]. The synthesized borosilicate zeolites were used as drug delivery systems (DDSs) for loading and release of doxorubicin (DOX) and their cytotoxicity was tested by MTT assay. The results proved that the borosilicate zeolites are biocompatible and can serve as pH-sensitive drug carriers. In order to study the effect of framework composition on the performance of these systems as DDSs, the incorporation of Fe^{3+} ions into the framework of borosilicates was studied. By incorporation of Fe^{3+} in zeolite framework, the efficiency of zeolites as DDSs falls drastically. However, the formation of extra-framework iron species (such as iron oxides) during the synthesis of zeolite leads to the higher loading and release efficiency of drug which shows the iron oxide- borosilicate composites are proficient DDSs [3, 4].

References:

[1] R. Millini et al., Top. Catal. 9 (1999) 13–34.
[2] J. Röseler et al., Appl. Catal. A Gen. 144 (1996) 319–333.
[3] M. Khatamian et al., Mater. Sci. Engin. C 78 (2017) 1212–1221.
[4] M. Khatamian et al., J. Mol. Liq. 242 (2017) 979–986.

Recent Progress of Dinuclear Organotin (IV) Complexes with Bis-hydrazones

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Abstract

In coordination chemistry, interest in the use of hydrazones as polyfunctional ligands has increased considerably. Acyl/aroyl hydrazones with the –C=NNHC(O)– functional group are a particular category of hydrazones. Among these derivatives, the chemistry of bis acyl/aroyl-hydrazones is seen to be of particular interest due to the possibility of creating various types of coordination modes. The flexibility of distance introduced between two coordinating units of these bifunctional hydrazones may result in interesting structural or reactivity features in the ligand and its metal complexes. Recently, the synthesis and structural investigation of binuclear organotin(IV) complexes of bis-hydrazones have received attention and we have also published several articles in this area [1-3]. Research into the organotin(IV) chemistry is a prolific area of chemical investigations. These compounds have found more industrial, agricultural and medicinal applications than any other organometallic compounds. In addition, they present an interesting structural variety, so that structural studies have always been prominent in organotin(IV) chemistry. Among these studies, the inclusion of two organotin units, instead of just one, in the same molecular entity may produce compounds with interesting biological and structural properties. As a part of our investigation dealing with the study of organotin(IV) complexes, we review the synthesis, structural chemistry and biological properties of binuclear organotin(IV) complexes with several bis-hydrazones. In most of these complexes, the dihydrazone ligand was symmetric and both tin atoms were in the same chemical environments, while in some others bis-hydrazone is asymmetric or contains two different donor environments. This is readily proven by observing one or two signal in ^{119}Sn NMR spectrum of the complex. Also, The X-ray crystallographic structures, *in vitro* antibacterial activity, interaction with DNA and *in vitro* cytotoxicities of some synthesized ligands and their complexes will be described.

References:

[1] M. Yousefi, T. Sedaghat, J. Simpson, H. Motamedi, M.R. Dayer, Polyhedron 155 (2018) 153.
[2] H. Zafarian, T. Sedaghat, H. Motamedi, D. Trzybiński, K. Woźniak, J. Organomet. Chem. 853 (2017) 184.
[3] H. Zafarian, T. Sedaghat, H. Motamedi, H.A. Rudbari, J. Organomet. Chem. 825 (2016) 25.

Cooperativity of chemical bonds or bonding interactions in metal complexes or inorganic triads

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Abstract

Cooperativity of non-covalent interactions has been extensively reported in the literature [1]. Cooperativity occurs in the well-known example of ice, where the oxygen-oxygen separation is shortened to 2.76 **Å** compared to 2.98 **Å** in the water dimer [2]. Recently, we reported a new equation for calculating total interaction energy in one noncyclic ABC triad and also new insights into cooperativity of noncovalent bonds [3]. Our next studies confirmed the expectation that the above proposed equation can be used in calculating the total interaction energy in any acyclic ABC system, regardless the nature of bonds between A, B and C fragments [4]. Our results also clearly show that whenever the fragmentation of any system into three fragments is possible we can find whether there is a cooperativity or anticooperativity between the corresponding bonds.

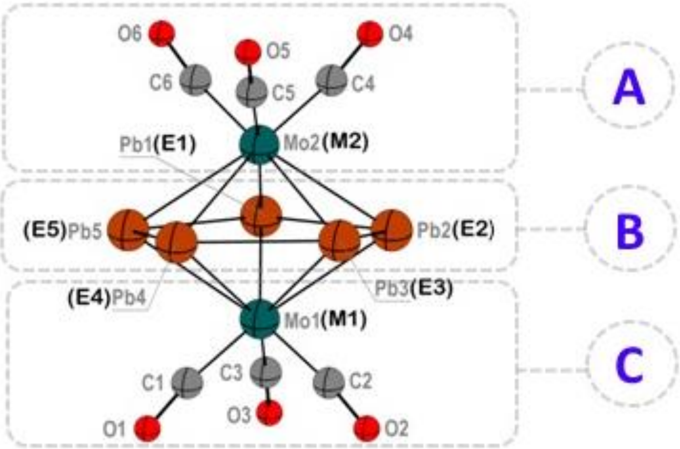

Fig. 1. Definition of A, B and C fragments for $[Pb_5\{Mo(CO)_3\}_2]^{4-}$ anion complex

References:

[1] A.S. Mahadevi, G. N. Sastry, Chem. Rev. 116 (2016) 2775−2825.

[2] T. R Dyke, J. S. Muenter, J. Chem. Phys, 60 (1974) 2929-2930.

[3] S. Salehzadeh, F. Maleki, J. Comput. Chem, 37 (2016) 2799–2807.

[4] Y. Gholiee, S. Salehzadeh, S. Khodaveisi, New J. Chem, 43 (2019) 7797--7805.

Metal and Metal Oxide synthesis by Electrical Explosion of Wire

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Abstract:

Metal nanoparticles (MNPs) and metal oxide (MONPs) nanoparticles were selectively produced in large quantities by the Electrical Explosion of Wire (EEW) process in different conditions. Transmission Electron Microscopy (TEM), laser particle size analyzing, X-ray diffraction (XRD), and FT-IR spectroscopy were carried out to characterize the purity, morphology, particle and crystallite size of the nanoparticles. The effects of conditional parameters on the particle size were analyzed. The results show that the wire diameter, feed rate, pulse time, voltage, and electrode distance are the main five factors. An ultimate Response Surface Methodology (RSM) design showed the particle size increases with decreasing voltage and increasing other factors.

References

[1] G. L. Dimas-Rivera, J. R. de la Rosa, C. J. Lucio-Ortiz, J. A. De los Reyes Heredia, V. González and T. Hernández, Materials, 7 (2014) 527-541.

[2] L. Liu; J. Zhao, W. Yan, Q. Zhang, IEEE T. Nanotechnol., 13 (2014) 842-849.

[3] S. H. Tong, Z. X. Bing, Z. Shen, Z. X. Lei, W. X. Xin, Acta Phys. Sin., 63 (2014) 145206.

[4] R.X.K. Gao, W.J.R. Haefer, L. R-Ping, IEEE T. Anten. Propag, 62 (2018) 2102 – 2108.

[5] K. Muzyka, K. Karim, A. Guerreiro, A. Poma, S. Piletsky, Nanoscale Res. Let., A 9 (2014) 154-161.

Preparation of $ZrFe_2O_4@SiO_2$ core-shell nanocomposite modified by meso-tetrakis(4-carboxyphenyl) porphyrin to oxidation of cyclohexane

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Abstract:
In this study, a new magnetic $ZrFe_2O_4@SiO_2$-TCPP nanocatalyst with high efficiency was used for the oxidation of cyclohexane to cyclohexanone (Ke) and cyclohexanol (Al). Optimization of the reaction conditions, as one of the most applicable Response Surface Methodologies (RSM), was executed by Central Composite Design (CCD) based on the applied mathematical modeling, and the results were analyzed by GC-Mass Analytical Testing Lab Services. The maximum Ke/Al products were 33.6 and 18.9%, respectively. The mesoporous $ZrFe_2O_4$ nanoparticles, with a nanocauliflower structure was synthesized via solvothermal method and it was coated with SiO_2 sell by tetraethyl orthosilicate (TEOS) to fabricate the $ZrFe_2O_4@SiO_2$ core-shell. Then, this composite was modified by 5,10,15,20-meso-tetrakis(4-carboxyphenyl) porphyrin (TCPP). FT-IR, XRD, FE-SEM, EDX, TEM, VSM, BET and fluorescence analyses were used to characterize the prepared nanomaterials. The new catalyst has many advantages such as very high activity, simple separation by a magnetic field, stability and recoverability.

Short Orals

Nature of S→M Bond in some Pharmaceutical Complexes of Group 11 Metals

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Abstract:

N-heterocyclic carbenes are well known σ-donor and their coordination chemistry with transition elements, particularly group 11 metals, would be noticeable. The first stable N-heterocyclic carbene (NHC) was synthesized by Arduengo et al. in 1991. Nowadays metal-NHC complexes appear as an emerging field of research on the development of novel metallodrugs because of their high stability and ease of derivatization. This study seeks to characterize the structure and nature of S→M bond in somepharmaceutical complexes of group 11 metals (M= Cu(I), Au(I), Ag(I)) in coordination with S atom of 3,4,5- three -O-acetyl-2 methyl acetato-1thio- β- D-pyranosato (Tgt) with general formula [Tgt→MNHC(R)] {M= Cu(I), Au(I), Ag(I), R= F, Cl, Br, H, CH_3, SiH_3 and 2,6 diisopropyl phenyl} at the Pbe/def2 TZVP level of theory. The strength and nature of donor‒acceptor bond between the Tgt and M-NHC(R) fragments in the complexes were studied by using NBO and energy decomposition analysis (EDA), as well as their natural orbitals for chemical valence variation (EDA-NOCV). The results show that the S→M bond interaction energies is conforming the well-known V-shaped trend for the transition metals of the first, second, and third row in the following order: Ag(I) < Cu(I) < Au(I). Also result showed that the nature of the S→M bond in [Tgt→M-NHC(R)] complexes is largely electrostatic, with a contribution of about 70% interaction energy [1,2].

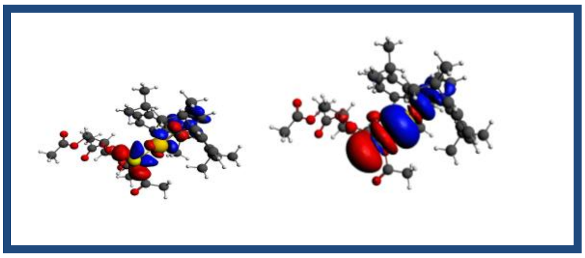
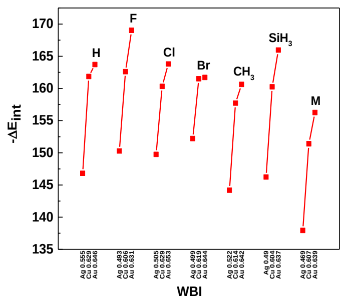


Fig 1. Deformation densities associated with the most important orbital interactionsfor [Tgt→ M-NHC(R)



Calculated ΔE_{int} and versus WBI of electron density (ρ) of [Tgt→MNHC(R)] {M=Cu(I), Ag(I), Au(I) , R= , H, F , Cl, Br, CH3, SiH3, 2,6 –diisopropyl phenyl }

References:

[1] L. Wukun, G. Ronald, Coordination Chemistry , 329 (2016) 191-213.
[2] M. Bayat, A. Sedghi, L. Ebrahimkhani, S.J. Sabounchei, Dalton Trans, 20 (2016) 207-220.

Improved photocatalytic degradation 4-Nitrophenol using novel nanostructured metal-doped Zeolite

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Abstract:
In this paper, Fe, Ce and Ti metals were subjected to the zeolite structure using post-synthesis treatment and identified by FT-IR, XRD, FESEM, EDX, BET spectroscopy techniques. Figure 1a showed the presence of peaks in related to CeO_2 and Fe_2O_3 which demonstrated the insertion of metals in zeolite structure. Fig. 1b, c shows FESEM and EDS analysis of catalyst which proved the preservation of zeolite structure with cubo-octahedral units based on metal doping. The improved photocatalytic activity was investigated in the photodegradation of 4-Nitrophenol [1,2]. Photocatalytic activity of this system depends on the catalyst loading, H_2O_2 content, pH, 4-Nitrophenol concentration and temperature effect [3]. The COD results reveal that 4-NP was degraded to simple materials. Pseudo-first order kinetic was suggested for photodegradation reaction.

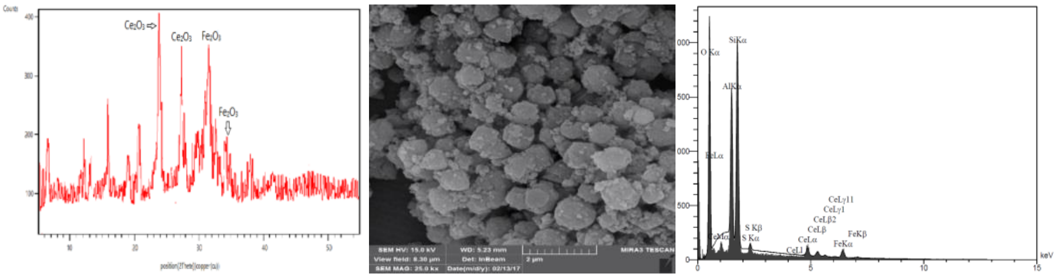

Fig. 1. a) XRD pattern of Ce-Fe-zeolite, b) FESEM and c) EDS analysis of Fe-Ce-zeoli

References:
[1] S. Ameen, M. S. Akhtar, Y. S. Kim, H. S. Shin, Applied Catalysis B: Environmental,103 (2011) 136-142.
[2] M. Moosavifar, M. Nikkhoo, F. Mansouri, Research on Chemical Intermediates, 42 (2016) 7417-7427.
[3] Y. Oumi, T. Manabe, H. Sasaki, T. Inuzuka, T. Sano, Applied Catalysis A: General, 388 (2010) 256–261.

Amino Acid-functionalized Hollow Mesoporous Silica Nanospheres as Efficient Biocompatible Drug Carriers for Anticancer Applications

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Abstract:

Herein, a series of new amino acid-functionalized hollow mesoporous silica nanospheres (HMSNs) by post-grafting methods were prepared. These new materials were characterized by different techniques and were studied as matrices for the antineoplastic drug (cisplatin) transport and delivery. The results demonstrate that the surface functionalization of the carriers has a remarkable positive influence on the loading efficiency and release rate of cisplatin. The highest drug entrapment efficiency and the most optimal release properties were observed when the (2-(butylamino) ethyl) glycine groups are grafted on the HMSNs surface (AFS-2-HMSNs sample). Moreover, the in vitro cytotoxic effect of both empty and cisplatin-loaded AFS-2-HMSNs sample (CDDP@AFS-2-HMSNs) on MCF-7 cells (human breast adenocarcinoma cell line) and HepG2 cells (human liver carcinoma cell line) were evaluated by MTT assay. The most important outcome is that the empty carrier revealed no cytotoxicity to cancer cells. However, CDDP@AFS-2-HMSNs caused a notable inhibition of cell viability which was affected from the dose and time. Our results demonstrate that the synthesized materials could be used as carriers for drug delivery with controlled release applications [1-5].

References:

[1] A. Yimit, O. Adebali, A. Sancar, Y. Jiang, Nature communications, 10 (2019) 309.

[2] Y. Min, C.Q. Mao, S. Chen, G. Ma, J. Wang, Y. Liu, Angewandte Chemie International Edition, 51 (2012) 6742-6747.

[3] P. Mura, M. Valleri, E. Fabianelli, F. Maestrelli, M. Cirri, International Journal of Pharmaceutics, (2019).

[4] Y. Li, J. Shi, Advanced Materials, 26 (2014) 3176-3205.

[5] Y. Gao, A.E. Kaziem, Y. Zhang, Y. Xiao, S. He, J. Li, Microporous and Mesoporous Materials, 255 (2018) 15-22.

Synthesis of Nano cluster {Mo_{132}} - polyacrylonitrile nanofibers for the extraction of methadone in human urine sample

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Abstract:

Polyacrylonitrile/{Mo_{132}} composite nanofibers mats was synthesized by an electrospinning technique using PAN and giant ball nano-polyoxomolybdate {Mo_{132}}. {Mo_{132}} [1] was mixed with PAN solution and then electrospun to produce bead-free nanofibers. The aim of this study is to evaluate the extraction abilitiy of electrospun composite nanofibers against methadone.

In many countries of the world, the selected treatment for opiates dependence is methadone maintenance therapy (MMT). Methadone (Fig. 1), also known as Methadose, Dolophine, Amidone, Symoron, Physeptone, Heptadon and many other names, is a synthetic analgesic drug which is commonly used to treat dependence on heroin and other opioids since the mid-1960s. Because methadone treatment replaces a short-acting opioid (heroin) with a long-acting opioid (methadone), it has been controversial since its inception, particularly with regard to adequate dose levels [2]. The surface morphology and other properties of the PAN/{Mo_{132}} nanofibers composite were characterized by various techniques, including SEM, TEM, FT-IR, UV-Vis. SEM images showed that the average diameter of the fibers was between 100-120 nm. [3]

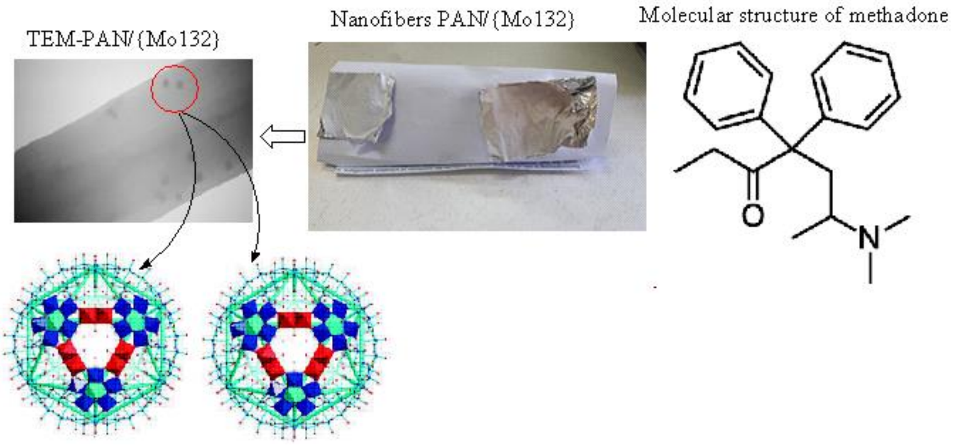

Fig. 1. Structure of methadone, Nanofibers PAN/{Mo_{132}} and TEM image of PAN/{Mo_{132}}

References:

[1] A. Muller, E. Krickemeyer, H. Bogge, M. Schmidtmann, .F. Peters, Angew Chem Int Ed, 37 (1998) 3359-3363.
[2] E. Ranjbari, A.A. Golbabanezhad-Azizi, M.R. Hadjmohammadi, Talanta, 94, 116-122.
[3] R. Haddad , M.T. Dusti, H.A. Hadi, M. Sadeghinia, Current Applied Polymer Science, DOI :10.2174/2452271603666190307161415

Electronic properties of $B_{12}N_{12}$ fullerene–like nanoclusters functionalized with Schiff bases: a DFT study

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Abstract:

In the present study, electronic properties of $B_{12}N_{12}$ nanocage functionalized with Schiff bases are studied by means of density functional theory (DFT) calculations at wB97XD/6-31+G(d,p) computational level. Adsorption of Schiff bases on the surface of $B_{12}N_{12}$ nanocage leads to one local minimum with the adsorption energy in the range of −63.61 and −157.37 kJ/mol. Effect of substitution of Schiff bases with electron-donating and electron-withdrawing groups on the adsorption energy, electronic properties, and thermodynamic parameters of studied complexes has been reported. In general, adsorption of $H_2C{=}N{-}C_6H_4{-}R$ Schiff bases on $B_{12}N_{12}$ nanocage is stronger than adsorption of $R_2C{=}N{-}C_6H_5$ moieties. The evaluation of thermodynamic parameters for adsorption indicates that formation of studied complexes through an exothermic reaction and spontaneous process at room temperature is feasible. The result of present study may be used for surface modification of $B_{12}N_{12}$ nanocage based on interaction with Schiff bases. Functionalization of nano structures will different molecular moeities have been reported recently [1-5].

References:

[1] V. Georgakilas, K. Kordatos, M. Prato, D.M. Guldi, M. Holzinger, A. Hirsch, J Am Chem Soc, 124 (2002) 760–761.
[2] J. Beheshtian, A.A. Peyghan, Z. Bagheri, J Mol Model, 19 (2013) 255–261.
[3] J. Beheshtian, A.A. Peyghan, Z. Bagheri, Comput Theor Chem 992, (2012) 164–167.
[4] K. Skinner, C. Dwyer, S. Washburn, Nano Lett, 6 (2006) 2758–2762.
[5] J. Beheshtian, A.A. Peyghan, Z. Bagheri, Struct Chem, 24 (2013) 1565–1570.

Green synthesis of copper oxide nanoparticles using *rosmarious officinalis* extract: towards Click-Chemistry

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Abstract:

Copper oxide nanoparticles (CuONPs) have been classified as an important metal oxide semiconductors with the special physical and chemical characteristics. CuONPs can be able to synthesize through different methods and techniques, such as sonochemical, precipitation, sol-gel, chemical bath deposition, hydrothermal approach, chemical reduction as well as reflux contestation. In this work, CuONPs were synthesized by a cost-effective, green and simple procedure using *rosmarious officinalis* extract at room temperature. These NPs were fully characterized by field-emission scanning electron microscopy (FESEM), Fourier transform infrared spectroscopy (FT-IR), UV-vis absorption and X-ray diffraction (XRD). These nanoparticles were applied in click chemistry and had an applicable and tunable results. [1-3]

References:

[1] M.B. Gawande, A. Goswami, F.X. Felpin, T. Asefa, X. Huang, R. Silva, X. Zou, R. Zboril, R.S. Varma, Chemical reviews, *116* (2016) 3722-3811.

[2] J. Kim, J. Park, K. Park, Chemical Communications, *46* (2010) 439-441.

[3] F. Alonso, Y. Moglie, G. Radivoy, Accounts of chemical research, *48* (2015) 2516-2528.

Comparison of magnetic properties, particle sizes, porosity and photocatalytic activities of $ZrFe_2O_4$ prepared via three methods

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Abstract:

Magnetic nanoparticles based on $ZrFe_2O_4$ [1] were prepared via three methods: solvothermal, microwave-assisted solvothermal and combustion [2,3]. By comparison, the latter two methods have reduced the synthesis time to 45 minutes by using a pressurized microwave reactor without the requirement of further post-treatments such as calcination, for combustion method, the time was less than 10 minutes. The characterization of the compound in terms of the structure, composition, morphology and magnetic properties was done by XRD, FE-SEM, EDX, VSM, BET, TGA and DRS, which emphasizes the mesoporous being of the particles. In application processes, the photocatalytic activity of the prepared compounds for degradation of the methylene blue was investigated by the UV-Vis spectroscopy [4]. The optimal particle size is one of the advantages of combustion and microwave-assisted solvothermal methods, but they have not exhibited photocatalytic activity as effective as the solvothermal technique.

References:

[1] Gangwar, A., et al., Journal of Magnetism and Magnetic Materials, 2016. 401: p. 559-566.
[2] Schmidt, R., J. Prado-Gonjal, and E. Morán, Boca Raton (USA): CRC Press Taylor & Francis Group, 2015: p. 561-572
[3] C.-H. Yan, Z.-G. Xu, F.-X. Cheng, Z.-M. Wang, L.-D. Sun, C.-S. Liao, J.-T. Jia, Solid State Communications, 1999. 111(5): p. 287-291
[4] Kharazi, P., R. Rahimi, and M. Rabbani. Materials Research Bulletin, 2018. 103: p. 133-141.

Ethylene glycol coated magnetic graphene oxide nanocomposite for MRI

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Abstract:

Nano graphene oxide is a good candidate for medical imaging purposes including magnetic resonance imaging (MRI). Thanks to the two dimensional layer structure of graphene oxide with high surface area, magnetic nanoparticles which are used in MRI can be placed on graphene oxide nanosheet [1]. Since magnetic nanoparticles can be toxic for medical purposes, placing of the nanoparticles on graphene oxide layers leads to less toxicity of them for biological conditions [2]. Additionally, usage of coating material around magnetic graphene oxide nanocomposite provides more biocompatibility and possibility of surface functionalization. The aim of this research was to investigate ability of ethylene glycol coated magnetic graphene oxide nanocomposite for using in MRI.

Magnetic graphene oxide was prepared with hydrothermal method and the structure, size, morphology, and cell toxicity was determined by use of XRD, TEM, SEM and MTT assay analyzes. In vitro MRI was carried out with a 1.5 tesla medical system and signal changes of the nanocomposite samples which were dispersed in agar were determined.

The results showed successfully prepared ethylene glycol coated magnetic graphene oxide nanocomposite with layer structure. No toxic effect on the cell culture was seen. The samples with higher amount of the magnetic graphene oxide nanocomposite showed higher signal changes relative to the control.

In conclusion, ethylene glycol coated magnetic graphene oxide nanocomposite is suitable for signal changing in MRI.

References:

[1] E. Shafaei, B. Divband, N. Gharehaghaji, Nanomed. J. 6(3) (2019).

[2] J. Lin, X. Chen, P. Huang, Adv Drug Deliv Rev. 105(Pt B) (2016) 242–254.

Design and fabrication of a new three dimensional Co-MOF@Sponge composite for highly selective visual sensing of inorganic acid gases

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Abstract:

Integration of metal-organic frameworks (MOFs) and functional materials is leading to the creation of new multifunctional composites which exhibit new properties that are superior to those of the individual components through the collective behavior of the functional units. This is a rapidly developing interdisciplinary research area [1, 2]. In this work a new three-dimensional Co-MOF@sponge composite has been prepared via immobilization of a novel Co-MOF on a porous melamine formaldehyde sponge (MFS). The composite has been used for visual detection of inorganic acid gases HCl, HNO_3, and H_2SO_4. In order to obtain an effective colorimetric MOF probe, the MOF was grown as a thin layer on the porous structure of melamine formaldehyde sponge using layer-by-layer growth of the metal nodes and organic linkers. The structure of the MOF and composite has been characterized by FT-IR, PXRD, CHN, SEM, and EDX mapping techniques. The results show high performance of the Co-MOF@sponge composite for selective visual sensing of inorganic acid gases by the naked eye.

References:

[1] Q.-L. Zhu, Q. Xu, Chem. Soc. Rev., 43 (2014) 5468.

[2] C. M. Doherty, D. Buso, A. J. Hill, S. Furukawa, S. Kitagawa, P. Falcaro, Acc. Chem. Res. 47 (2014) 396.

Posters

Synthesis, Spectral Studies and Application of Schiff-Base Derived Ligand For Sensing of Hydrogen Carbonate Anion

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Abstract:

The Schiff-base ligands, owning good donor properties, are very important in coordination chemistry [1]. Azo-benzenes are used in the chemical industry as dyes and pigments, drugs, food additives, liquid crystals, photochemical molecular switches, and nonlinear optics [2]. In this study, at first, the synthesis and characterization of Schiff-Base ligand (L1), containing N = N and C = N dye units with OH and NH groups, from the condensation reaction 2-amino-3-methylpyridine has been reported with salicylic aldehyde derivatives.

Then, the sensor behavior of the (L_1) ligand against the HCO_3^- anion was investigated by the UV-Vis (Fig.1), ^{1}H—NMR techniques. The (L_1) ligand exhibited significant color and spectral variations with respect to the HCO_3^- anion in DMF / H_2O solution (95: 5) (Fig.2). A significant change in the color of the DMF / H_2O solution of the other anions, such as: F^-, Cl^-, Br^-, HSO_4^-, N_3^-, NO_2^-, $H_2PO_4^-$, SCN^-, ClO_4^- and NO_3^- was not observed.

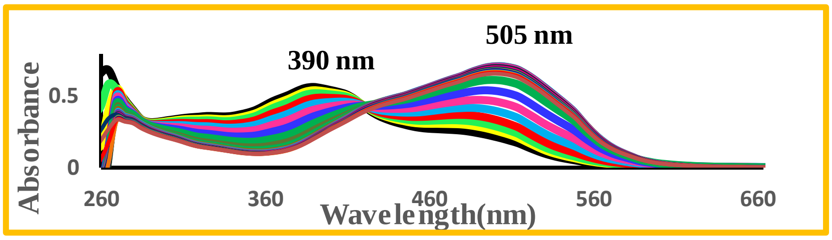

Fig.1. the Sensor behavior of the L_1 ligand against the anion HCO_3^-

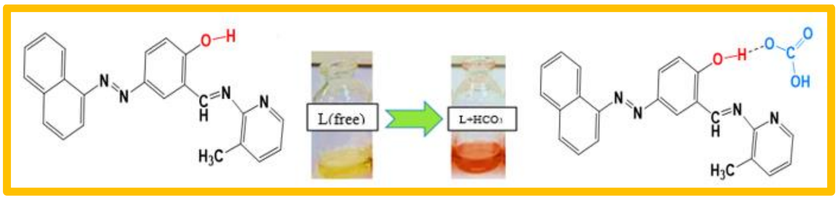

Fig. 2 . scheme of Ligand L_1

The nature of the interaction of (L_1) receptor with hydrogen Carbonate anion was confirmed through hydrogen bonding. By using the changes in the absorption spectrum, the stability constant (*Ka*) and the stoichiometric ratio of the host-guest complexes were determined with the Bensi-Hildebrand diagram and the Jobs plot curve method, respectively.

References:

[1] M. Orojloo, P. Zolgharnein, M. Solimannejad, S. Amani, Inorganica Chimica Acta 467 (2017) 227–237.
[2] E. Merino,Chem. Soc. Rev. 40 (2011) 3835–3853.

Synthesis and spectroscopic characterization of sensor for naked-eye detection of cyanide ion in solution media using a new Schiff-base based on thiophene

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Abstract:

Development of anion sensors is of great interest in supramolecular chemistry due to their chemical and biological importance [1]. Schiff base ligands are considered because they are easily prepared by the condensation between aldehydes and imines [2,3]. Among the various anions, cyanide is one of the most concerned anion, because it is known as one of the most rapidly acting and powerful poisons [4]. In this research, a new reactive ligand such as ethyl 2-{[1-(2-hydroxyphenyl) methylidene] amino}-4, 5, 6, 7-tetrahydro-1-benzothiophene-3-carboxylate was synthesized by a condensation reaction. In the first step, amine was synthesized from salicyl aldehyde substituted thiophene compounds. The synthesized receptor was detected by UV-Vis, FT-IR spectroscopy, ^{1}H-NMR and melting point. Sensitivity and reactivity behavior of receptor with different anions was determined in the presence of different solvents. Also, the sensor sensitivity to various anions was investigated by UV-Vis (Fig.1) and ^{1}H-NMR spectroscopy. The receptor exhibited significant color and spectral changes in the CN^- anion in the DMF solvent. However, a significant change in the color of other anions, such as F^-, Cl^-, Br^-, AcO^-, $H_2PO_4^-$, HSO_4^-, HCO_3^-, ClO_4^-, N_3^-, NO_3^-, NO_2^-, SO_4^{2-}, SCN^-, OH^- in DMF was not observed.

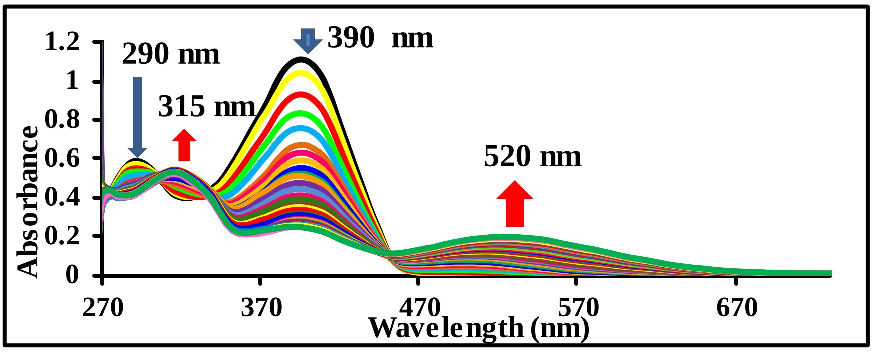

Fig.1. the sensor behavior of the ligand against the anion CN^-

Referencces:

[1] D.Yubin, et al. Organic and Biomolecular Chemistry 10.21 (2012) 4201-4207

[2] Osman, H.Ahmed . Transition Metal Chemistry 31.1 (2006) 35-41.

[3] M.Orojloo, S.Amani, Comptes Rendus Chimie 20.4 (2017) 415-423.

[4] Park, G.Jin, et al. Tetrahedron70.17 (2014) 2822-2828.

The first report of supported copper catalyst on biochar nanoparticles for the synthesis of tetrazoles as antimicrobial agents

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Abstract:

Biochar is a carbon-rich solid which its surface were covered by high density of carbonyl, hydroxyl and carboxylic acid functional groups. In this work, biochar nanoparticles were prepared from pyrolysis of chicken manure and further a new copper catalyst was supported on its surface (Cu-ABA@biochar) as reusable and environmental biocatalyst. The structure of this catalyst has been characterized by SEM, EDS, WDX, XRD, TGA and AAS techniques. SEM images of this catalyst demonstrate that particle size is less than 100 nm in diameter. The catalytic activity of this nanocatalyst was studied in the synthesis of tetrazole derivatives. Tetrazole products were obtained in high TOF and TON values in the presence of Cu-ABA@biochar, which indicate the high efficiency of this catalyst. The biological activity of obtained tetrazoles was screened against several Gram-positive & Gram-negative bacteria strains which these compounds were found to posses promising activity. This catalyst was reused for several runs without significant loss of its catalytic activity or copper leaching. Heterogeneity and stability of this nanocatalyst was confirmed by hot filtration test and reusing of catalyst. Despite several advantage of this work, it is the first time that biochar was applied as support for fabrication of copper catalyst. [1]

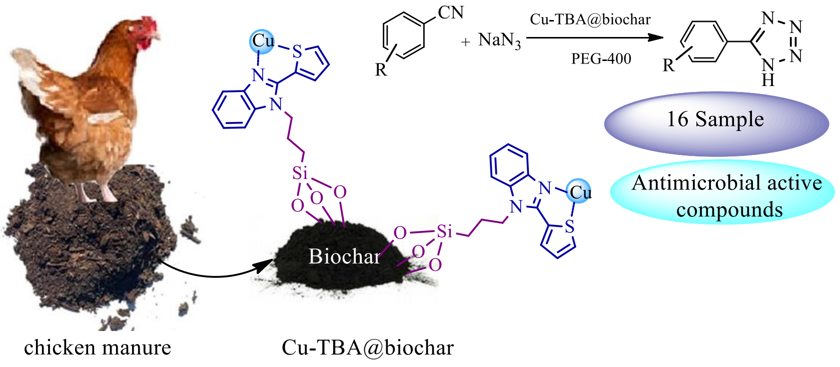

Fig.1 preparation method of biochar nanoparticles

References:

[1] L.V. Zwieten , S. Kimber, S. Morris, K.Y. Chan, A. Downie, J. Rust, S. Joseph, A. Cowie, Plant and Soil, 327 (2010) 235–246.

[2] M. Ahmad, A. U. Rajapaksha, J. E Lim, M. Zhang, N. Bolan, D. Mohan, M. Vithanage, S. S. Lee, Y. S Ok, Chemosphere, 99 (2014) 19-33.

[3] C. J. Atkinson, J. D. Fitzgerald, N. A. Hipps, Plant Soil, 337 (2010) 1–18.

Comparative study of physico-chemical properties of two nano-magnetic compounds, $CaO@Fe_3O_4$ and $Fe_3O_4@CaO$ and their catalytic role on Biodiesel preparation

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Abstract:

In this project, two nano-magnetic composites from Calcium Oxide and Iron (II, III) Oxide as nano-core-shell materials ($CaO@ Fe_3O_4$ and $Fe_3O_4@CaO$) were synthesized by hydrothermal method and characterized by general techniques such as FTIR, XRD, FESEM, EDS, MAP and BET. The chemical and physical properties of these nano-compounds were studied and compared with each other. What was very interesting in this research was the type of Metal Oxide as a core part. By changing of core from Fe_3O_4 to CaO; 1) the crystal size decreased from 41.60 to 36.82 nm. 2) the morphology was significantly changed, $CaO@ Fe_3O_4$ got misty mountain like shape but other compound has got tiny spherical. 3) surface area and pore volume decreased as: $CaO@Fe_3O_4$ is Macroporous and other compound is Microporous. 4) Fe_3O_4 was better than CaO as core due to more amount of shell. Both nano-magnetic composites were efficiently performed trans-esterification process with sun flower oil and Methanol without any additional base compounds. Prepared Biodiesel was characterized by ^1H, ^{13}C-NMR and GC apparatuses. Also these results corresponded with prepared Biodiesel by NaOH as a standard.[1-5]

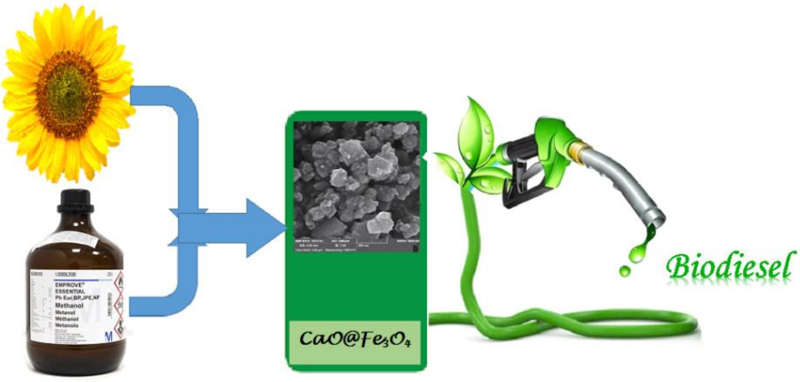

Fig.1

References:

[1] H.R. Mardani, M. Forouzani, R. Emami, Asian Journal of Green Chemistry, (2019).
[2] S.Y. Kim, B. Ramaraj, K. Yoon, Surface and Interface Analysis, 44 (2012) 1238-1242.
[3] J.S. An, W.J. Han, H.J. Choi, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 535 (2017) 16-23.
[4] G. Leofanti, M. Padovan, G. Tozzola, B. Venturelli, Catalysis Today, 41 (1998) 207-219.
[5] K. Liu, Y. Qin, Y. Muhammad, Y. Zhu, R. Tang, N. Chen, H. Shi, H. Zhang, Z. Tong, B. Yu, ournal of Alloys and Compounds, 781 (2019) 790-799.

Biosynthesized of silver nanoparticles using of Rosemarry extract assisted by microwave irradiation and study its photocatalytic application

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Abstract:

Today, releasing of persistent organic and inorganic pollutants in the environmental bodies like atmosphere, lakes, rivers, and soils is the largest environmental problems that leads to serious effects such as ozone hole, high average of carbon dioxide and so on. These pollutants are difficult to remove by traditional water treatment procedures. Therefore, it was necessary to find a feasible way to eliminate these hazardous pollutants by using low-cost materials such as: metallic nanoparticle and their compounds. Here, we report use of the green synthesized nanostructured silver particles in photodegradation of Methylene Blue (MB). The silver nanoparticles (Ag NPs) utilized as photocatalyst were synthesized using extract of Rosemarry leaves assisted by microwave irradiation. In this study, we don't need to add any surfactant and stabilizer, because all materials in the plant extract like flavonoids, sugars and other antioxidants act as reductant for silver ions and as protective layer for the formed particles. Formation of Ag NPs from the reduction silver ions by Rosemarry extract was confirmed by using UV-visible spectroscopy with the appearance of Surface Plasmon Resonance (SPR) bands around (421 nm). Field emission scanning electron microscope (FESEM), energy-dispersive X-ray spectroscopy (EDS), SEM-mapping, Fourier-transform infrared (FT-IR), X-ray diffraction analysis (XRD), and transmission electron microscopy (TEM) were applied to characterize the green Ag NPs synthesis. The report exhibit that the bio-synthesized Ag NPs are the suitable candidate as a photocatalyst for removing organic dye (MB) as a pollutant. The degradation of MB increase up on to 95.7% during 10 min. Effect of diverse experimental conditions such as initial pH, concentration of dye, and contact time was studied on the degradation process.[1,2]

References:

[1] A.A. Fairuzi, N.N. Bonnia, R.M. Akhir, M.A. Abrani, H.M. Akil, IOP Publishing, 105 (2018) 012018.
[2] J. John, C.T. Aravindakumar, S. Thomas, Scholarena Journal of Biotechnology, 4 (2017) 1.
[3] I. Fatimah, Journal of Advanced Research, 7 (2016), 961-969.

Azo-azomethine ligand anchored onto MCM-41: Synthesis, characterization and applications

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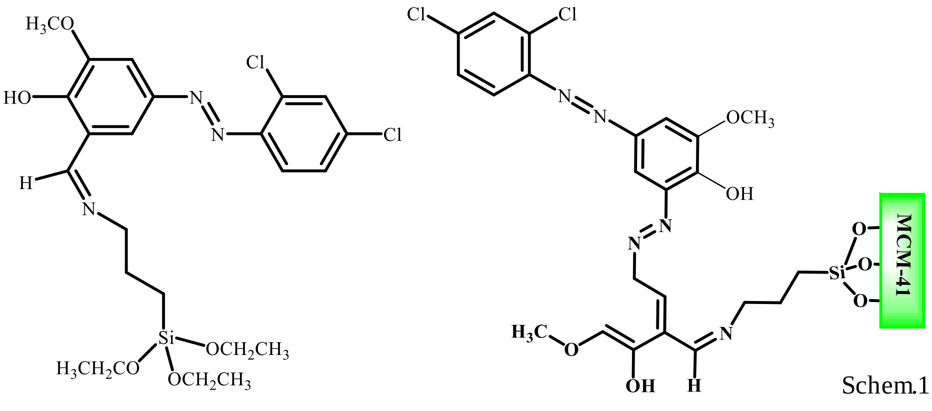
Abstract:

New molecular azo-azomethine receptor, **HL**, was synthesized via condensation reaction of 2-hydroxy-3-methoxy-5-((2,4-dichlorophenyl)diazenyl)benzaldehyde with 3-aminopropyl triethoxysilane (3-APTES) in EtOH. **HL** was characterized using standard spectroscopic techniques (FT-IR, ^{1}H NMR and UV-Vis). The sensing ability of **HL** was investigated towards the inorganic anions in DMSO and DMSO/H_2O (1:4 v/v) media. Also, new azo-azomethine receptor immobilized in MCM-41, **S-MCM**, has been prepared by reaction of amino-modified MCM-41 support with 2-hydroxy-3-methoxy-5-((2,4-dichlorophenyl)diazenyl)benzaldehyde in anhydrous EtOH. The mesoporous hybrid material, **S-MCM**, was characterized by elemental analysis, Fourier-transform infrared spectra, powder X-ray diffraction (XRD), scanning electron microscopy (SEM), and nitrogen (N_2) adsorption–desorption (BET). **S-MCM** was applied for detection of anions in aqueous and semi-aqueous media.[1,2]



Schem.1

HL **S-MCM**

References:

[1] S. Mahadavi Hezaveh, H. Khanmohammadi, M. Zendehdel, Spectrochim. Acta A, 199 (2018) 21-31.

[2] G. Sánchez, D. Curiel, I. Ratera, A. Tárraga, J. Vecian, P. Molina, Dalton Trans, 42 (2013) 6318-6326.

Uperparamagnetic $Fe(OH)_3@Fe_3O_4$ nanoparticles: An efficient and recoverable catalyst for tandem oxidative amidation of alcohols with amine hydrochloride salts

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Abstract:

Magnetic $Fe(OH)_3@Fe_3O_4$ nanoparticles were successfully prepared and characterized. This magnetic nanocomposite was employed as an efficient, reusable and environmentally benign heterogeneous catalyst for the direct amidation of alcohols with amine hydrochloride salts. Several derivatives of primary, secondary and tertiary amides were synthesized in moderate to good yields in the presence of this catalytic system. The catalyst was successfully recycled and reused up to six times without significant loss of its catalytic activity.[1-3]

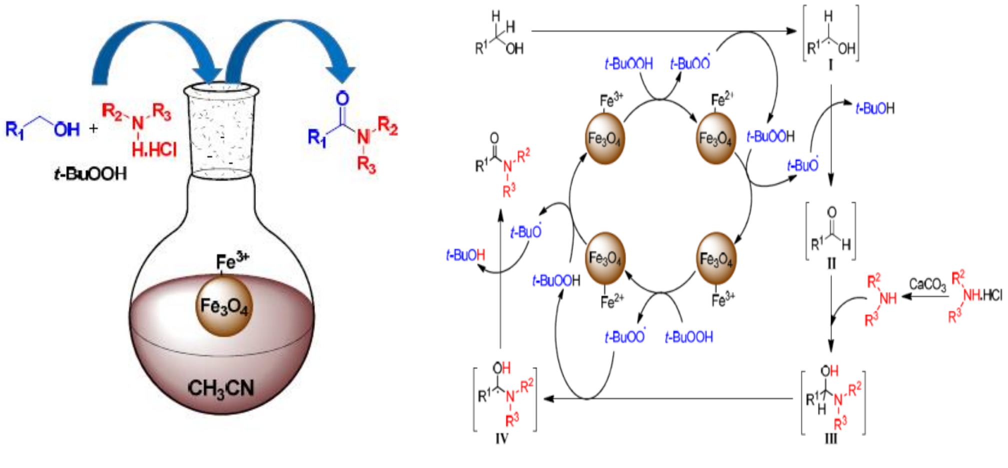

Fig.1 $Fe(OH)_3@Fe_3O_4$ nanoparticles as an efficient catalyst

References:

[1] K. Azizi, M. Karimi, F. Nikbakht, A. Heydari, App. Catal. A., 482 (2014) 336.
[2] M. Arefi, D. saberi, M. Karimi, A. Heydari, ACS Combinatorial science, 17 (2015) 341.
[3] M. Karimi, D. Saberi, K. Azizi, E. Ghonchepour, A. Heydari, Tetrahedron Lett., 56 (2015) 2674.

Erbium-Organic Framework as Heterogeneous Lewis Acid Catalysis for Hantzsch Coupling and Tetrahydro-4H-Chromene Synthesis

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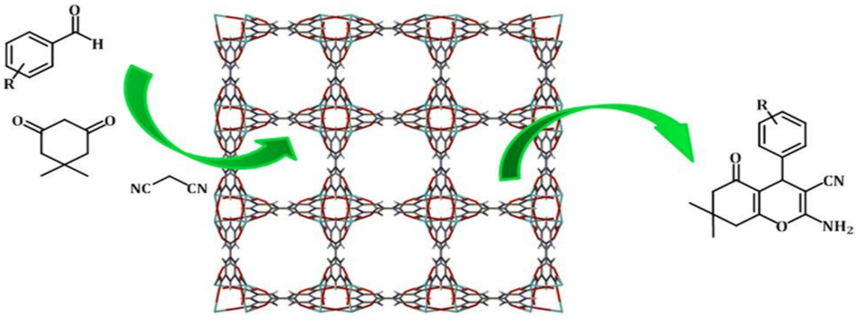
Abstract:
An Erbium-organic framework was prepared by hydrothermal reaction. The prepared framework was characterized by Fourier transform infrared spectroscopy (FT-IR), Scanning electron microscopy (SEM), and X-ray powder diffraction (XRD). The framework has open metal sites at Er(III) centers, thus providing an accessible Lewis acid center for electrophile activation. Accordingly, the synthesized framework was used as Lewis acid heterogeneous catalyst for Hantzsch coupling reaction and tetrahydro-4H-chromene synthesis. The reaction condition has been optimized by variation of the reaction time, temperature, solvent and catalyst concentration. A variety of tetrahydro-4H-chromenes was synthesized and characterized by FT-IR and 1H NMR spectroscopy. Er-MOF, as a Lewis acid heterogeneous catalyst, showed excellent selectivity and high yield for these transformations.[1,2]



Scheme.1 Synthesis of tetrahydro-4H-chromene

References:
[1] H. Ghasempour , A.A. Tehrani, A. Morsali , J. Wang, P.C. Junk, Crystengcomm, 18 (2016) 2463.
[2] A.A. Tehrani, S. Abedi, A. Morsali, J. Wang, P.C. Junk, J Mater Chem A, 3 (2015) 20408.

Terbium–organic framework as heterogeneous Lewis acid catalyst for β aminoalcohol synthesis: Efficient, reusable and green catalytic method

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Abstract:

A terbium–organic framework (Tb-MOF) was prepared using a previously reported procedure. Tb-MOF was characterized using Fourier transform infrared spectroscopy, scanning electron microscopy, powder X-ray diffraction and surface area analysis. Tb-MOF was employed as a heterogeneous Lewis acid catalyst for the synthesis of β-aminoalcohols. Also, the effect of ultrasonic irradiation was examined in the catalytic aminolysis of styrene oxide. The reaction conditions were optimized by variation of reaction time, catalyst concentration and solvent. Avariety of β-aminoalcohols were synthesized and characterized. The Tb-MOF catalyst showed excellent selectivity and high yield for these transformations.[1,2]

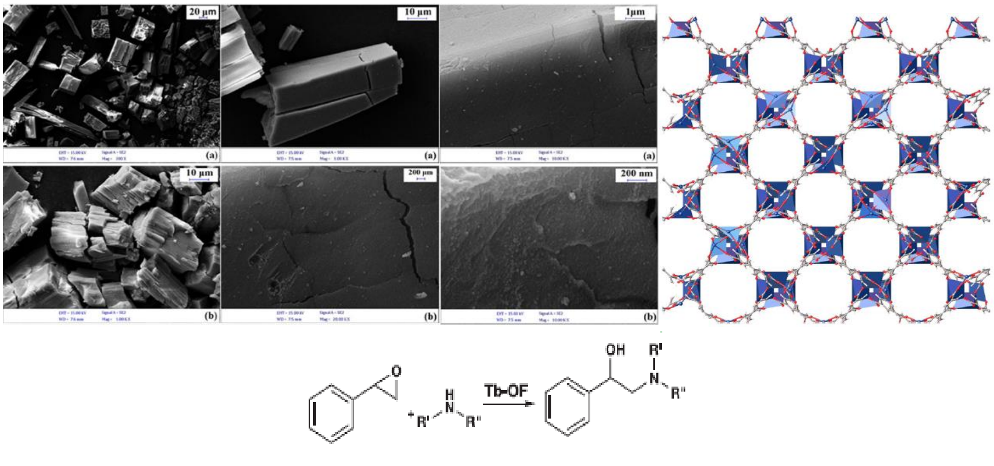

Fig.1 A terbium–organic framework as catalyst

References:

[1] H. Ghasempour , A.A. Tehrani, A. Morsali, J. Wang, P.C. Junk, Crystengcomm, 18 (2016) 2463.
[2] A.A. Tehrani, S. Abedi, A. Morsali, J. Wang, P.C. Junk, J Mater Chem A, 3 (2015) 20408.

Copper-Amino Groups Complex Supported on Silica Coated Magnetite Nanoparticles: Efficient Catalyst for Oxidative Amidation of Methyl Arenes

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Abstract:

Magnetite nanoparticles coated with mesoporous silica, Fe_3O_4@SiO_2, were prepared. Surface functionalization of this core-shell nanocomposite with (3-aminopropyl) trimethoxysilane (APTMS) followed by its reaction with $Cu(OAc)_2$ was resulted to develop a new heterogeneous copper complex (Fe_3O_4@SiO_2-APTMS-Cu). The structure and composition of synthesized nanocatalyst were characterized by FTIR, SEM, VSM, TEM, XRD, and ICP analyses. Catalytic activity of the synthesized catalyst was probed in oxidative amidation reaction of methyl arenes with amine hydrochloride salts. Various primary, secondary, and tertiary amides were prepared by this method. Magnetic properties of this catalyst lead to easy separation as well as providing significant recyclability of it. The catalyst is reusable for 6 times without significant decrease in its catalytic activity.[1-3]

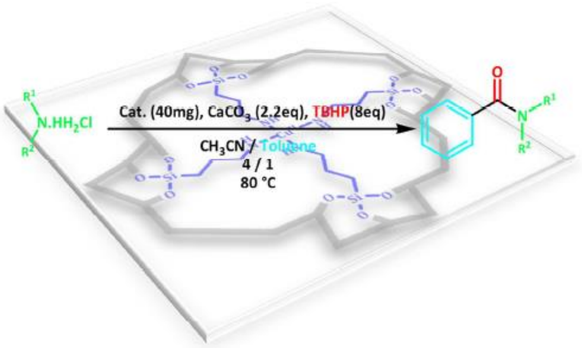

Fig.1 Fe_3O_4@SiO_2-APTMS-Cu as catalyst

References:

[1] K. Azizi, M. Karimi, F. Nikbakht, A. Heydari, App. Catal. A., 482 (2014) 336.
[2] M. Arefi, D. saberi, M. Karimi, A. Heydari, ACS Combinatorial science, 17 (2015) 341.
[3] M. Karimi, D. Saberi, K. Azizi, E. Ghonchepour, A. Heydari, Tetrahedron Lett., 56 (2015) 2674.

Efficient Fluorescence Sensing of Fe^{3+} Ions Using a Luminescent Functionalized Metal-Organic Framework

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Abstract:

Metal-organic frameworks are a class of attractive materials for fluorescent sensing. Here, we report the exploration of fluorescent Zn-based amine/azine-functionalized MOF, TMU-17-NH_2, ([Zn(NH_2-BDC)(4-bpdb)].2DMF; NH_2-BDC = amino-1,4-benzenedicarboxylic acid, 4-bpdb = 1,4-bis(4-pyridyl)-2,3-diaza-2,3-butadiene) for highly selective and sensitive detection of Fe^{3+} in DMF solution. TMU-17-NH_2 shows fast recognition of Fe^{3+} ion with a response time of <1 min and detection limit of 0.7 µM (40 ppb), and the luminescence is completely quenched in 10^{-3} M DMF solution of Fe^{3+}. Furthermore, the static quenching constant is calculated to be upper than 41000 M^{-1} by the fluorescence titration experiment in low concentration of Fe^{3+}. No interferences from 250 µM As^{3+}, Cd^{2+}, Zn^{2+}, Co^{3+}, Ni^{2+}, Cu^{2+}, Pb^{2+}, Mn^{2+} and Al^{3+} were found for the detection of Fe^{3+}. The efficient fluorescent quenching effect is attributed to the photoinduced electron transfer between Fe^{3+} ions and the amino-functionalized ligand in this MOF. Moreover, the introduced azine N donors in the 4-bpdb ligand of TMU-17-NH_2 additionally donate their lone-pair electrons to the Fe^{3+} ions, leading to significantly enhanced detection ability. Furthermore, the regenerated TMU-17-NH_2 still has high selectivity for Fe^{3+} ions, which suggests that the functionalized TMU-17-NH_2 is a promising luminescent probe for selectively sensing iron ions.[1,2]

References:

[1] P. Nelson, Important elements, J. Chem. Educ., 68 (1991) 732.

[2] L.M. Hyman, K.J. Franz, Chem. Rev., 256 (2012) 2333-2356.

Synthesis of a new complexes of Mn(II), Cd(II) and Zn(II) metals with the interaction of asymmetrical amine

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Abstract:

Schiff's bases play a significant role in the development of chewing chemistry by forming stable complexes with most intermediate metals. During our journey with coordination chemistry for last several years, we have frequently encountered very interesting consequences whenever we use N-(2-aminoethyl) piperazine to make Schiff-bases. In most of the cases terminal nitrogen atom of the piperazine moiety gets protonated. In this work an unexpected condensation between the uncoordinated NH piperazine fragment with 2-pyridinecarboxaldehyde was detected. In this work we report the synthesis and characterization of new Mn(II), Cd(II) and Zn(II)complexes have been prepared via the Mn(II), Cd(II) and Zn(II)with an asymmetrical amine N1-Pyridin-2-ylmethyl-N1-[2-(4-pyridin-2-ylmethyl-piperazin-1-yl)-ethyl]-ethane-1,2-diamine,. The complexes have been characterized by elemental analysis, IR , H NMR. And X-ray crystal Mn(II) complex structure(fig. 1).[1,2]

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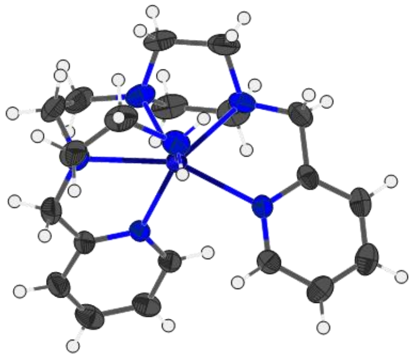

Fig. 1: X-ray crystal Mn(II) complex structure

References:

[1] H. Keypour, N. Rahpeyma, P. Arzhangi ,M. Rezaeivala , Y. Elerman, O. Buyukgungor, L. Valencia, Polyhedron,29 (2010) 1144.

[2] H. Keypour, M. Rezaeivala, L. Valencia, P. Perez-Lourido, Polyhedron, 27 (2008) 3172.

The first report of biochar as heterogeneous support for immobilization of Pd as efficient and reusable biocatalyst in C-C coupling reactions

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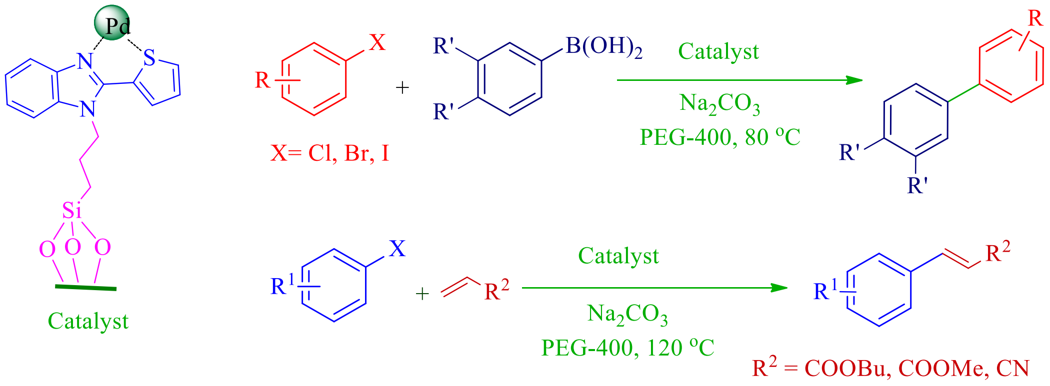
Abstract:

Biochar is made via pyrolysis of biological source such as woody materials, agricultural wastes, green waste, animal manures and other waste products, therefore it is inexpensive and environmentally friendly. Biochar can be used as a support for immobilization of catalyst or other substances due to existence of high density of carbonyl, hydroxyl and carboxylic acid groups on its surface. In this work, surface of biochar nanoparticles (BNPs) was modified by 3-choloropropyltrimtoxysilane (3-CPTMS) and further 2-(thiophen-2-yl)-1H-benzo[d]imidazole (TBA) was anchored on its surface. Then, palladium nanoparticles were fabricated on the surface of modified BNPs and further its catalytic application was studied as recyclable biocatalyst in carbon-carbon coupling reactions such as Suzuki–Miyaura and Heck–Mizoroki cross-coupling reactions. The structure of this catalyst was characterized by SEM, EDS, TGA, N_2 adsorption–desorption isotherms, XRD, and AAS techniques. This catalyst can be reused for several times without decreasing in the catalytic efficiency. Despite several advantages of this work, application of biochar as catalyst support for the first time is a major novelty of the present work.[1,2]



Schem.1 carbon-carbon coupling reactions

References:

[1] L. V. Zwieten , S. Kimber, S. Morris, K. Y. Chan, A. Downie, J. Rust, S. Joseph, A. Cowie, Plant and Soil, 327 (2010) 235–246.

[2] M. Ahmad, A. U. Rajapaksha, J. E Lim, M. Zhang, N. Bolan, D. Mohan, M. Vithanage, S. S. Lee, Y. S Ok, Chemosphere, 99 (2014) 19-33.

[3] C. J. Atkinson, J. D. Fitzgerald, N. A. Hipps, Plant Soil, 337 (2010) 1–18.

Synthesis, characterization and spectroscopic studies of new Zn(II) complex of 1, 10-Phenanthroline-based Schiff base ligand

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Abstract:

A novel 1, 10-phenanthroline based Schiff base, 3-(((1,10-phenanthrolin-5-yl)imino)methyl)benzene-1,2-diol (**H_2L**) receptor has been designed, synthesized and characterized using standard spectroscopic methods (FT-IR, ^{1}H NMR and UV-Vis) Fig.1. Zn(II) complex of the receptor was also synthesized by 1:1 reaction of **H_2L** with $ZnCl_2$ in absolute ethanol. The **H_2L** and its Zn(II) complex were applied as multi-ion responsive scaffolds for the sensing of both anions and cations via chromogenic methods in DMSO:H_2O (9:1) media. **H_2L** was displayed excellent selectivity for CN^- ion over other anions such as F^-, Cl^-, Br^-, I^-, $H_2PO_4^-$, OAC^- , N_3^- , $N0_2^-$, IO_3^- and HSO_4^-.

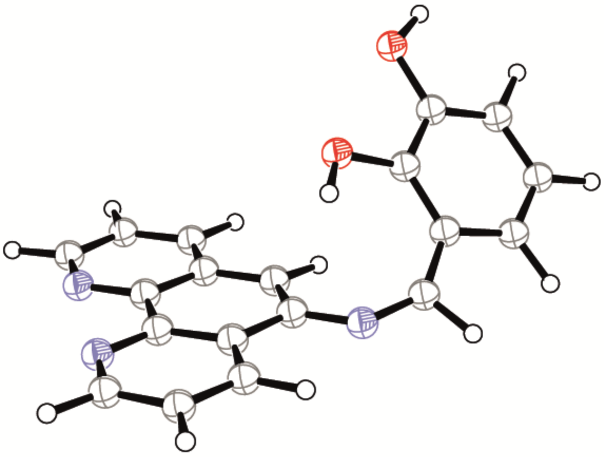

Fig. 1- **H_2L**

References:

[1] E. Merino, Chem. Soc. Rev, 40 (2011) 3835.

[2] B. L. Feringa, R. A. Van Delden, N. Koumura, E. M. Geertsema, Chem. Rev, 100 (2000) 1789.

[3] S. Alghool, H. F. Abd El-Halim, A. Dahshan, J. Mol. Struct, 983 (2010) 32.

A new nickel complex supported on MCM-41 as an efficient and recyclable catalyst in the organic reactions

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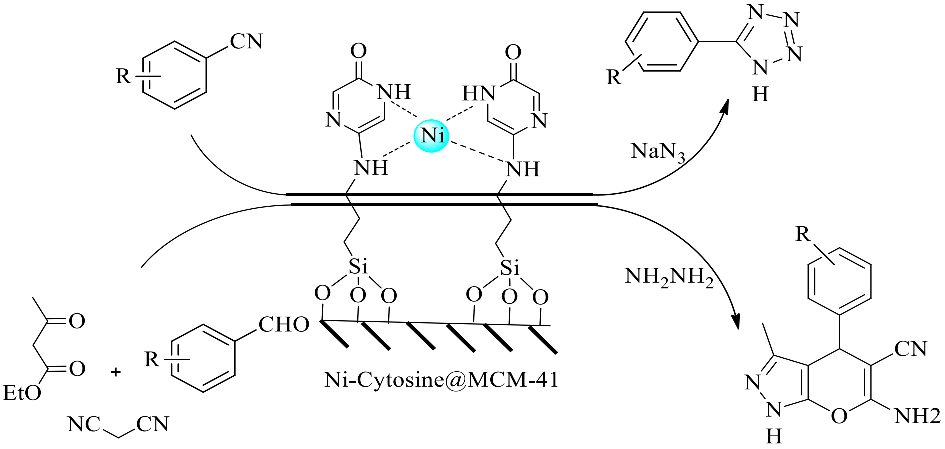
Abstract:

A new complex of nickel was anchored onto mesoporous channels of MCM-41 (Ni-Cytosine@MCM-41). This nanocatalyst has been characterized by N_2 adsorption–desorption isotherms, SEM, EDS, XRD, TGA, FT-IR, and AAS techniques. The BET results indicated that the pore volume and average pore diameter of Ni-Cytosine@MCM-41 are lower than the MCM-41 which is due to the grafting of organic species and Ni-complex onto mesoporous channels of MCM-41. Further, this catalyst was identified using low angle X-ray diffraction patterns. The spectra display hexagonal symmetry with the peaks that relate to 2θ values of 2.85^0 (1 0 0), 4.75^0 (1 1 0) and 5.45^0 (2 0 0), which indicates the functionalization of MCM-41 and successful formation of catalyst (Ni-Cytosine@MCM-41). This catalyst was applied as highly efficient, heterogeneous and recoverable nanocatalyst in the synthesis of tetrazole and pyranopyrazole derivatives. All products were obtained in high TOF and TON values, which reveal the high activity of this catalyst. This catalyst can be reused for several times without significant loss of its catalytic efficiency or nickel leaching [1-4].



Schem.1 Ni-Cytosine@MCM-41 as a catalyst

References:

[1] A. Ghorbani-Choghamarani, P. Moradi, B. Tahmasbi, polyhedron, 163 (2019) 98.
[2] A. Ghorbani-Choghamarani, P. Moradi, B. Tahmasbi, RSC Adv, 6 (2016) 56638.
[3] X. Xiong, C. Yi, X. Liao, S. Lai, Tetrahedron Lett, 60 (2019) 402.
[4] B.J. Khairnar, D.V. Mane,B.R. Chaudhari, J. Applicable Chem, 8 (2019) 425.

Synthesis of MOF $[Zn_2\ (1,4\ bdc)_2\ \ (dabco)]_n$ as a control and Drug delivery

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Abstract:

Metal-organic framework (MOF) make up an emerging class of porous crystalline materials that consist of multI topic organic linkers and inorganic nodes. In recent years, MOFs have attracted considerable attention for their potential applications in many areas such as gas storage, separation, catalysis, optics, photonic, ion exchange, molecular array, biomedicine, sensing and drug delivery(1). In the present study synthesis procedure, the porous MOF $[zn_2(1,4\ bdc)_2\ \ (dabco)]_n$ was prepared via solvothermal . The zn^{2+} ion was used as a connector, 1,4-diazabicyclo[2,2,2] octane (dabco) as a bridging ligand, and 1,4 benzene dicarboxylic acid (H_2 bdc) as a chelating ligand.in a typical reaction, $Zn(OAc)_2.2H_2O$, bdc and dabco were added to DMF. The reactant were sealed and stirred for 72h.The reaction mixture was then filtered. The withe crystal were washed with DMF to remove any metal and ligand remained, and dried in a vacuum. Powder X-ray diffraction (PXRD) of sample was measured, which proved its crystalline structure. The IR absorption spectra of sample were recorded in the range of 400-4000 cm^{-1} with KBr pellets. The produced drug-loaded MOF $[cox/zn_2(1,4\ bdc)_2\ \ (dabco)]_n$ was then studied as a drug delivery system. Also the presence of drug was confirmed in the MOF by, XRD patterns, FTIR spectra and TGA(2). Release profiles of drug, approximately with 5 mg of samples loaded was suspended in 5mg of PBS. Release drug was gently and maximum release was in 28h. Quantification of the drug in solution was performed by Uv spectrophotometr using quartz cuvette.[1,2]

References:

[1] Z.wang, G. Chen, K. Ding, Chem. Rev. 109 (2009) 322.

[2] D.Farrusseng, first ed., Wiley-vch, New York.

Synthesis and characterization of some transition metal complexes with pyridinium ylide and application of its palladium (II) complex in Suzuki-Miyaura coupling reaction

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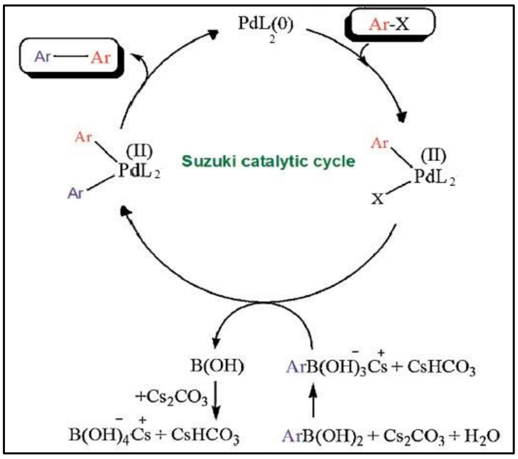
Abstract:

Pyridinium ylides are able to form stable complexes and could be characterized by spectroscopic techniques. They can behave as ambidentate ligands because the carbanion located at the Cα of the ylide is able to donate electron density to a transition metal. This work reports the synthesis and catalytic properties of new palladium complex which prepared by reaction of new pyridinium ylides (**Y**) and $PdCl_2$. The reaction of pyridine with 2-Bromo-4'-fluoro acetophenone in dry chloroform produces new pyridinium salt (**S**). The action of Na_2CO_3 on **S** compound leads to a new type of stable ylide. The reaction of **Y** with palladium (II) Chloride in dry methanol as a solvent led to the formation of C-coordinated dimeric complex $[PdY_2Cl_2]$. Characterization of the Pd(II) complex was Optimized by IR, ^{1}H and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom. Also this complex has been found to act as efficient catalysts for the Suzuki cross-coupling reaction. Various aryl bromides were coupled with aryl boronic acids in DMF, under air, in the presence of 0.2 mol% of the catalyst to afford corresponding cross-coupled products in good to excellent yields. [1-3]



Schem.1 Suzuki-Miyaura coupling reaction

References:

[1] G. Wittig, D. Krauss, A. Liebigs, 679 (1964) 34.

[2] S.J. Sabounchei, A. Sedghi, M. Bayat, M. Hosseinzadeh, A. Hashemi, A. Yousefi, R.W. Gable, J. Mol. Struct, 1175 (2019) 346.

[3] S.J. Sabounchei, M.S. Hashemi, R. Karamian, S.H. Moazzami Farida, P.G. Derakhshandeh, R.W. Gable, R.W., K. Van Hecke, J. Coord. Chem, 71 (2018) 3277.

A new Schiff‑base complex of copper supported on MCM-41 as an organic–inorganic hybrid nanocatalyst in the organic reactions

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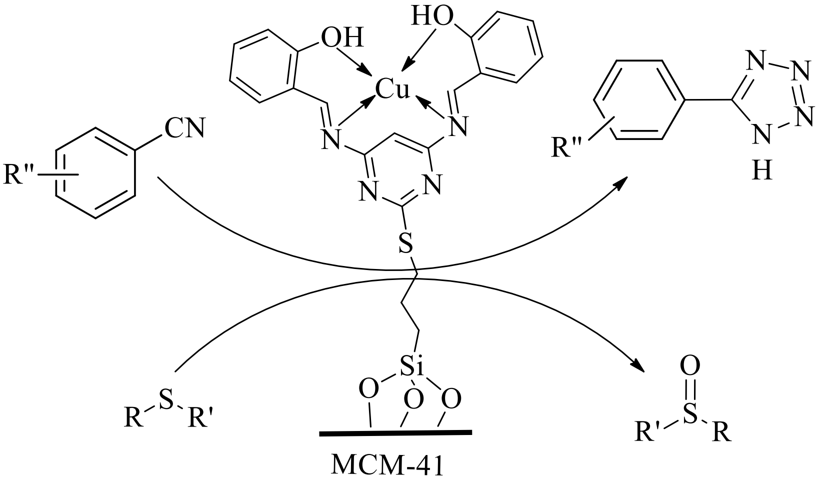
Abstract:

MCM-41 as a mesoporous structure of the silica including regular and hexagonal cannels with high density of hydroxyl groups could be available for immobilization of metal ions. Nontoxicity, availability, high specific surface area (more than 1200 m^2/g), large and uniform pore size, thermal and mechanical stability are unique properties of MCM-41 which have received much attention in various fields. In this work, mesoporous MCM-41 nanoparticles were synthesized and a new Schiff base complex of copper was immobilized on its inner surface (Cu-Schiff-base@MCM-41) and further its catalytic application was studied in selective oxidation of sulfides and synthesis of 5-substituted tetrazoles. The structure of this nanocatalyst has been characterized by N_2 adsorption–desorption isotherms, SEM, EDS, XRD, TGA, FT-IR, and AAS techniques. This catalyst can be reused for several times and the all products were obtained in high TOF and TON values.[1-3]



Schem.1 Cu-Schiff-base@MCM-41as a catalyst

References:

[1] M. Hajjami, L. Shiri, A. Jahanbakhshi, Appl. Organometal. Chem, 29 (2015) 668.

[2] S. Layek, R. Ganguly, D.D. Pathak, J. Organomet. Chem, 870 (2018) 16.

[3] P.K. Samanta, R. Biswas, T. Das, M. Nandi, B. Adhikary, R.M. Richards, P. Biswas, J. Porous Mat, 26 (2019) 145.

New Schiff base complex of zirconium on mesoporous MCM-41 as highly efficient nanocatalyst for the synthesis of tetrazoles and sulfoxides

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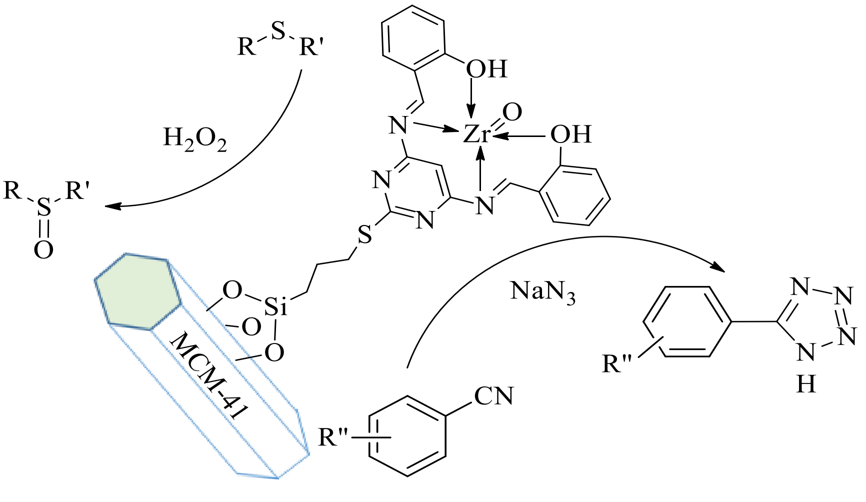
Abstract:

Heterogeneous catalysts have used in various organic reactions and industrial processes due to their stability, recoverability and recyclability. Nanomaterials can be applied as a bridge between homogeneous and heterogeneous catalysis due to their high surface area to volume ratio, remarkable efficiency, stability and recoverability. For example, MCM-41 is great and useful material for the heterogenization of homogeneous catalysts because of its unique properties such as large specific surface area, ease of functionalization, homogeneous hexagonal pore arrays with pore diameters, stability in high temperature, and versatile separation from reaction media. In this work, a zirconium Schiff‑base complex was anchored on functionalized MCM-41 (Zr-Schiff‑base@MCM-41) and applied as efficient and reusable nanocatalyst for the synthesis of 5-substituted 1H-tetrazoles using [2+3] cycloaddition reaction of various organic nitriles with sodium azide (NaN_3) in green solvent. Also this catalyst was applied as a versatile catalyst for selective oxidation of sulfides to sulfoxides using hydrogen peroxide as oxidant. Characterization of the catalyst was performed using N_2 adsorption–desorption isotherms, SEM, EDS, XRD, TGA, FT-IR, and AAS techniques [1-3].



Schem.1 Zr-Schiff-base@MCM-41 as a catalyst

References:

[1] A.G. Choghamarani, P. Moradi, B. Tahmasbi, polyhedron, 163 (2019) 98.

[2] M. Nikoorazm, A.G. Choghamaranai, M. Khanmoradi, P. Moradi, J. Porous Mate, 25(2018) 1831.

[3] M. Hajjami, L. Shiri, A. Jahanbakhshi, Appl. Organometal. Chem, 2015, 29, 668.

Simulation of the new combined process of Ca-method and Na-method to produce high purity calcium hypochlorite

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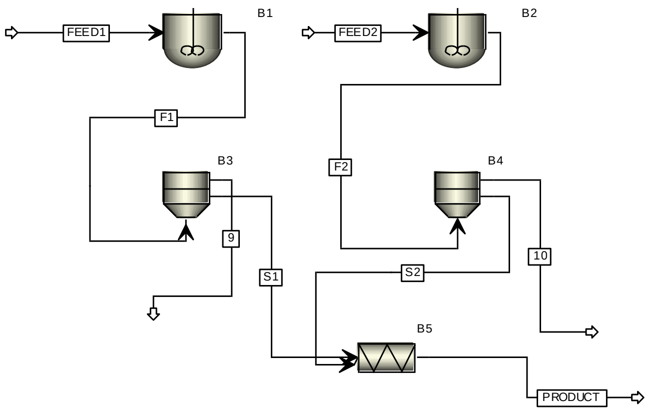
[b] CCPC innovation center
[c] University of applied science & technology; CCPC branch
*E-mail: kalateh60@yahoo.com

Abstract:

In the chlor-alkali industries, the major products, including, chlorine and hydrogen gases, and also sodium hydroxide are produced by electrolysis of the saturated brine.

One of the most important minor products in these industries is the calcium hypochlorite. The production process has a lot of problems such as environmental issues including the high wastewater volume which is the most significant one. This causes that the production reduces in our country despite the key role of this product in the water and wastewater industries.

Based on the patented plan in Chloran Chemical Production Company, these problems are resolved by a new process method in which the calcium hypochlorite is produced by combination of the Ca-method and Na-method processes and whole the wastewater is used as the precipitating agent in the secondary purification of the saturated brine and as the raw material in the calcium chloride production unit. In this article, we are trying to approve the possibility of this new process by Aspen plus simulating software.[1,2]



References:

[1] Yee San Su; Delmar "Trey"Morrison III; Russell A.Ogle. Journal of Chemical Health and Safety, 16 (2009) 21-25.

[2] Thomas F. O'Brien; Tilak V. Bommaraju; Fumio Hine; Handbook of Chlor-Alkali Technology, 2005 Springer Science+Business Media, Inc.

[3] Iranian Patent "Production of Neutral Calcium Hypochlorite Dihydrate by Combination of Ca-method and Na-method Processes" M. Hamoun; A. Kalateh; Chloran Chemical Production Company; Patent No.: 93617, 2017.

Synthesis and characterization platinum (IV) complexes containing phthalazine ligands

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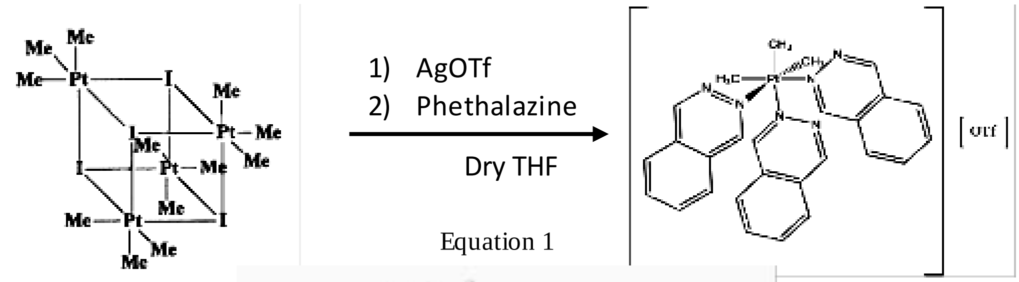
Abstract:

Platinum (IV) complex $[PtMe_3(phth)_3]^+X^-$,**1**, has been prepared from the reaction of trimethyl platinum (IV) complex $[PtMe_3I]$ and 3 equivalents phthalazine. Complex **1** characterized using NMR spectroscopy and X-ray crystallography. Complex **1** in solid state shows yellow emission upon excitation under UV-lamp. The crystal structure of **1** shows coordination of three phthalazine ligand to the platinum center. As shown in equation 1 complex **1** has three coordinated nitrogen atoms that providing the possibility of coordination to the second metal center. Attempts for preparation hetero binuclear complexes containing bridging phthalazine ligand using **1** and other late transition metals are in progress in our group.[1]



Equation 1

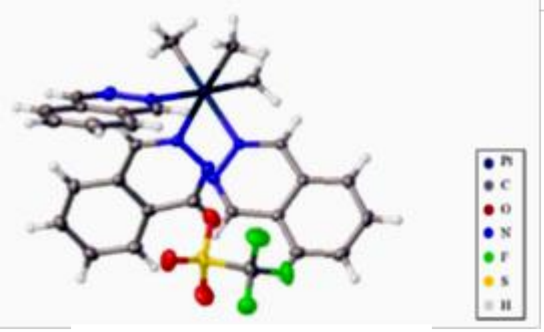


Fig1. Crystal structure of complex

References:

[1] H. Molaee, M. Nabavizadeh, M. Jamshidi, M. Vilsmeier, A. Pfitzner, M.S Sangari, *Dalton Transactions*, 46 (2017) 16077-16088.

BioInorganic Chemistry Investigation on encapsulated Cysteine derivative

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Abstract:
Recently Cysteine has been introduced as an agent of suppression of μ- and m-calpain activities and followed by that neuroprotective compound. The main objective of this research was to investigate the neuroprotective potential of the encapsulated Cysteine derivatives into polymeric nanocarriers (NCs). The copolymer-based synthesized Cysteine-loaded nanocarriers were prepared from coprecipitation method at constant temperature followed by evaporation of an organic solvent. To the best of our knowledge, it is the first time to investigate the biocompatibility and neuroprotective potential of Cysteine derivatives loaded into PEG-b-PCL (poly (ethylene glycol)-block-poly (ε−caprolactone) methyl ether). The average size of the polymeric/empty NCs was 89 nm and for PEG-b-PCL/Synthesized derivative of Cysteine was 126 nm. The Drug Loading efficiency was 81%. The concentration of Polymeric NCs was 2.1 x 10^{10} particles/ml and the zeta potential of polymeric/empty and polymeric/ Synthesized derivative of Cysteine NCs -5 mV and -11 mV respectively. Biocompatibility and Neuroprotective potential of NCs were evaluated in the SH-SY5Y human neuroblastoma cell line using cell viability and toxicity assays. The concentration of polymeric NCs below 1 x 10^{10} particles/ml can be considered as a safe concentration for the cell line. Also the Synthesized derivative of Cysteine encapsulated into polymeric NCs have more neuroprotective effect compared to free Cysteine at lower concentration, and therefore, have a significant neuroprotective potential against Z-VAD-fmk and St-evoked SH-SY5Y cell damage.[1-3]

References:

[1] N. Rabiee, M. Rabiee, Drug Delivery Letters, 8 (2018) 242-247.
[2] N. Rabiee, M. Kiani, M. Bagherzadeh, M. Rabiee, S. Ahmadi, Nanoparticle (NP)-Based Delivery Vehicles, (2019).
[3] M. Karimi, M.R. Mansouri, N. Rabiee, M.R. Hamblin, Morgan & Claypool Publishers, (2018).

Preparation and Application of Mesoporous Activated Carbons from Waste Sesame as Green Absorbent for Removal of Azithromycin

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[b]Food and Drug Laboratory Research center, Food and Drug Administration, Ministry of health and Medical Education

*E-mail: marazavimehr@gmail.com

Abstract:

Activated carbon decorated with magnetite (ACMG) nanoparticles composites have been prepared by facile method via impregnation of AC obtained sesame oil wastes with stable dispersion of superparamagnetic MG nanoparticles followed by drying. These composites exhibit both magnetic and porosity behavior which can be easily optimized by controlling the weight ratio of two phases. The structural, thermal and morphological properties of these as synthesized ACMG samples were characterized by powder XRD, FTIR, and SEM techniques. The ACMG powder has been used for water purification having Azithromycin (AZ) as an impurity. The response surface methodology (RSM) with historical design was used to investigate the adsorption properties of Azithromycin onto synthesized composite. The nanoporosity of these composites allow rapid adsorption of AZ and their magnetic behavior helps in single step separation of AZ adsorbed ACMG particles by the application of external magnetic field. According to the achieved result, magnetic activated carbon as an inexpensive adsorbent, have promising application in the removal of antibiotics from solution and also can be effectively utilized in industrial application. [1]

Fig.1. Preparation of ACMG

References:

[1] B. Zhang, J. Xu, P. Xin, Y. Han, B. Hong, H. Jin, X. Peng, J. Li, J. Gong, H. Ge, Z. Zhu, X. Wang, Journal of Solid State Chemistry, 221 (2015) 302-305.

[2] A. Asfaram, M. Ghaedi, S. Hajati, A. Goudarzi, E.A. Dil, Ultrason. Sonochem. 34 (2017) 1-12.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Evaluation of activated carbons based on Palm Kernel Shell as absorbent of Cr (VI)

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Abstract:

Chromium is a heavy metal in wastewater that should be removed from the environment due to negative effects on living organisms and environmental impacts. The potential of palm kernel shell (PKS), as agricultural waste, to remove Cr (VI) from aqueous solution was evaluated in a one at a time process. Effective parameters such as pH (2–8), temperature (20–80 °C), contact time (10-120 min), adsorbent concentration (0.1–1 g/L), and initial Cr (VI) concentration (10-100 mg/L) were all studied to attain the maximum removal efficiency. The results showed that a strong dependence of the adsorption capacity on pH was observed, the adsorption capacity increases as pH value decreases and the optimum pH value is pH= 2.0. The other optimal conditions for maximum adsorption efficiency are temperature 40 °C, contact time 45 min, adsorbent concentration 0.5 g/L and initial Cr(VI) concentration 10 mg/L. The equilibrium data for chromate adsorption well fitted to Freundlich equation, with maximum adsorption capacity of 125 mg/g. Removal efficiencies of 100% were achieved in 120 min at a Cr (VI) dose of 10 mg/L.[1,2]

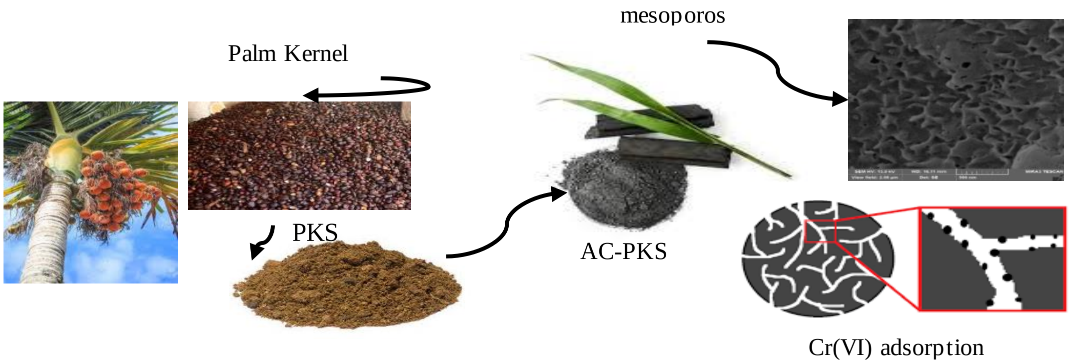

Fig.1

References:

[1] R. Labied, O. Benturki, A. Ya, E. Hamitouche, A. Donnot, Adsorption Science & Technology, 36 (2018) 1066–1099.

[2] M.K. Rai, G. Shahi, V. Meena, R. Meena, S. Chakraborty, R.S. Singh, B.N. Rai, Resource-Efficient Technologies, 2 (2016) S63–S70.

Glucose Oxidase Immobilized On Novel Multifunctional Silver Dendritic Hierarchical Nanostructure: An Efficient and Robust Biocatalyst

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*Email: Moghadamm@sci.ui.ac.ir

Abstract:

Glucose oxidase enzyme (GOX) (oxygen 1-oxidoreductase) catalyzes the oxidation of *β*-D-glucose to gluconic acid. GOX has found several commercial applications including used in an automatic glucose assay kit in conjunction with catalase and chiefly in biosensors for the detection and estimation of glucose in industrial solutions and in body fluids such as blood and urine [1]. Immobilized enzymes are used as biocatalysts for analytical purposes in diagnostics and for preparative purposes in large scale industrial methods [2,3]. Immobilization can enhance the half-life, improve the stability, and increase the catalytic activity as well as recovery and reusability of an enzyme. Herein, we demonstrated synthesis of silver dendritic hierarchical nanostructure as unique and convenient support for immobilization of enzyme [4-6]. Then, an important enzyme, GOX, was immobilized on the nano carrier to produce robust biocatalysts for oxidation of *β*-D-glucose to gluconic acid. The biocatalyst was characterized by different analytical techniques. The results of biocatalyst systems exhibited the substantial enhancement of reactivity, reusability, and stability of GOX due to this strategy.[1-6]

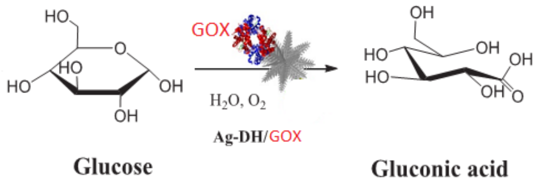

Fig.1 GOX for oxidation of *β*-D-glucose to gluconic acid

References:

[1] A. Liese, L. Hilterhaus, Chem Soc Rev, 42 (2013) 36-49.
[2] C. Mateo, J.M. Palomo, G. Fernandez-Lorente, J.M. Guisan, R. Fernandez-Lafuente ,Enzyme Microb Technol, 40 (2007) 1451-63.
[3] A. Dyal, K. Loos, M. Noto, S.W. Chang, C. Spagnoli, K.V. Shafi, J Am Chem Soc, 125 (2003) 1684-5.
[4] C.X. Kan, J.J. Zhu, X.G. Zhu, J Phys D: Appl Phys, 41(2008) 155304.
[5] J.N. Tiwari, R.N. Tiwari, K.S. Kim, Prog Mater Sci, 57 (2012) 724-803.
[6] B. Wiley, Y. Sun, Y. Xia, Acc Chem Res, 40 (2007) 1067-76.

Synthesis of nickel sulfide nanoparticles using a new precursor, characterization and investigation of photocatalytic properties

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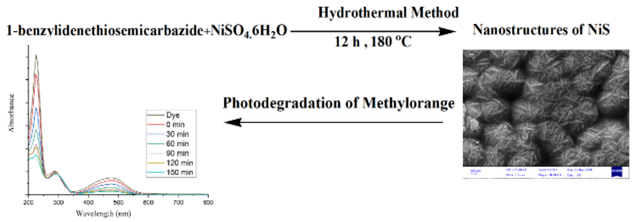
Abstract:

Nanomaterials have very special properties. Two important properties, which distinguish them from other groups; include increased surface of substances and quantum effects. Among the wide range of mineral compounds, metal sulfides are used in various fields. The basic elements are in fact the same nanoscale elements whose properties vary in nanoscale mode with their properties on a larger scale. Among metal sulfids, nickel sulfide, which has been used extensively as a catalyst, IR detectors, rechargeable lithium batteries, solar storage and catalysts. To date, limited reports have been published on the production of nickel sulfide. In this project, along with the preparation of nanosized nickel sulfide, it's photocatalytic properties was studied. In a simple and efficient way, a one-step hydrothermal method was used to synthesize NiS using $Ni(SO_4)_2.H_2O$ a source of nickel and a new synthesized thio Schiff base ligand as a source of sulfur. The synthesized NiS was characterized by FT-IR, XRD and EDAX analysis. The morphology and size of particles were investigated by SEM images. To determine the photocatalytic ability of as-synthesizes NiS, color removed of methylorange was studied.[1-5]



References:

[1] Y. Xia, Y. Xiong, B. Lim and SE. Skrabalak, Angew. Chem., Int. Ed. 48 (2009) 60-103.
[2] H.M. Chen, R.S. Liu, J. Phys. Chem. C., 115 (2011), 3513-3527.
[3] A. Sobhani, M.S. Niasari, Superlattices and Microstructures, 59 (2013) 1-2.
[4] R. Karthikeyan, D.Thangaraju, N. Prakash, Y. Hayakawa, CrystEngComm, 17 (2015), 5431-5439.
[5] M. Sabbaghan, A.S. Shahvelayati, Ceram. Int, 42 (2016) 3820-3825

Synthesis of a new polyoxotungstate-based inorganic-organic hybrid and invastigation of its catalytic activity in azide-alkyne cycloaddition reaction

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Abstract:

Polyoxymetalates (POMs) are known as inorganic metal oxide clusters, which because of their unique physical and chemical properties are widely used in various scientific-research fields such as catalysis, electronics, magnetism, optics, medicine, and etc. Many various methods are applied to improve the catalytic performance of POMs, including the stabilization of these particles on silicates, metal-organic frameworks (MOFs) and preparation of inorganic-organic hybrid material with these components. In this work, first, polyoxotungstate-based inorganic-organic hybrid was synthesized by in-situ protocols. For this purpose, benzimidazole (bim) and polyoxotungstate are used as a linker and POM, respectively. The obtained precipitate was characterized by FT-IR, CHN, PXRD and ICP techniques and finally, the catalytic activity of the synthesized particles was investigated in the azide-alkyne cycloaddition (AAC) reaction, and the effect of different parameters such as temperature, solvent, time and catalyst content on reaction efficiency were studied.[1-3]

References:

[1] H. An, Y. Hou, L. Wang, Y. Zhang, W. Yang, S. Z. Chang, Inorg. Chem,56 (2017) 19, 11619–11632.
[2] H. Liu, C. Qin, Y. Wei, L. Xu, G. Gao, F. Li, X. Qu, Inorg. Chem,47 (2008) 4166–4172.
[3] M. Bagherzadeh, H. Hosseini, Coord. Chem,70 (2017) 2212_2223.

Synthesis of mercapto functionalized Zr-MOFs for the enhanced removal of Hg^{2+} ions from water†

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Abstract:

Having access to clean water is a mandatory requirement for the proper development of living beings [1]. So , addressing the removal of contaminants from aquatic systems should be a priority research topic in order to restore ecosystem balance and secure a more sustainable future [2]

Mercapto functionalized Zr-MOFs have been developed via postsynthetic modification for selective adsorption of Hg^{2+} ions. Thioglycolic acid (TGA) was used as the modulator and functionalized molecule to synthesize the mercapto functionalized Zr-MOFs (Zr-MOFs-TGA). In comparison with the Zr-MOFs without modulator (UiO-66 and UiO-66-NH_2), our synthesized Zr-MOFs-TGA because of using NH_2-BDC with S-containing modulators and having more coordinating groups, leads to a much higher adsorption capacity for Hg^{2+} ions. Specially, UiO-66-TGA had an adsorption capacity for Hg^{2+} ions up to 214.6 mg/g, which is much higher than that of UiO-66 (28 mg/g). Additionally, the Zr-MOFs-TGA can be used to reduce the Hg^{2+} ions concentrations (10-500 ppm) from water. Moreover, the synthesized Zr-MOFs-TGA also exhibited good selectivity and chemical stability.

References:

[1] M Mon ,J. Mater. Chem. A, 6 (2018) 4912.
[2] L. Xu, , Springer Berlin Heidelberg, Berlin, Heidelberg, 2015.

Synthesis and Characterization of New Cu(I) and Ag(I) Complexes Containing Bis(diphenylphosphino)methane and NN bidentate ligand.

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Abstract:

Binuclear transition-metal complexes containing bidentate bridging ligands, L-L, have been the focus of much investigation in the last few years. Particularly, many examples with two bridges of the diphosphine $Ph_2PCH_2PPh_2$ (dppm), including a variety of metals, oxidation states, and stereochemistries, have been described. They are generally characterized by the presence of an eight-membered ring $M(\mu\text{-L-L})_2M'$, in different conformations. The stereochemistry of the complex, the presence of metal- metal bond interactions and the nature of the second ligand in the structure effect on the photophysical properties of the binuclear complex which is very important in various applications such as OLEDs and optical devices [1]. In this work we have synthesized a new binuclear Cu(I) and Ag(I) complexes by treatment of $[Cu(MeCN)_4].PF_6$ and $[Ag(MeCN)_4].BF_4$ with dppm as a bridging ligand and another NN bidentate ligand at room temperature in dichloromethane which gives $[Cu_2(dppm)_2(NN)_2].PF_6$ and $[Ag_2(dppm)_2(NN)_2].BF_4$ respectively. The complexes were characterized by ^1H,^{13}C-NMR in solvent phase and X-ray crystallography in the solid state. These complexes demonstrated interesting photophysical properties as shown in Fig .1.

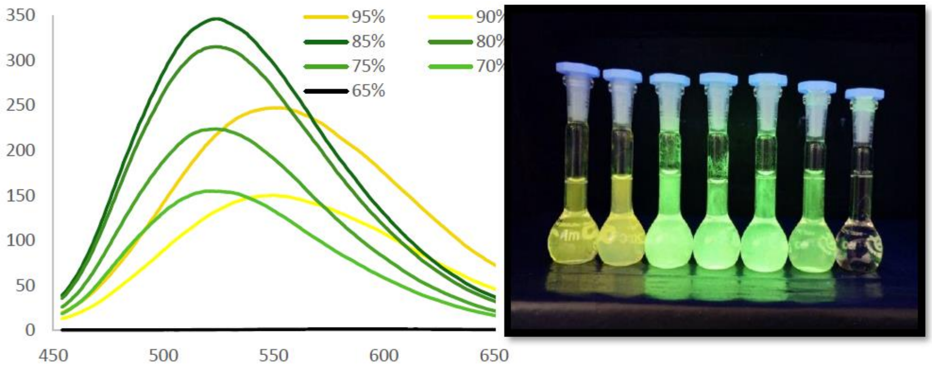

Fig 1. Emission spectra of aggregated solution of $[Cu_2(dppm)_2(NN)_2].PF_6$

References:

[1] H.He, Y.S.Luo, B.S.Di, J.L.Chen, L.C.Ho, H.R.Wen, S.J.Liu, J.Y.Wang, W.Y.Wong, Inorg. Chem., 56 (2017) 10311-10324.

Synthesis and Characterization of ZnO Nanoparticles by Using A Zn(II) Schiff Base Complex

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Abstract:
In this work, first a metal Schiff base complex of Zn (II) was synthesized by using $Zn(NO_3)_2$, $4H_2O$ and a bidentate Schiff base ligand (Fig. 1)[1]. The structure of this compound was characterized by some spectroscopic methods. In the other part of this work, nanosized ZnO (NPs) were prepared by calcination of this metal complex. The structure of ZnO (NPs) was characterized by some usual techniques, such as X-ray diffraction analysis (XRD), field emission scanning electron microscopy (FESEM), elemental analysis (MAP), Fourier Transform Infrared spectroscopy (FT-IR) and energy dispersive X-ray spectroscopy EDS[2].

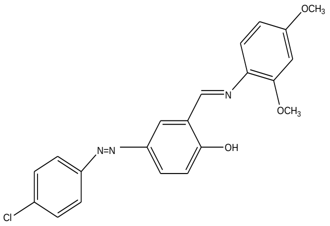

Fig.1. The structure of Schiff base ligand

Fig.2. shows the SEM image of ZnO (NPs) and Figure 3 shows the XRD pattern of ZnO (NPs). By Scherer's formula, the average size of the nano-sizes of the complex was calculated >100 nm.[2].

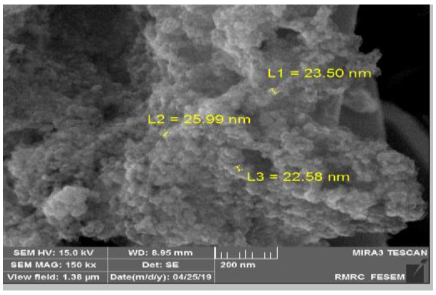

Fig. 2. The SEM image of nano-sized ZnO

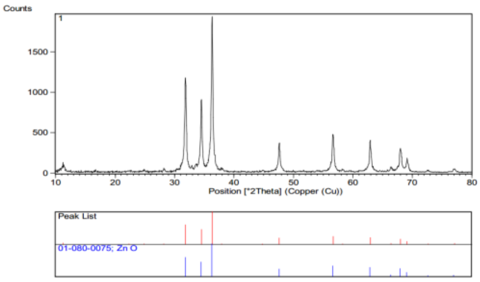

Fig. 3. The XRD pattern of nano-sized ZnO

References:

[1] A. Vogel, A Text-Book of Practical Organic Chemistry, Longman, New York, (1956) 620.

[2] H. Korideck, A. Kassis, R. Kumar, S. Sridhar, G. Makrigiorgos, R. Cormack, Nanomedicine, 9 (2013) 25.

Nature of C→E and E→M Bonds in [NHC(R)→ER_2→$M(CO)_5$] Complexes

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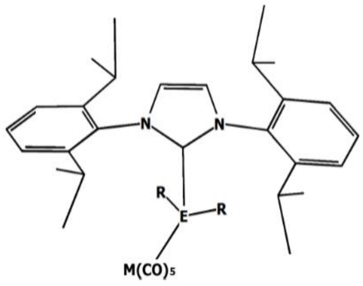
Abstract:

The heavy group 14 methylene analogues, EH_2, (E = Ge and Sn) have been stabilized via efficient methods, thus enabling the chemistry of these novel inorganic hydrides to be explored in depth [1]. The first stable transition-metal complex involving the heavy methylene congener,SnH_2, as a ligand was synthesized by Rivard and his co-workers in 2011 [1]. Also a theoretical study on some adducts of [NHC(CH_3)→ER_2] was reported by us in 2017. [2]. Herein a theoretical studies on structure and nature of the C→E and E→M bonds in some [NHC(R)→ER_2→$M(CO)_5$]; (E=Ge,Sn,Pb)R=(CH_3, H, F, Cl, Br)M=(Cr, Mo, W) complexes has been reported (Scheme.1). The structures of latter complexes are investigated at M06 /def2-SVP level of theory. The natures of C→E and E→M bonds in the complexes are analyzed with NBO, EDA as well as ETS-NOCV at the mentioned level of theory. Results Show that changing E atom from Ge to Pb with considering the same R substituents and M atom, led to decreasing in the values of interaction energies between the NHC(R) and $ER_2M(CO)_5$ fragments in [NHC(R)→ER_2→$M(CO)_5$]; (E=Ge, Sn, Pb; R=CH_3, H, F, Cl, Br; M=Cr, Mo, W) complexes. Results also confirm that the nature of E→M bond in the complexes studied is largely electrostatic with a contribution of about 50% in total interaction energies.



Schem1. Schematic representation of the [NHC(R)→ER_2→$M(CO)_5$]; (E=Ge, Sn, Pb; R=CH_3, H, F, Cl, Br; M=Cr, Mo, W) complexes investigated here

References:

[1] E. Rivard, J. Ferguson, J.Am. Chem. Soc, 133 (2011) 777–779.
[2] M. Bayat, E. Soltani, J. Polyhedron, 123 (2017) 39-46.

Synthesis of magnetically separable copper nanocatalyst and their application as an efficient catalyst for Sonogashira and Suzuki cross-coupling reactions

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Abstract:
A copper complex was immobilized on Schiff base modified magnetic Fe_3O_4@SiO_2 nanoparticles by covalent linkage. The obtained nanoparticles were identified with various characterization methods. The nanocatalyst shows good activity toward Sonogashira and Suzuki cross-coupling reaction in environmentally friendly solvent (H_2O/DMF) under mild conditions [1]. The catalyst shows not only high catalytic activity, but also offers many practical advantages such recyclability and air stability. Expectedly, the nanocatalyst can be applied in large-scale industrial synthesis. The SEM micrographs of the products Fe_3O_4 and nanocatalyst are given in Fig. 1(a) and Fig. 1(b) respectively. It was found that the nanoparticles were present as uniform particles with spherical morphology. SEM images reveal that Fe_3O_4 particles are aggregated particles having rough external surfaces (Fig. 1(a)) [2]. Silica coating makes the particles exhibit smooth and spongy surfaces (Fig. 1(b)) which indicatives the successful coating of silica over the magnetic nanoparticles. However, the nanocatalyst particles still fall in the nano-size range.

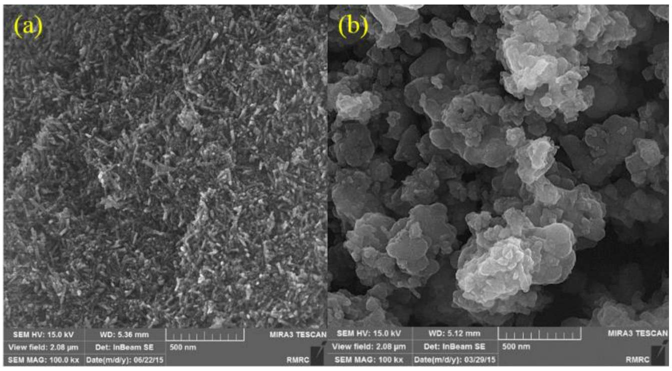

Fig. 1.(a) SEM images of Fe_3O_4 and (b) nanocatalyst

References:
[1] V. Polshettiwar, C. Len, A. Fihri, Coordination Chemistry Reviews, 253 (2009) 2599.
[2] C.I. Fernandes, M.D. Carvalho, L.P. Ferreira, C.D. Nunes and P.D. Vaz, J. Journal of Organometallic Chemistry, 2 (2014) 760.

Synthesis and spectroscopic studies of some mercury(II) complexes of an symmetrical bidentate Schiff base ligand

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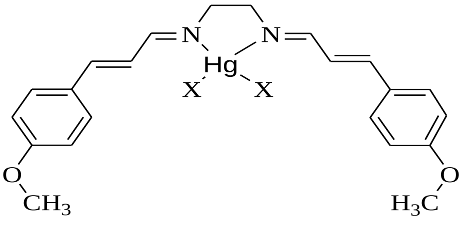
Abstract:
Schiff base ligands are one of the most important classes of donor compounds forming metal coordination materials. Various applications of the Schiff base complexes may be the reason for development in synthesis of these types of compounds with different structures [1]. The Schiff base ligands and its complexes have showed a broad range of biological activities such as antibacterial, antitumor, antifungal, DNA cleavage systems and anti-infammatory. Among the different methods that have been used for the synthesis of nano structures, the sonochemical procedure has become popular due to the rapid synthesis, product quality, environmentally friendly and low cost [2].

In this work, we report some new mercury(II) Schiff base complexes $HgLX_2$ (where X = halide and/or pseudohalide and L is a bis[(4-methoxyphenyl)acryaldehydene)-ethylenediamine were synthesized and characterized by molar conductance, thermal analyses, UV–visible spectra, FT-IR spectra, ^1H NMR and ^{13}C NMR spectra. The mercury compounds in nano-structure size were also prepared by sonochemical method. The nano-structure compounds were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The antimicrobial activity of the ligand and its mercury complexes against four gram positive and gram negative bacteria and also two fungi was assessed by the disk diffusion method.



Scheme 1. The structure of [$HgLX_2$] complex.

References:

[1] G. Mahmoudi, A. Morsali, M. Zeller, Inorg Chim Acta. 362 (2009) 217.

[2] M. Montazerozohori, S. MojahedJahromi, A. Masoudiasl, P. McArdle, SpectrochimActa A. 138 (2015) 517.

Synthesis, characterization, antimicrobial and theoretical investigation of a new mercury bromide complexes

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Abstract:

Mercury is an extremely toxic element that is naturally present in the environment and also as a result of human activities. Analysis of biosystems with mercury ion becomes a problem of particular importance in view of the established toxic influence of this metal, associated with Cd and Pb to the group of the most toxic environmental pollutants. Recently, an increase in the concentration of this metal in living organisms has been observed. Its toxicity derives from the fact that it is rapidly localized intracellularly, mainly in the liver, and then bound to metallothionein forming a complex that is slowly transferred to the bloodstream to be deposited in the kidneys. This metal competes with Zn and blocks active sites of metal–enzymes and as a relatively soft acid it can dislodge Zn(II) in cysteine-coordinated zinc compounds or Ca(II) ions in bone cells. Therefore, investigation of possibility of its coordination to various ligand especially nitrogen donor ligand can be useful for following its pathway in biological system[1-3]. In this work we report synthesis and characterization of some new zinc halide complexes formulated as $HgLBr_2$ (L= Schiff base ligand). The Schiff base ligand was prepared by a condensation of chlorobenzaldehyde and 2-aminoethylethylenedianie in 2:1 molar ration in ethanol for 3h at room temperature. The zinc complexes were synthesized by direct reaction of the ligand and zinc salt in 1:1 molar ratio in ethanol. Furthermore the ligand and its complexes have been screened for their antibacterial and antifungal activities and the data reveal that the complexes have higher activity than the free ligand. Finally, optimized structures, molecular parameters and vibrational frequencies were calculated at the B3LYP/LANL2DZ level of theory.

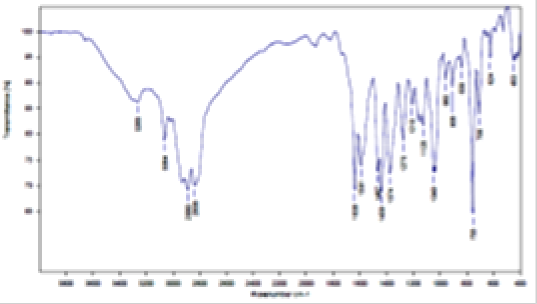

Figure 1- The FT/IR of ligand

References

[1] B. Gao, M. Wan, J. Men, Y. Zhang, Appl. Catal. A: Gen., 10 (2012) 156.
[2] M. H. Habibi, E. Shojaee, G. S. Nichol, Spectrochim. Acta Part A, 98 (2012) 396.
[3] M. Montazerozohori, F. Parsi, A. Masoudiasl, R. Naghiha, M. Montazer Zohour, Inorg. Nano-Met. Chem., 47(2017) 881.

The effect of hydrochloric acid on particle size in synthesis of UiO-66 by hydrothermal method and investigation on photocatalytic properties

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Abstract:

In this study, UiO-66 was synthesized by hydrothermal method in acidic solution by different concentrations (0/25 – 1 mol) of hydrochloric acid to enhance the particle surface [1]. Also, the photocatalytic properties of UiO-66 under UV light irradiation was investigated by photodegradation of methylene blue (25 ppm) pollutants, (80% degradation in 70 min). The Synthesized UiO-66 were identified and characterized by fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron micrograph (SEM), Nuclear magnetic resonance (NMR) and BET.

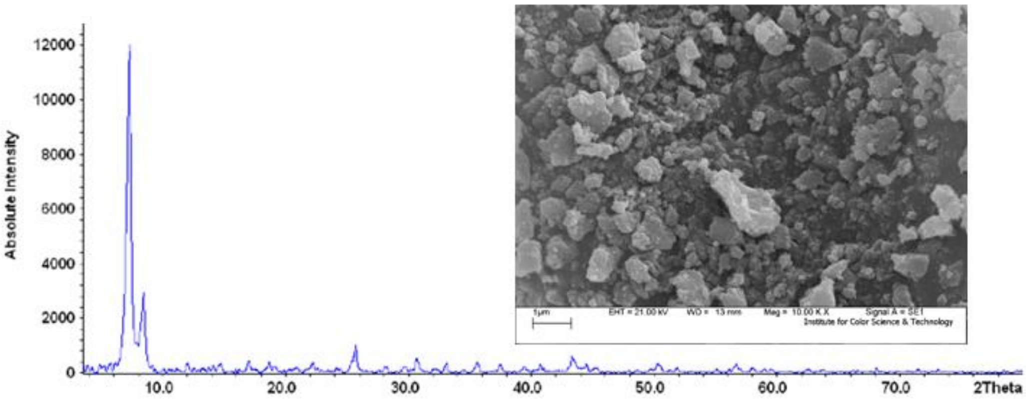

Fig.1. XRD and SEM of UIO-66 was synthesized by 1 mol of hydrochloric acid.

References:

[1] G.Zahn, P.Zerner, J.Lippke, F.L.Kempf, S.Lilienthal, C.A.Schröder, & P.Behrens, CrystEngComm, 16(39) (2014) 9198-9207.

Synthesis of New Luminescent MOf and application as a sensor in detection of Cr(VI) Oxyanions

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Abstract:

Mofs have attracted a lot of attention because of their extraordinary features, like Removal contaminants, fluorescence detection, gas storage and separation, drug delivery, chemical sensing, heterogeneous catalysis [1]. MOFs as a luminescent sensors responses towards small molecules, gas molecules, ions (cations and anions), pH, humidity, temperature, and biomolecules [2]. Cr(VI) is one of the cations that very dangerous for humans. especially for people working in the steel and textile industry. The effects of Cr(VI) on the human body These include stomach ulcers, skin inflammation, and skin sensitivities [3]. In this work we synthesized a new Cd Mof with a n donor Schiff base ligand and a carboxylic acid linker which have high selectivy for Cr(VI) Oxyanions in Aqueous Media. Also Compared to similar reports have a high Quenching constants (Ksv) .

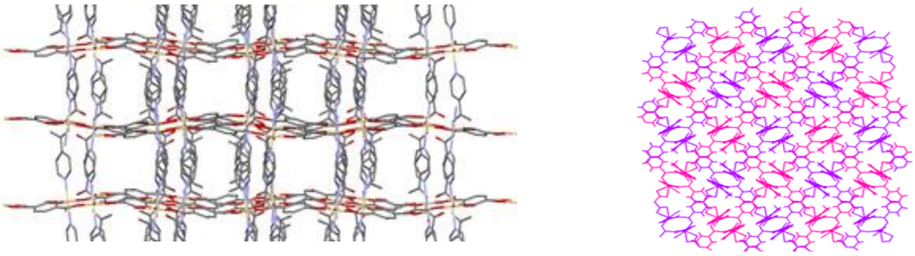

Fig.1. From right: 2-fold interpenetration of pcu nets, packing network of MOF

References:

[1] V.Guillerm, D.Kim, J.F.Eubank, R.Luebke, X.Liu, K.Adil, M.S.Lah, M.Eddaoudi, Chem. Soc. Rev. 43 (2014) 6141−6172.

[2] X.Wang, L.Zhang, J.Yang, F.F.Liu, F.Dai, R.Wang, D.J.Sun, Mater. Chem. A, 3 (2015) 12777−12785.

[3] T.Y.Gu, M.Dai, D.J.Young, Z.G.Ren, J.P.Lang, Inorg. Chem. 56 (2017) 4668−4678.

Synthesis and spectroscopic characterization of a new phosphoric triamide: $[2,3\text{-}F_2–C_6H_3C(O)NH]P(O)[NC_5H_{10}]_2$

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Abstract:

NMR spectroscopy is the most important analytical tool for chemists who work on synthesis. In recent years, this powerful and valuable tool has been used to identify phosphoramide compounds [1-4]. In this regard, a new phosphoric triamide with formula $[2,3\text{-}F_2–C_6H_3C(O)NH]P(O)[NC_5H_{10}]_2$ (**1**, Fig. 1) was synthesized and characterized by ^1H, $^{13}C\{^1H\}$, $^{31}P\{^1H\}$ NMR and IR spectroscopy.

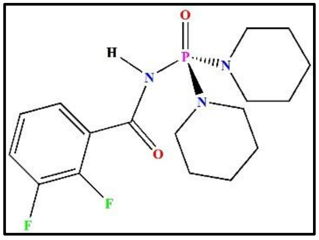
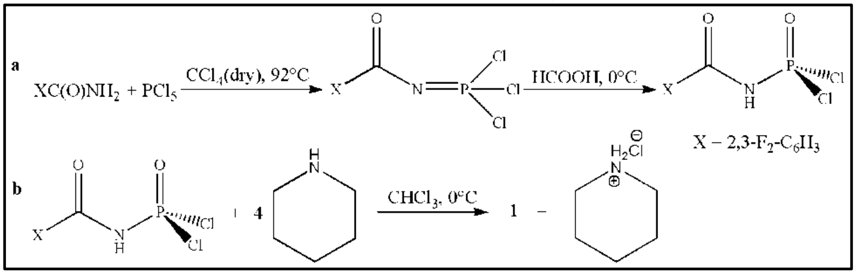


Fig 1. Molecular structure of compound **1**

Reaction of phosphorus pentachloride and 2,3-difluorobenzamide in dry CCl_4 at 365 K (3 h) followed by treatment with formic acid at 273 K (ice water bath) leads to the formation of $2,3\text{-}F_2–C_6H_3C(O)NHP(O)Cl_2$ (scheme 1a) as a white solid. This precursor containing two phosphorus-chloride bonds is then reacted with piperidine (in a molar ratio of 1:4, respectively) in $CHCl_3$ at 273 K for 4 h to give compound **1** (scheme 1b).



Scheme 1. Synthesis of compound **1**

In the ^{13}C NMR spectrum of this compound, three-bond distance coupling with the phosphorus atom is observed for corresponding carbon atoms of piperidine rings ($^3J(P,C) = 4.7$ Hz), but two-bond distance coupling $^2J(P,C)$ not observed. Due to the coupling with both fluorine atoms, each of the three adjacent unsubstituted carbon atoms of the $2,3\text{-}F_2–C_6H_3–$ fragment show the second-order spectra.

References:

[1] K. Gholivand, Z. Shariatinia, M. Pourayoubi, Zeitschrift für anorganische und allgemeine Chemie, 631 (2005) 961-967.
[2] K. Gholivand, N. Oroujzadeh, Z. Shariatinia, Heteroatom Chemistry, 21 (2010) 168-180.
[3] M. Pourayoubi, S. Shoghpour Bayraq, A. Tarahhomi, M. Nečas, K. Fejfarová, M. Dušek, Journal of Organometallic Chemistry, 751 (2014) 508-518.
[4] B. Vahdani Alviri, M. Pourayoubi, A. Saneei, M. Keikha, A. van der Lee, A. Crochet, A. A. Ajees, M. Nečas, K. M. Fromm, K. Damodaran, T. A. Jenny, Tetrahedron, 74 (2018) 28-41.

Adsorption of As^{3+}, Hg^{2+}, Cd^{2+}, and Pb^{2+} by acid activated exfoliated bentonite clay functionalized with thiol group

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Abstract:

At the present time, water pollution is a very dangerous and prevalent problem in our world [1], caused by perilous and toxic heavy metal ions as a result of innumerable industrial actions. These days, due to the industry's development, we understand a sharp rise in industrial wastewater containing a high amount of heavy metals such as Hg (II), As (III) [2], Cd (II), and Pb (II), particularly in developing countries This study investigated on developing an effective method of using thiol functionalized acid activated exfoliated bentonite clay with good performance to eliminate four toxic heavy metals (As^{3+}, Hg^{2+}, Cd^{2+}, and Pb^{2+}) from water. A unique, low-cost, and locally accessible adsorbent with great adsorption capacity comprising exfoliated organofunctionalized bentonite clay from Qazvin, Iran, was synthesized. To increase the adsorption productivity of acid activated bentonite (AB), clay was exfoliated (EAB) and then immobilized in toluene with addition of MPTMS as a modifier (MEAB). The MEAB greatly increased removal of 4 target ions. This research confirmed that MEAB shows identical or even better adsorption capacities compared to other conventional adsorbents and that the binding capacity of heavy metal ions is about four times higher compared to unfunctionalized samples [3]. As a consequence, this new functionalized exfoliated bentonite may be a good alternative to economical adsorbents for the removal of toxic and perilous heavy metals.

References:

[1] S.K. Yadanaparthi, D. Graybill, R.V. Wandruszka, J. Hazard. Mater, 171 (2009) 1–15.
[2] A. Chen, X. Xin, J. Xu, Y. Bian, Desal. Water Treat, 77 (2017) 342–348.

[3] Z. Xia, L. Baird,N. Zimmerman, M. Yeager . Appl. Surf. Sci, 416 (2017) 565–573.

Synthesis and characterization of inorganic nanostructures for application in provskite solar cells

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Abstract:

Nowadays, there is no doubt about harmful effect of fossil fuels(coal, oil, gas) on environment and public health. These harmful consequences include the danger to plants, animals and human being .Many people each year lose their life due to the air pollution[1]. To solve these issues renewable energies such as wind, solar, biomass, geothermal, hydroelectric energy and other forms have become the subject of extensive studies. One of the most important types of renewable energy is solar. In order to use solar energy solar photovoltaics, the device that convert the energy of sunlight into electricity by photovoltaic effect, are used[2]. Solar cells have different catagories such as silicons, thin films, nanostructure and so on. Perovskite solar cells are new generation the kind. These solar cells have demonstrated power convention efficiency of more than 22%[3-4]. In this article, synthesis and characterization of inorganic nanostructure for increasing power convention efficiency is studied. Orthorhombic structure of rare earth perovskite type oxide $LaFeO_3$ nanoparticles with light absorption properties in visible range was synthesized. The prepared nanoparticles was characterized by several measurements such as X-ray diffraction. This inorganic perovskite is used to fabricate perovskite solar cell devices.

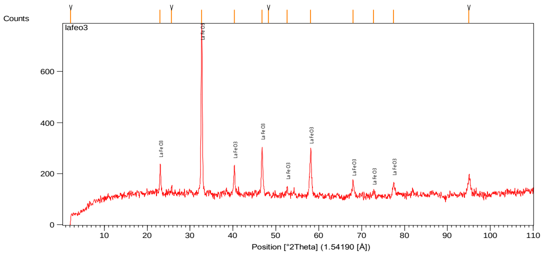

Fig.1 The XRD pattern of $LaFeO_3$

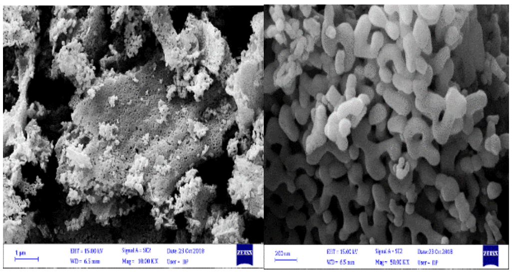

Fig.2 The SEM image of $LaFeO_3$

References:

[1] O. Jamal, W.A. Jabera, A.B.Taieseer, A.A. Alawina, S.Al-Lubania, A.Al-Bashirb, Renewable and 500 Sustainable Energy Reviews 73 (2017) 452–459.
[2] A. Lind, E. Rosenberg, P. Seljom, K. Espegren, A. Fidje, K. Lindberg, Energy Policy 60 (2013) 364-377.
[3] M.Saliba, J.P.Correa-Baena, M.Graetzel, A.Hagfeldt, and A.Abate, Angew. Chem. Int. Ed (2017)
[4] L.Tzounis, T.Stergiopoulos, A.Zachariadis, C.Gravalidis, A.Laskarakis, and S.Logothetidis, Mater. Today 4 (2017) 5082–5089.

Synthesis and spectroscopic studies and Naked-eye detection of hydrogen carbonate ions in aqueous media based on an azo-azomethine chemosensor

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Abstract:

Azo compounds are an interesting class of organic compounds which have found wide application in the field of chemicals sciences. Dyes are also found in food, pharmaceutical, paints, polymers, and standard materials used in adsorption chromatography [1]. They are increasingly used in textile, leather and plastic industries [2]. Anions play an essential role in the field of biology, industry and environmental science. [3]. Colorimetric chemosensors are attractive due to enhanced selectivity, sensitivity, low cost, convenient operation and fast detection character [4]. bicarbonate is, as the dominant buffering system in the human body. And has been celebrated for years as a multi-use household item and additive in food and dental products [5].

In this work, we have synthesized a new optical and colorimetric properties of chemosensor 4-((E)-(2,5-dichlorophenyl)diazenyl)-2-((E)-((4 hydroxyphenyl)imino) methyl)phenol (L) for hydrogen carbonate ions by the naked–eye detection and UV–vis spectroscopy. This ligand reveals visual changes toward HCO_3^- anions in aqueous media. No considerable color changes were observed against the addition of any other anions. The sensitivity and selectivity of receptor to bicarbonate anion were specified with UV-vis spectroscopy and ^1H NMR titration methods. The detection limit of the receptor towards HCO_3^- have 2.17×10^{-7} mol L^{-1}. Therefore this chemosensor is sensitive to detect bicarbonate anion in aqueous solutions. Stability constants of these complexes were determined by Benesi–Hildebrand plot technique. Stoichiometry of the complexes was determined as (Ligand/anion) 1:1 with Job's plot technique. The designed chemosensor may be applied for the quick detection of hydrogen carbonate anions in the basic pH range.

References:

[1] G.R. Ferreira, L.F.C. de Oliveira, J. Molecular. Structure. 1146 (2017) 50-56.
[2] M. Sarigul, S. E. Kariper, P. Deveci, H. Atabey, D. Karakas, M. Kurtoglu, J. Molecular. Structure. 1149 (2017) 520-529.
[3] Z. Li, S. Wang, P. Deveci, L. Xiao, X. Li, X. Jing, X. Peng, L. Ren, Inorg. Chim. Acta. 479 (2018) 147-153.
[4] E. Normaya, M. Fazli, M. Norazmi Ahmad, K. H. K. Bulat, J. Molecular. Structure. 1184 (2019) 538-545.
[5] M. A. Farha, S. French, J. M. Stokes, E. D. Brown, ACS Infect. Dis. 4 (2018) 382-390.

Study on structural, morphology, optical and photocatalytic activity of a novel mesoporous $ZrFe_2O_4@SiO_2$ core-shell nanocomposite modified with APTES and TCPP

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Abstract:

In this study, the mesoporous $ZrFe_2O_4$ with nanocauliflowers structure was first synthesized via solvothermal method [1,2]. Then the core-shell composite of $ZrFe_2O_4@SiO_2$ was successfully prepared by a simple wet route using tetraethyl orthosilicate (TEOS) as precursor of silica [3]. Furthermore, the core-shells were modified with tetrakis (4-carboxyphenyl) porphyrin (TCPP) for improving the photocatalytic activity [4] and 3-aminopropyltriethoxysilane (APTES) was used as the linker which TCPP could be easily grafted to it [5]. The samples characterizations were performed by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), nitrogen adsorption and desorption isotherms (BET), vibrating sample magnetometer (VSM), diffuse reflectance spectroscopy (DRS).

The photocatalytic activity of $ZrFe_2O_4@SiO_2$-NH_2-TCPP on the degradation of methyl orange (MO) was shown the excellent catalytic activity in comparison of nanocomposite without linker. The higher surface area is beneficial to raise the number of active sites for degrade methyl orange.

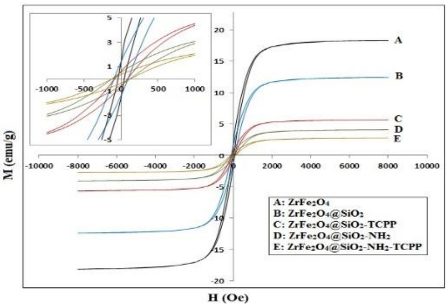

Fig.1. the magnetic properties of the nano magnetic particles reduced due to the presence of APTES and TCPP.

References:

[1] A. Gangwar et al., Journal of Magnetism and Magnetic Materials 401 (2016) 559-566.

[2] M. Sorescu, T. Xu, A. Wise, M. Díaz-Michelena, M. E. McHenry, Journal of Magnetism and Magnetic Materials 324 (2012) 1453-1462.

[3] M. Abbas, S. Torati, C. Lee, C. Rinaldi, C. Kim, J Nanomed Nanotechnol 5 (2014) 1-8.

[4] M. Rabbani, F. Rafiee, H. Ghafuri, R. Rahimi, Materials Letters 166 (2016) 247-250.

[5] F. Liu, F. Niu, Y. Su, Y. Yang, RSC Advances 5 (2015) 18128-18136 .

[6] P. Kharazi, R. Rahimi, and M. Rabbani, Materials Research Bulletin 103 (2018) 133-141.

Comparison of Photocatalytic efficiency of Magnetic and non-magnetic Ceria -Cs salt of Polyoxometalate Nanocomposites

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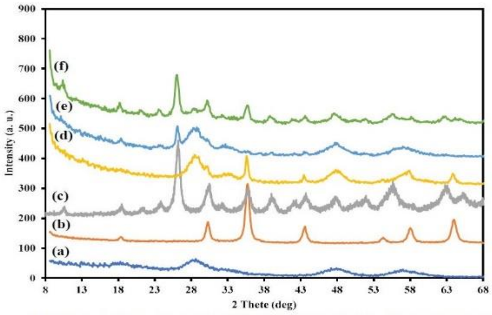
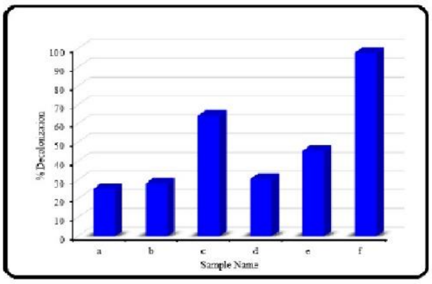
Abstract:

Now a day, effluent of dyes recommends a challenge for environmental safety and daily operations of the industry [1]. There are many methods to remove the effects of pollutants which are included absorption techniques, reverse osmosis, electrochemical and photocatalytic [1]. Over the past decade, Metal oxides have wide range of applications in catalysis, environmental science and material science [2]. Ceria (CeO_2) is one of the most significant rare earth metal oxide that has different applications in some fields [3]. Polyoxometalates are a kind of metal clusters, because of their various structures and unique properties. Newly, one of the most significant current discussions are easier separating and recycling of catalysts. Hence, the magnetic nanoparticles (NPs) have been attracting a lot of attention in chemical process (e.g., catalysis, photocatalysis, energy storage and etc.) [4]. Therefore, these NPs can play an important role for recycling and separating of magnetized catalysts by an external magnetic field. The aim of this research are comparison of magnetic and non- magnetic ceria/ Cs- salt of Polyoxometalate composites in order to investigation the efficiency of as-synthesis toward improving photocatalytic activities. The prepared magnetic ceria/ Cs- salt of Polyoxometalate composites displayed significantly enhanced photocatalytic activity toward CR degradation under 210 min visible light irradiation than others.



The PXRD pattern for (a) CeO_2, (b) Fe_3O_4, (c) Cs-$PW_{12}O_{40}$, (d) Fe_3O_4@CeO_2,(e) CeO_2/Cs- $W_6Mo_6O_{40}$ (f) Fe_3O_4@CeO_2/Cs-P $W_6Mo_6O_{40}$



The percentage of decolorization of a) CeO_2/Cs-$PMo_{12}O_{40}$, b) CeO2/Cs-$PW_{12}O_{40}$, c) CeO/Cs-$PMo_6W_6O_{40}$, d) Fe_3O_4@CeO_2 /Cs-$PMo_{12}O_{40}$, e) Fe_3O_4@CeO_2/Cs-$PW_{12}O_{40}$ and f) Fe_3O_4@ CeO_2/Cs-$PMo_6W_6O_{40}$

References:

[1] J.G. Huang, S.S. Chu, J.J. Chen, Y. Chen, Z.M. XieBioresour. Technol. 161 (2014) 465-468.
[2] M. A. Rauf, M.A. Meetani, A. Khaleel and A. Ahmed. Eng. Chem. J. 157 (2010) 373–378.
[3] C. T. Campbell, C. H. F. Peden, Science. 309 (2005) 713−714.
[4] A. Trovarelli, Catalysis Reviews—Science and Engineering. 38 (1996) 439–520.
[5] D. Wang, D. Astruc, Chem. Rev. 114 (2014) 6949–6985.Z

Synthesis and Characterization of a Zn (II) Schiff base Complex

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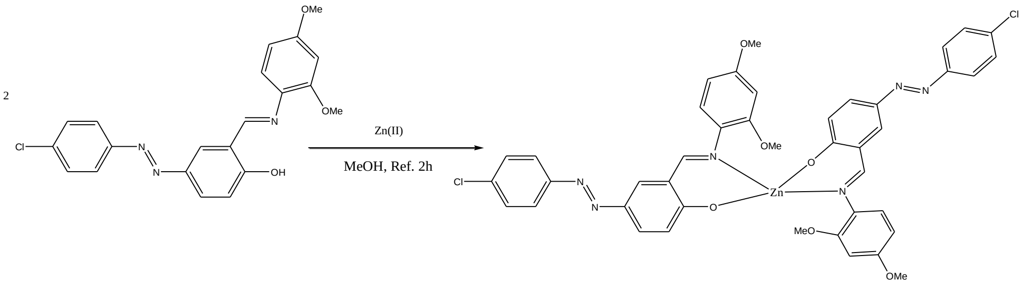
Abstract:

Schiff base ligands have been considered as important compounds in the development of coordination chemistry [1]. The transition metal complex exists in a wide range of metalloenzymes that catalyze diverse metabolic reactions in bacteria, fungi, algae, plants and animals [2].

In this study, we synthesized and characterization of a Zn(II) Schiff base complex (Scheme 1) by the reaction of a Zn(II) ions with a bidentate Schiff base ligand Cl (C H_4)N2(C_6H_3(OH)(CH=N-$C_6H_3(OCH_3)_2$ (**HL**) in MeOH as a solvent. The ML_2 Schiff base complex was characterized by by FT-IR, UV–Vis, ^{1}HNMR, ^{13}C NMR and elemental analysis.



Scheme 1. The structure of Schiff base ligand and its Zn(II) complex

References:

[1] M.Shakir, M.Azam, Y.Azim, S.Parveen, A.U.Khan, J. Polyhedron, 26 (2007) 5513.

[2] M.R.Pedrosa, J.Escribano, R.Aguado, R.Sanz, F.Arnaize, J. Polyhedron 29 (2010) 841.

The effects of various activation methods on UiO-66 Metal–Organic Framework.

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Abstract:

UiO-66 is a high important prototypical zirconium-based metal–organic framework (MOF) compound because of its excellent stabilities not typically found in common porous MOFs. In the crystal structure, each Zr metal center is fully coordinated by 12 organic linkers to form a highly connected framework [1]. In this work showed that by changing the Synthesis methods and the synthesis time, the linker vacancies can be modified systematically, leading to dramatically enhanced porosity. The results showed a porous metal–organic framework based on benzene 1,4-dicarboxylic acid ligand that its specifications are dependent on different activation methods [2]. A key aspect to the realization of high porosity is the removal of guest molecules from the framework while still maintaining its structural integrity ("activation"). The highlights utilized strategies for activating MOFs are: (i) conventional heating and vacuum; (ii) solvent-exchange; (iii) supercritical CO_2 ($scCO_2$) exchange; (iv) freeze-drying; and (v) chemical treatment [3]. The surface area of prepared sample via conventional heating and vacuum method increased from 50 m^2/g to 570 m^2/g, via the solvent-exchange method increased from 570 m^2/g to 870 m^2/g and via the freeze-drying method increased from 870 m^2/g to 1200 m^2/g.

References:

[1] H.Wu, Y.S.Chua, V.Krungleviciute, M.Tyagi, P.Chen, T.Yildirim, W.Zhou, Journal of the American Chemical Society, 135(28) (2013) 10525-10532.

[2] Y.P.He, Y.X.Tan, J.Zhang, Inorganic chemistry, 51(21) (2012) 11232-11234.

[3] J.E.Mondloch, O.Karagiaridi, O.K.Farha, J.T.Hupp, CrystEngComm, 15(45) (2013) 9258-9264.

Antibacterial activity investigation of CuBDC loaded silk fibers

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Abstract:

Metal-organic frameworks (MOFs) are porous, hybrid materials comprising metal ions linked by organic binding ligands. Infinitely extended metal–ligand networks with metal nodes and bridging organic ligands are called coordination polymers or metal–organic frameworks (MOFs). MOFs consist of metal atoms or metal clusters as nodes, which are linked through organic ligands (linkers)[1]. Since in the last years the antibiotic therapy has become a public health problem[2], we decided to work on a nanostructure which relates to this matter. Antimicrobial agents are capable of destroying pathogenic microorganisms and are used to sterilize water and preserve food, as well as in the form of drugs[3]. Metal-organic frameworks could be a good option because of the diversity of their applications which antibacterial property is one of them[1]. This work is concentrated on the antibacterial property of CuBDC MOF. A good substrate for CuBDC is silk fibers. First silk fibers were activated in NaOH. In a separate experiment 1, 4-benzenedicarboxylic acid (BDC) and $CuNO_3$ were solved in DMF and silk fibers were immersed in resulting solution with reflux condition. After 24 hours the CuBDC loaded silk fibers with blue color were separated and washed with DMF. Then the fabric sample was dried at room temperature. Different analysis such as IR, XRD and SEM confirmed the formation of CuBDC on the silk fibers. Finally antibacterial activity of fabric sample was investigated against Escherichia coli (Gram-negative bacterium) and Staphylococcus aureus (Gram-positive bacterium).

References:

[1] C.Janiak, J.K. Vieth,. New Journal of Chemistry, 34(11) (2010) 2366-2388.
[2] G.Wyszogrodzka, et al, Drug Discovery Today, 21(6) (2016) 1009-1018.
[3] R.K.Alavijeh, et al, Polyhedron, 156 (2018) 257-278.

Synthesis and characterization of Pt(Ⅱ)-Ag(Ⅰ) clusters containing $(PPh)_2Py$ ligands

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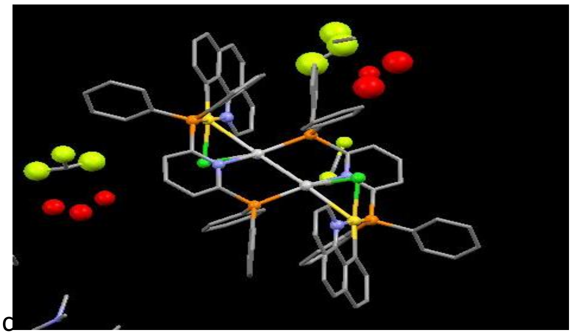
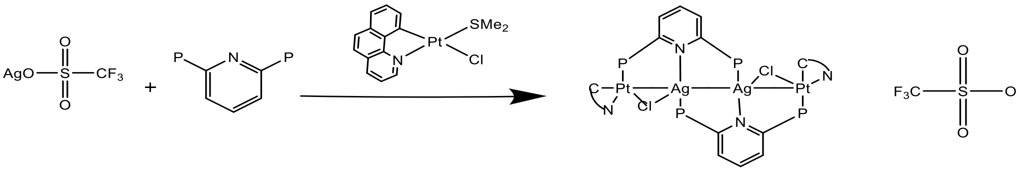
Abstract:

Metal clusters occupy a prominent position in chemistry. In addition to the interest arising from the potential utility of metal clusters in catalysis and the preparation of new materials, there has also been significant interest in exploiting the remarkable structural and bonding properties of these compounds. Metal-metal dative bonds play an important role in the synthesis of metal clusters, and electron-rich Platinum(II) complexes can expand opportunities for the formation of metal-metal dative bonds [1].

In this work, the tetranuclear Pt(Ⅱ)-Ag(Ⅰ) cluster $\{Pt_2Ag_2[(\mu\text{-}PPh)_2Py](\mu\text{-}Cl)_2(bhq)_2\}(OTf)_2$ has been prepared by reaction of AgOTf , 2,6-(bisdiphenylphosphino)prydine and $Pt[(bhq)(SMe_2)Cl]$ in 1:1:1 molar ratio. The structure of the cluster is determined using ^{31}PNMR and ^{1}HNMR spectroscopy and its crystal structure was further determined by X-ray crystallography [Fig1.]. This cluster shows yellow emission in solid state.





Scheme 1.

References:

[1] S.Jamali, Z.Mazloomi, Nabavizadeh. Inorg. Chem. 49 (2010) 2721–2726.

Preparation of Metal-Organic framework Nano Composite made from functionalized HKUST-1 and Magnetic Nanoparticles as an adsorbent of Cadmium heavy metal from aqueous solution.

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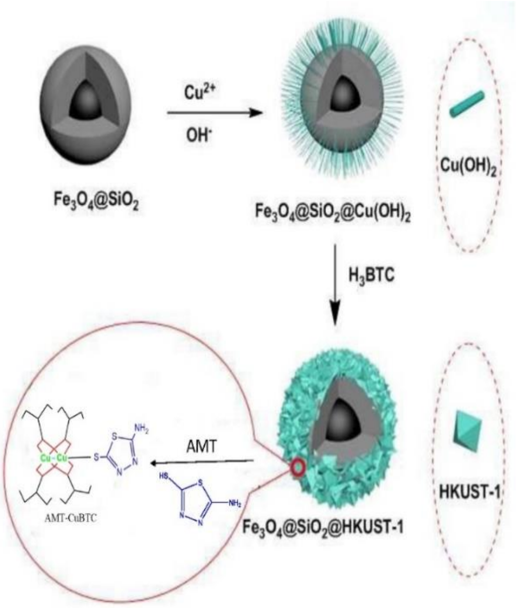
Abstract:

A Metal-Organic Framework, Fe_3O_4@SiO_2@CuBTC@AMT synthesized by post synthesis modification of CuBTC by solvothermal method [1]. CuBTC, a nano-intrusive framework with an unsaturated Cu^{2+} center that can be chemically modified, forms around nano-magnetite. In this work, covalent post-synthesis modification was performed by adding 2-amino-5-mercapto-1,3,4-tiatidiazole to CuBTC frameworks [2]. In the presence of Fe_3O_4@SiO_2@CuBTC@AMT adsorbent at pH =7 and 60 minutes, the adsorption and selectivity percentage of cadmium metal was achieved 55.6 % and 95.66%, respectively.



Scheme.1 Preparation of Fe_3O_4@SiO_2@CuBTC@AMT

References:

[1] K. Schlichte, T. Kratzke, S. Kasei, Microporous Mesoporous Mater., 73 (2004) 81.
[2] L. Huamg, M. B. Chen, B. Hu, Mater. Chem. A., (2013) 00, 1.

Solvent polarity influence on NMR parameters a $(OC)_4$Cr-biscarbene complex: A Computational investigation

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Abstract:

In this study, using the MPW1PW91 method, quantum chemical calculations were used to analyze the solvent effect on NMR parameters of a $(OC)_4$Cr-biscarbene complex at the ground state (S_0) and first singlet excited state (S_1). Using the self-consistent reaction field theory (SCRF) based on the Polarizable Continuum Model (PCM), the solvent effects were examined. Selected solvents are dichloromethane, tetrahydrofuran, cyclohexanone, propanonitrile, and acetonitrile. The ^{13}C NMR chemical shifts of the complex were calculated for both gas and solution phases. One-bond nuclear spin-spin coupling constants of Cr-CO and $Cr\text{-}C_{Carbene}$ bonds were estimated [1-3]. The correlations of these parameters and solvent polarity functions including both the dielectric constant (ε) and refractive index (n_D) of the liquid medium were explored further. In addition, the most significant Ramsey terms involved significantly in ^{1}J(Cr-CO) and $^1J(Cr\text{-}C_{Carbene})$ values were determined [4-6]. Finally, the correlations between ^{1}J(Cr-CO) and $^1J(Cr\text{-}C_{Carbene})$ and Cr-CO and $Cr\text{-}C_{Carbene}$ bond distances were studied [7].

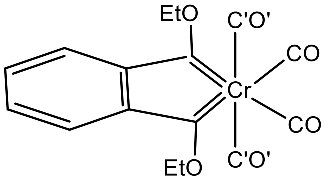

Fig.1 $(OC)_4$Cr-biscarbene complex

References:

[1]. M. A. Sierra, Chem. Rev., 100 (2000) 3591.
[2]. D. I. Bezuidenhout,S. Lotz,D. C. Liles,B. v. d. Westhuizen, Coordination Chemistry Reviews, 256 (2012) 479.
[3]. E. O. Fischer,W. Roll,U. Schubert,K. Ackermann, Angew. Chem. Int. Ed. Engl., 20 (1981) 611.
[4]. E. O. Fischer,W. Roll,N. H. T. Huy,K. Ackermann, Chem. Ber. , 115 (1982) 2951.
[5]. U. Schubert,K. Ackermann,N. H. T. Huy,W. Roll, J. Organomet. Chem., 232 (1982) 155.
[6]. J. B. Foresman,M. Head-Gordon,J. A. Pople,M. J. Frisch, J. Phys. Chem., 96 (1992) 135.
[7]. R. J. Bartlett,G. D. Purvis, Int. J. Quantum Chem., 14 (1978) 561.

Novel carrier for delivery of drug and simultaneous fluorescence imaging

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Abstract:

Drug delivery systems are one of the most promising applications for human health care and represent an ever-evolving field for biomedical materials science [1]. In the area of drug delivery, looking for appropriate non-toxic carriers which is efficient for drugs delivery to the body is a crucial challenge [2].

NMOFs possess some unique properties that enable them to perform as promising nanoplatforms for drug delivery and bioimaging. Firstly, NMOFs are compositionally and structurally diverse, allowing the facile synthesis of NMOFs with different compositions, shapes, sizes, and chemical properties. Secondly, NMOFs are biodegradable due to the presence of relatively labile metal ligand bonds; this feature makes it possible to rapidly degrade the composite material and release the loaded drug or probe [3].

In summary, our experimental procedure involves the following steps: the hydrothermal method used to the synthesis of NMOF and the solvothermal method employed for the synthesis of N-CNDs. Then, hybrid nanocomposite (NMOF@N-CNDs) produced by the incorporation of the N-CNDs into NMOF. Afterwards, drug loaded into nanocomposite. So, this drug delivery vehicle can employ for simultaneous drug release and cell fluorescence imaging. Fluorescence imaging showed in Figure 1.

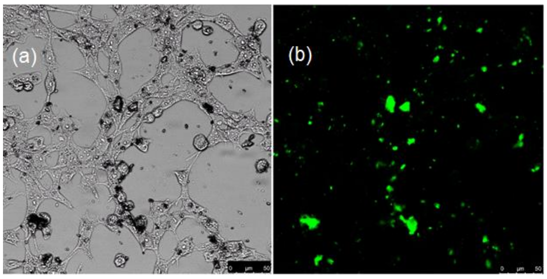

Fig.1. Fluorescence imaging: CLSM images of A549 cells incubated with drug loaded UiO-66-NH_2@N-CNDs for 24 h. (a) The differential interference contrast (DIC) image. (b) The green fluorescence showing internalized drug loaded UiO-66-NH_2@N-CNDs.

References:

[1] VP.Torchilin, Nat Rev Drug Discov, 4 (2005) 145-60.
[2] ME.Davis, Z.Chen, DM.Shin, Nat Rev Drug Discov, 7 (2008) 771-82
[3] S.Keskin and S.Kızılel, Ind Eng Chem Res, 50(4) (2011) 1799-1812.

CTAB cation surfactant affection on distribution metal particles on KIT-6 silica support with mesopores in methanol steam reforming process

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Abstract:

Hydrogen as a source of clean energy is a proper substitude for fossil fuel because of high potential energy among different processes of hydrogen production, steam reforming (SR) the feeds like Alcohols, Ethers and some hydrocarbons are very useful and efficient.[1]

In this research KIT-6 pores silica has synthesized successfully with mesopores as a catalitic support in the hydrothermal method, then certain amount of copper and cerium are placed on support by CTAB cation surfactant-assisted impregnation methods. Catalysts catalitic activity in methanol steam reforming in different temperatures 275, 300, 325 °C , 1 atmosphere pressure , mole ratio water to methanol 2/1 was done in a fixed-bed reactor.

The CeO_2-Cu/KIT-6 synthesized catalyst with surfactant-assisted impregnation methods was done more effectively. At 300 °C temperature in a way that %92 methanol conversion and selectivity H_2 and CO receptively%99 and 0.9.

In order to determination of structural and surface characteristics of synthesized catalysts different methods were used such as XRD, BET and FE-SEM.[2]

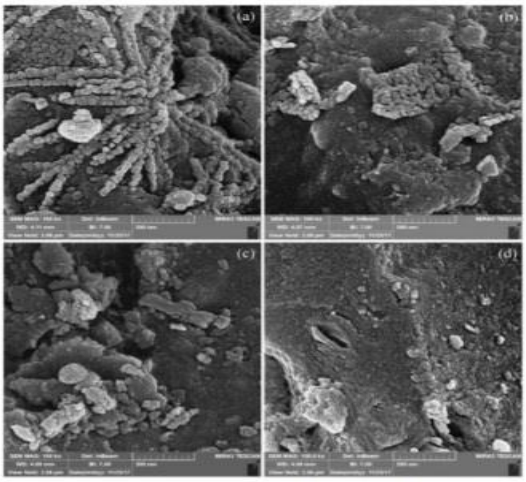

Fig. 4 – FESEM images of KIT-6 (a), Cu/KIT-6 (b), Ce–Cu/KIT-6 (c), Ce–Cu/KIT-6(CT) (d).

References:

[1] H.Ji, J.Lee, E.choi, and L.seo, International Journal of Hydrogen Energy, 43 (2018) 3655-3663.

[2] T.Majid, A.Hossein, R.Armin, S.Mobina, International Journal of Hydrogen Energy, 4 (2018) 10926-10937.

Cation-exchanged nano-zeolite 13X for water vapor adsorption from air

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Abstract:

Around 13 sextillions (10^{21}) liters of water exist in the atmosphere which is considered as a recyclable natural source to resolve the water crisis in dry areas of the world [1]. Because of their certain average pore diameters, zeolites adsorb water molecules in preference to other gases while restricting larger molecules. Moreover, exchangeable compensation cations such as Li^+, K^+, Ba^{2+}, Mg^{2+}, and Ca^{2+} can be added to the zeolite structure which is expected each one shows a great attraction to link with water molecules [2]. This study concerns the synthesis of nano-zeolite 13X and its modification by a hygroscopic salt (magnesium chloride) to investigate its water vapor adsorption capacity. At first, nano-zeolite 13X with gel formula of 5.5 Na_2O:1.0 Al_2O_3:4.0 SiO_2:190 H_2O was synthesized by microwave heating of precursors as sodium aluminate, sodium silicate, NaOH and distilled water at 90 °C for several hours. The final white product was characterized using techniques as XRD, FT-IR, SEM, and EDX. Then, 2g of nano-zeolite was shaken with different solutions of magnesium chloride (10 to 50 wt%) for 24 hours and calcined at 300 °C for 2 hours. A set-up was designed to measure the adsorbed content of water by the adsorbent. Airstreams with different initial humidity passed through a column containing adsorbent and the measurement of input and output humidity was continued until saturation happened. According to the obtained data of the adsorption diagram, with 14.6 g/m^3 absolute humidity, this adsorbent could adsorb 131% water of its own weight in one minute.

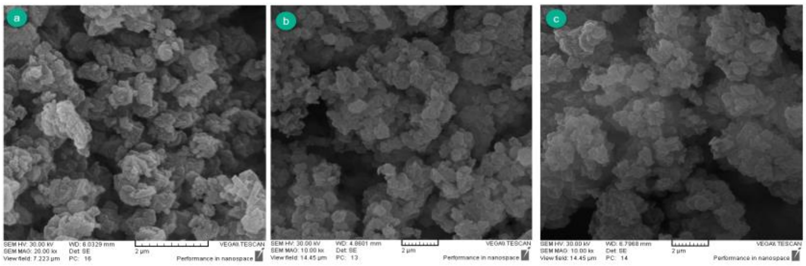

Fig.1. SEM images of **a)** nano-zeolite 13X **b)** composite of nano-zeolite 13X and $MgCl_2$(10%) **c)** composite of nano-zeolite 13X and $MgCl_2$(50%)

References:

[1] F. Fathieh, M. Kalmutzki, E. Kapustin, P. Waller, J. Yang, Practical water production from desert air, Sci. Adv. 4(6) (2018).

[2] Y. Yuan, H. Zhang, F. Yang, N. Zhang, X. Cao, Inorganic composite sorbents for water vapor sorption: A research progress, Renew. Sust. Energ. Rev. 54 (2016) 761-776.

Microwave-assisted water harvesting by composite adsorbent of zeolite 13X and activated carbon

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Abstract:

Water scarcity is a critical challenge in dry and desert climates while a plentiful quantity of water is present in the form of vapor in the air. So, water harvesting from air has attracted great attention in recent years. Essential concern of many studies is focused on sorption technique due to being a high-yield, low-energy-consuming, and eco-friendly technology [1]. Zeolite 13X is one of the most traditional adsorbents showing high water adsorption capacity because of its hydrophilic nature and large surface area. To promote zeolite features, many attempts have been made via modification. In this research, a composite of microporous zeolite 13X and activated carbon was provided, then adsorption and desorption of water vapor from air humidity were investigated through conventional and microwave heating methods. Zeolite was synthesized via hydrothermal reaction of appropriate aluminosilicate hydrogel. For the synthesis of composite adsorbent, a particular amount of activated carbon was added to the zeolitic hydrogel at room temperature. The obtained gel stirred for 24 hours and subsequently transferred to an autoclave at 95°C for 20 hours. The product was characterized using techniques as XRD, SEM, FT-IR, and EDX. A set-up was designed to measure the amount of water adsorbed by the sorbents. Airstreams with different initial humidity passed through a column containing adsorbent and the measurement of input and output humidity was continued until saturation occurred. According to the obtained data from adsorption diagram, with 15 (g/m^3) absolute humidity, the adsorbent could adsorb 144% water of its own weight in five minutes.

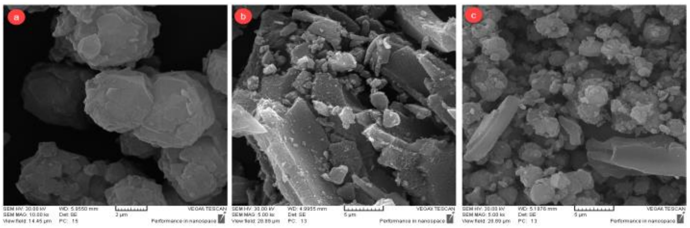

Fig.1 SEM images of **a)** micro-zeolite 13X **b)** raw activated carbon **c)** composite of micro-zeolite 13X and activated carbon

References:

[1] Y. Yuan, H. Zhang, F. Yang, N. Zhang, X. Cao, Inorganic composite sorbents for water vapor sorption: A research progress. Renew. Sust. Energ. Rev. 54 (2016) 761-776.

[2] J. Kim, C. Lee, W. Kim, J. Lee, J. Kim, J. Suh, Adsorption equilibria of water vapor on alumina, zeolite 13X, and a zeolite X/activated carbon composite. J. Chem. Eng. Data. 48 (1) (2003) 137–141.

Synthesis, Characterization and Antibacterial Activity Study of MOF-5 and MOF-2

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Abstract:

Metal-Organic Frameworks (MOFs) are known as porous coordination polymers (PCPs) which are compounds constructed from the self-assembly of metal ions or metal clusters and organic linkers [1]. Their high porosity, large surface area and tunable shape are some of the attractive properties of MOFs [2]. MOFs have three-dimensional lattices that can form a web-like structure around microbes, therefore making them effective from all angles. Because of these features, MOFs have the potential for investigation as antibacterial agents [3].

Zn_4O (BDC) $_{3)}$ $_{MOF}$-5) and $[Zn_2(BDC)_2(H_2O)_2(DMF)_2]_n$ (MOF-2) are two MOFs with same reagents but different formulas and structures. The structure of MOF-5 is derived from a simple cubic six-connected net in two stages: the nodes (vertices) of the net are replaced by clusters of secondary building units; second, the links (edges) of the net are replaced by finite rods (`struts') of BDC molecules. The core of the cluster consists of a single O atom bonded to four Zn atoms, forming a regular Zn_4O tetrahedron. Each edge of each Zn tetrahedron is then capped by a CO2 group to form a $Zn_4(O)(CO_2)_6$ cluster [4]. MOF-2 is a 2D (4,4) layered framework consisting of paddle-wheel $Zn_2(COO)_4$ SBUs which are bridged by BDC^{2-} linkers [5]. It is interesting to study antibacterial activity of these two MOFs and compare their antibacterial activities based on their structures. Thus, these two MOFs were synthesized by same method but different ratio of reagants. Then their structures were characterized by FT-IR, PXRD, TG-DTA and SEM analysis. Finally antibacterial activity of them was studied and compared against gram-positive (Staphylococcus aureus) and gram- negative (Escherichia coli) bacterias.

References:

[1] V. Bagchi, D. Bandyopadhyay, J. Organomet. Chem. 694 (2009) 1259-1262.
[2] S. A. A. Razavi, M. Y. Masoomi, T. Islamoglu, A. Morsali, Y. Xu, J. T. Hupp, O. K. Farha, J. Wang, P. C. Junk, , Inorg. Chem., 56 (2017) 2581–2588.
[3] R.K. Alavijeh, S. Beheshti, K. Akhbari, A. Morsali, Polyhedron, 156 (2018) 257-278.
[4] Hailian Li, Mohamed Eddaoudi, M. O'Keeffe, O. M. Yaghi, Nature,402 (1999) 276–279.
[5] Z. Chen, S.Xiang, D.Zhao,B.Chen, , Cryst.GrowthDes. 9 (2009) 5293–5296.

Selective hydrogenation of phenol to cyclohexanone by palladium on alumina/lanthanide oxides

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Abstract:

The industrial production of cylcohexanone commonly involves the oxidation of cyclohexane or the hydrogenation of phenol. For industrial processes using a simple, clean, and low price method is critical. In this work, we leverage high selectivity, environmental friendliness, and lower energy consumption of palladium supported on mixture of alumina and lanthanide oxides (such as Lanthanum, Cerium, Europium, Terbium and Holmium) with different mole ratios and employed them for one stage hydrogenation of phenol to Cyclohexanone under mild conditions (80°C and 3 bars H_2) [1]. Under experimental conditions in this paper, by using Gas Chromatography, 99.8% conversion of phenol with 96.3% selectivity to cyclohexanone was obtained with Pd supported on alumina/lanthanum oxide/cerium oxide with mole ratio of 9:1:1 at 80°C and 3 bar H2 pressure [2]. For characterization of prepared catalysts scanning electron microscopy (SEM), X-ray diffraction (XRD), and volumetric isothermal nitrogen gas adsorption-desorption method (BET) were used.

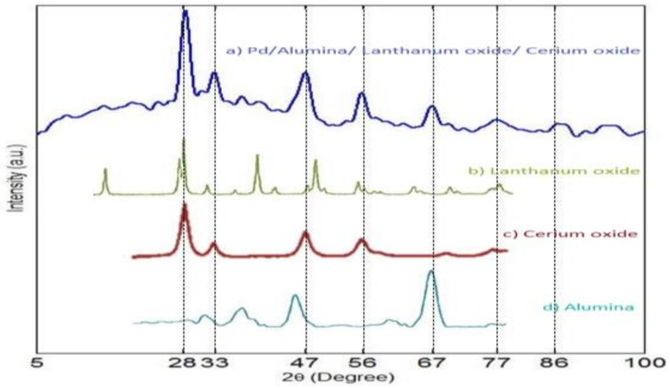

Fig.1. XRD pattern of Pd/Alumina/ Lanthanum oxide/ Cerium oxide (a), reference of Lanthanum oxide (b), Cerium oxide (c), and Alumina (d)

References:

[1] Xiang, Yi-zhi, et al, Reaction Kinetics, Mechanisms and Catalysis 100, no. 1 (2010) 227-235.
[2] G.Neri, et al. Applied Catalysis A: General 110, no. 1 (1994) 49-59.

Synthesis and characterization of a new Ruthenium complex based on various supports; investigation of electrocatalytic properties of prepared complex and nanocomposites in reduction of CO_2 to CO

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Abstract:
The current energy supply of human society is mainly based on fossil fuels like coal, oil and gas which are related to several problems. The reserves are decreasing and their final depletion seems to be just a matter of time. In addition, the combustion of fossil fuels leads to the emission of CO_2, which is considered as a main source for global warming caused by the greenhouse effect [1]. The demand for energy is steadily increasing. Renewable energy appears to be the only sustainable solution. However, since the availability from renewable sources such as wind and solar energy are variable and often do not meet with the time and local needs, efficient energy storage and transport are also critical issues. Therefore recycling of carbon dioxide by catalytic conversion to gaseous or liquid fuels using renewable energy has received increasing interest in the past years [2].

Up to now, mainly ruthenium-based systems have been reported for their ability to electrochemically or photochemically accelerate the reduction of CO_2 to CO. Carbon monoxide itself can be used as a precursor compound for fuel synthesis processes, where CO and H_2 are mixed as syn-gas to form hydrocarbons such as methane or methanol by fischer- tropsch process[1,2].

Here, we report the synthesis and structural characterization of a new mononuclear polypyridyl Ru(II) complex, $[Ru(tptz)(ACN)Cl_2]$ (where tptz = 2,4,6-tris(2-pyridyl)-1,3,5-triazine and ACN = Acetonitrile). The electrocatalytic reduction of CO_2 to CO by the complex was investigated using cyclic voltammetry (CV) in CH_3CN solution. Ruthenium complex/various supports nanocomposites prepared and the effect of support on the electrocatalytic performance of prepared nanocomposite investigated. The electrocatalytic activity of products investigated by circle voltammetry. We utilized density functional theory (DFT) to investigate a potential pathway and reaction mechanism of CO_2 reduction in a catalytic cycle.

References:

[1] X. Yun Wang, S. Qin Liu, K. Long Huang, Q. Ju Feng, D. Lai Ye, B. Liu, J. Long Liu, G. Hua Jin, Chin. Chem. Lett. 21 (2010) 987..

[2] L. Tong, Y. Wang, L. Duan, Y. Xu, X. Cheng, A. Fischer, M.S.G. Ahlquist, L. Sun. Inorg. Chem. 51 (2012) 3388.

Synthesis and characterization of N_6 macroacyclic Schiff-base ligand contaning piperazine moiety and its Mn (II) complex

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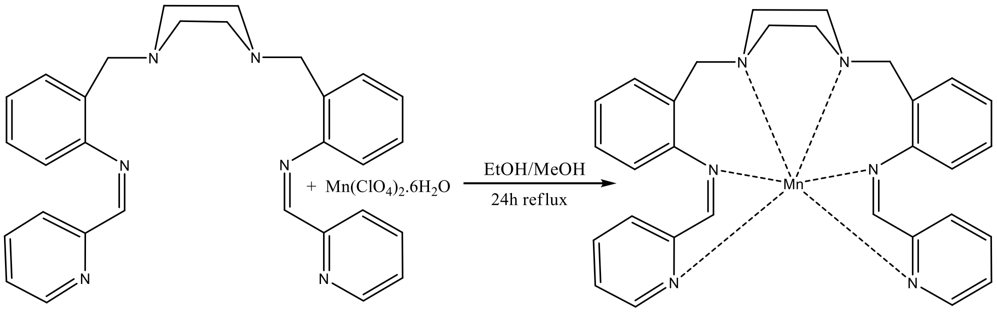
In this report we have synthesized one macroacyclic Schiff-base ligand L with the N_6 donor system from condensation of 2-formylpyridine and 2,2'-(piperazine-1,4-diylbis(methylene))dianiline (A). IR spectrum of ligand exhibited a υ(C=N) vibration in 1634 cm^{-1}. The elemental analysis, ^1H and ^{13}C NMR and the presence of a peak at 474 m/z in the mass spectrum of ligand (L) confirm the synthesis of ligand. The Mn (II) complex was synthesized by direct reaction of manganese (II) metal ion and ligand L. In the IR spectrum, υ(C=N) of the complex appears in the 1617 cm^{-1}, and also in mass spectrum of complex the presence of peak at 728 m/z confirms the synthesis of complex. The elemental analysis confirms the synthesis of complex [1-2].



Scheme.1 Synthesis of macroacyclic Schiff-base ligand /Mn (II) complex

Reference:

[1] M. Rezaeivala, H. Keypour, Coord. Chem. Rev. 280 (2014) 203.

[2] H. Keypour, M. Mahmoudabadi, A. Shooshtari, M. Bayat, M. R. Karamian, M. Asadbegy, R. William Gable, Inorg. Chim. Acta, 478 (2018)176.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
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H_2 uptake ability of ($Li_2C_8H_6$) dilithium pentalenide

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Abstract:
The hydrogen uptake ability of dilithium pentalenide (DLP) has been studied by means of density functional theory (DFT) method at B3LYP-D3/6-311++G (d, p) computational level. The results indicate that up to eight hydrogen molecules are adsorbed over DLP with hydrogen storage capacity of 12.12 wt%, higher than the year 2020 target from the US department of energy (DOE). The average values for adsorption energy of hydrogen lies in the range of -0.134eV/H_2 and -0.090eV/H_2 for 1H_2-DLP and 8H_2-DLP complexes respectively, locate the favorable range under the physical adsorption at near ambient conditions. Findings of present study may be create motivation for design of promising hydrogen storage materials in future.uptake of H_2 molecule will different molecular moieties have been reported recently [1-4].

References:

[1] L. Schlapbach, A. Züttel, Hydrogen-storage materials for mobile applications, in: Materials for Sustainable Energy, n.d. 265–270.
[2] C. Tabtimsai, W. Rakrai, B. Wanno, Hydrogen adsorption on graphene sheets doped with group 8B transition metal: A DFT investigation, Vacuum. 139 (2017) 101–108.
[3] Y. Zhang, X. Cheng, First-principles study of hydrogen storage on Li12F12 nano-cage, Chemical Physics Letters. 672 (2017) 105–111.
[4] Y. Zhang, X. Cheng, Hydrogen storage property of alkali and alkaline-earth metal atoms decorated C24 fullerene: A DFT study, Chemical Physics. 505 (2018) 26–33.

Preparation of magnetic ferrite-polymer nanocomposite modified with porphyrin

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Abstract:

Spinel ferrite nanoparticles are very important materials because of their interesting magnetic and electrical properties with good chemical and thermal stabilities [1]. In recent years, a great deal of studies has been devoted to polyaniline due to its unique properties, high environmental stability, easy polymerization and low cost of monomer [2]. Furthermore, porphyrin derivatives are the most promising sensitizers due to their high absorption coefficient within the solar spectrum, non-poisonous nature of porphyrin and compatibility with the environment [3, 4]. In this regard, synthesis of nanocomposite based on copper ferrite, polyaniline and porphyrin is an ideal approach for preparation of well performing and readily separable nanocomposite. In this work, copper ferrite magnetic nanoparticles were synthesized via solvothermal synthetic route. Copper ferrite-polyaniline magnetic nanocomposite was prepared by in situ chemical oxidative polymerization of aniline in the presence of ferrite particles. In the next stage, copper ferrite which coated with polyaniline was successfully modified with tetrakis (4-carboxyphenyl) porphyrin. FT-IR spectra, XRD patterns, UV-Vis spectra, VSM curves, TGA/DTA analysis, EDS test, SEM images confirmed the architecture of the prepared nanocomposite. The magnetic saturation (Ms) values of $CuFe_2O_4$, $CuFe_2O_4$@PANI and TCPP/$CuFe_2O_4$@PANI, determined from the hysteresis loops measurements were 96, 27 and 15 emu/g, respectively. The VSM magnetization curves of the samples were displayed in Fig. 1. Due to the excellent magnetic properties of the prepared samples, the nanocomposite could be easily separated by an external magnetic field.

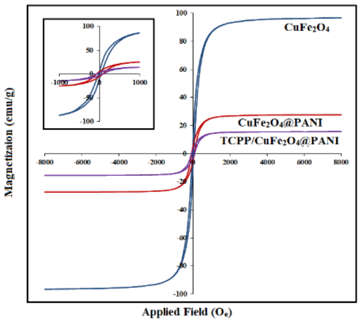

Fig. 1. The magnetization curves of $CuFe_2O_4$, $CuFe_2O_4$@PANI and TCPP/$CuFe_2O_4$@PANI

References:

[1] S. Sun, H. Zeng, D. B. Robinson, S. Raoux, P. M. Rice, S. X. Wang, , G. Li, J. Am. Chem. Soc. 126(1) (2004) 273-279.
[2] S. Sultana, Rafiuddin, M. Z. Khan, K. Umar, J. Alloys Compd. 535 (2012) 44–49.
[3] Y. Chen, A. Li, Z.-H. Huang, L.-N. Wang, F. Kang, Nanomaterials 6 (2016) 51.
[4] M. Rabbani, M. Heidari-Golafzani, R. Rahimi, Mater. Chem. Phys.179 (2016) 35-41.

Synthesis, Characterization and photoluminescence studies of A New Schiff Base Ligand Containing 2-Thiophenecarboxaldehyde and Its Zirconium(IV) Complex

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Abstract:

Schiff bases are an important class of organic compounds. This kind of ligands have significant importance in chemistry, especially in the development of Schiff base complexes [1]. Schiff bases with sulfur and nitrogen donor atoms in their structures act as good chelating agents [2]. Coordination of such compounds with metal ions often enhance their biological activities. Schiff base complexes have been of interest in coordination chemistry for many years due to their facile synthesis and wide applications. In this research, we reported synthesis and characterization of a new Schiff base ligand containing 2-thiophenecarboxaldehyde and 2-aminoethanethiol. This ligand was synthesized in methanol at 60 ºC. Also, zirconium(IV) complex was synthesized by the reaction of ligand and zirconium chloride in 1:1 molar ratio. The compounds were characterized by different spectroscopies and elemental analysis. The most important peaks in FT-IR spectra are due to the imine group at 1630 and 1617 cm^{-1} for Schiff base ligand (Fig. 1) and its complex, respectively. Furthermore, in ^{1}H NMR the hydrogen of imine group were appeared at 8.47 and 8.40 ppm for the ligand and its complex.

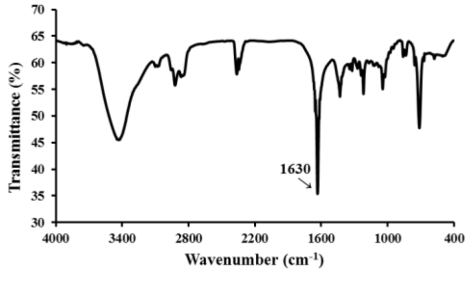

Fig. 1: FT-IR spectra of Schiff base ligand

References:

[1] C.P. Johnson, J.L. Atwood, J.W. Steed, C.B. Bauer, R.D. Rogers, Inorg. Chem. 35 (1996) 2602-2610.

[2] B. Shafaatian, Z. Ozbakzaei, B. Notash, S.A. Rezvani, Spectrochim. Acta A 140 (2015) 248-255.

Effect of preparation methods on copper ferrite nanoparticles: A comparison between combustion and solvothermal methods

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Abstract:

Spinels are a class of binary transition metal oxides arranged in a close packed cubic lattice with general formulation $A^{2+}B_2^{3+}O_4$, where A is a divalent cation and B is a trivalent cation [1]. Because of their attractive magnetic, electronic, thermal and catalytic properties, copper ferrites have been widely used in variety of applications such as magnetic material, catalyst, and so on [2].

In the present study, magnetic nanoparticles of copper ferrite were synthesized by two different routes which are combustion method and solvothermal method. At first, Magnetic nanoparticles of copper ferrite was synthesized by combustion method using stoichiometric amount of copper (II) and iron (III) nitrates with known amount of glycine, as a fuel. In the next step, copper ferrite magnetic nanoparticles were also synthesized via solvothermal synthetic route by using $FeCl_3 \cdot 6H_2O$, $CuCl_2$, ethylene glycol and ammonium acetate. The X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FT-IR) studies confirm the spinel phase, and cation ion distribution for both methods. The copper ferrite nanoparticles which prepared by solvothermal method were structurally uniform spherical magnetic particles and display good crystallinity. The SEM images of the as synthesized samples are shown in Fig. 1.

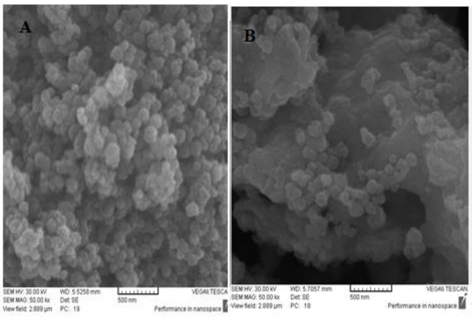

Fig. 1. SEM images of $CuFe_2O_4$ magnetic nanoparticles synthesized by A) combustion method B) solvothermal method

References:

[1] L. B. Zakiyah, E. Saion, N. M. Al-Hada, E. Gharibshahi, A. Salem, N. Soltani, S. Gene, Materials Science in Semiconductor Processing 40 (2015) 564–569.

[2] Y. Shen, Y. Wu, H. Xu, J. Fu, X. Li, Qi. Zhao, Y. Hou, Materials Research Bulletin 48 (2013) 4216–4222.

Controlled synthesis and photocatalytic activity of TiO_2@MIL-100 (Fe) microspheres

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Abstract:

TiO_2@MIL-100 (Fe) microspheres with a controllable method were synthesized by incorporating MIL-100(Fe) on TiO_2 using a versatile step-by-step self-assembly strategy. The XRD patterns and FT-IR spectra of TiO_2@MIL-100 (Fe) indicated the co-existence of TiO_2 and MIL-100(Fe). Moreover, loading of MIL-100 (Fe) on TiO_2 have increased the surface area as observed in BET experiment. The SEM and TEM images demonstrated the formation of MIL-100(Fe) shells on the TiO_2 microsphere. According to UV-Vis DRS data, imparting of MIL-100 (Fe) on TiO_2 microsphere caused to a red shift in absorption edge of catalysts and the band gap energy altered from 3.2 eV for TiO_2 particles to 2.2 eV for TiO_2@MIL-100 (Fe) microsphere. The synthesized composite indicated superior photocatalytic activity in the removal of methylene blue (MB) from water under visible light. The complete degradation of 40 mg/L MB was attained by using synthesized microstructure within 120 min, while commercial TiO_2 (P-25) degraded only 36.6% of MB under similar conditions.

References:

[1] A. H. Cheshme Khavar, Gh. Moussavi, A.R. Mahjoub, App. Sur. Sci. 440 (2018) 963–973.
[2] C.-F. Zhang, L.-G. Qiu, F. Ke, Y.-J. Zhu, Y.-P. Yuan, G.-S. Xu, X. Jiang, J. Mater. Chem. A 1 (2013) 14329-14334.

Synthesis and characterization of a 14-membered macrocyclic copper (II) complex

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Abstract:

Macrocycles are an important class of ligands in transition metal chemistry since they can provide beneficial thermodynamic and kinetic properties to their metal complexes. There are a board range of applications for these types of ligands and their complexes, such as metal ion-selective reagents [1], precursors for luminescent compound formation, MRI contrast agents and radiopharmaceuticals [2].

In this work, a new macrocyclic copper complex of 1,3,6,10,12,15-hexaazatricyclo[13.3.1.1^{6,10}]eicosane (ACE), [Cu(ACE)NO$_3$]NO$_3$, was prepared by template synthesis, followed by ion exchange reaction and its spectral and structural properties was investigated. The complex is an intermediate product which can be formed during the ion exchange reaction of its non-ionic [Cu(ACE)(NO$_3$)$_2$] compound. In the structure of the complex (figure 1), the copper atom has a distorted square pyramidal geometry with CuN$_5$ environment. The complex has Jahn-Teller distortion.

m.p. 199 °C. Anal. Calcd for $C_{14}H_{30}CuN_8O_6$ (%): C, 35.78; H, 6.43; N, 23.84. Found: C, 35.90; H, 6.51; N, 23.96. IR (KBr, cm^{-1}): 3269 m (ν N−H), 2935 m (ν_{as} CH$_2$), 2860 m (ν_s CH$_2$), 1465 m (δ_{as} CH$_2$), 1403 s (δ_s CH$_2$), 1360 s (ν_4 NO$_3$), 1320 s (ν_4 NO$_3^{free}$), 1268 m (ν_1 NO$_3$), 1086 m (ν_2 NO$_3$), 1046 m (ν C−N), 818 m (ν_6 NO$_3$).

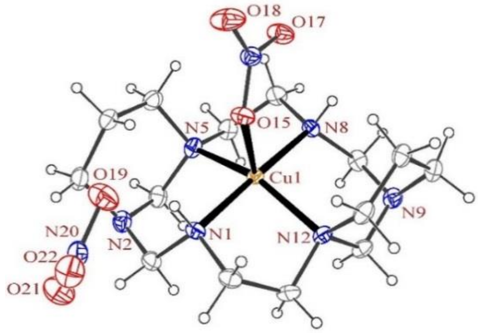

Fig.1. An ORTEP plot of the complex, showing thermal ellipsoids at 50% probability.

References:

[1] D. E. Fenton, Chem. Soc. Rev., 28 (1999) 159 .
[2] B. P. Burke, S. J. Archibald, Annu. Rep. Prog. Chem., Sect. A: Inorg. Chem., 109 (2013) 232.

Expanding Applications of Zeolite Imidazolate Framework: Synthesis of Zeolite A-ZIF-8 Composite and Investigation of its Properties

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Abstract:

Metal–organic frameworks (MOFs) are permanently microporous materials with crystalline structures synthesized by assembling metal ions with organic ligands in appropriate solvents. MOFs are typically characterized by large internal surface areas, uniform and tunable cavities [1].

One particularly interesting category of MOFs is the zeolite imidazolate frameworks (ZIFs) [2]. ZIFs, based on an imidazolate linker and metallic nodes, can adopt symmetrical porous structures analogous to zeolites. For example, ZIF-8 has been synthesized from 2-methylimidazole and a zinc precursor in the sodalite form [3].

In this study, Zeolite A-ZIF-8 was synthesized by inclusion of Zn^{2+} into the cages of zeolite A followed by solvo-thermal linkage of 2-methylimidazolate (MeIM) moiety.

The obtained composite was characterized by means of X-ray powder diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FT-IR). SEM imaging showed that nano-sized ZIF-8 crystallites were successfully formed inside and over the surface of zeolite A. Meanwhile, EDS analysis showed presence of all of the anticipated elements in the sample. FTIR analysis and XRD patterns also approved correctness of the expected structure. Potential application of this newly devised composite is currently under investigation in our laboratory.

References:

[1] G. Lu, Sh. Li, Zh. Guo, O. K. Farha, Br. G. Hauser, X. Qi ,Y. Wang, X. Wang, S. Han, X. Liu, J. S. DuChene, H. Zhang ,Q. Zhang, X. Chen, J. Ma, S. Ch. J. Loo, W. D. Wei, Y. Yang J. T. Hupp, F. Huo, J. Nat. Chem. 4 (2012) 310-316.

[2] S. K. Nune, P. K. Thallapally, A. Dohnalkova, Ch. Wang, J. Liu, G. J. Exarhos, Chem. Commun. 46 (2010) 4878-4880.

[3] K. S. Park, Z. Ni, A. P. Coˆte´, J. Y. Choi, R. Huang, F. J. Uribe-Romo, H. K. Chae, M. O'Keeffe, O. M. Yaghi,. Org. Chem. 103 (2006) 10186-10191.

Nano Polymeric Biodegradable of Alginate-Arginine for Breast Anticancer Drug Delivery

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Abstract:
Natural polysaccharides could easily form biodegradable nanogels, owning good stability in biological fluids due to the existence of the low driving forces for their aggregation. Compared to other nanocarriers, nanogels usually have good biocompatibility, high aqueous dispersibility, and well-defined stable structure [1]. Alginate is one of the most abundant biodegradable natural linear polysaccharide derived from gulfweed, bacteria or seaweed of brown algae, composed of 1–4 linked α-L-guluronic (G) and β-D-mannuronic (M) acid residues. It has been recognized in biomedical applications, owing to its non-antigenicity, nontoxicity, satisfactory biocompatibility, favorable biodegradability, and pH sensitivity [2].

The main goal of the project was to produce SA/Arg nanoparticles loaded with PTX. After synthesis of nanoparticles by gelation method, the structure of the FT-IR spectra was identified. Also, using the DLS and SEM images, the approximate diameter of nanoparticles, bulk density and morphology were investigated. The magnitude of the zeta potential of -12.2 mV reduces the accumulation of nanoparticles in suspension. The zeta potential of more than 30 mV indicates the stability of nanoparticles, which prevents their accumulation. The encapsulation efficiency, was between 74.63 and 95.83.

The SEM image of the synthesized nanoparticles represents a spherical shape with a good distribution and no accumulation and very fine nanoscale size. The FT-IR spectrum is used to confirm the binding of sodium alginate and arginine, and the formation of amide bonding, as well as the cross-linking of calcium cations with carboxylate alginate and carbonylamide groups.

Laboratory studies showed that PTX controlled release of nanoparticles lasted about 96 hours. The PTX drug is absorbed by calcium alginate-arginine (CA-Arg) by covalent coupling, which results in the release of the drug by destroying the stereochemicals by hydrolysis in phosphate buffer with pH = 5. Alginate cross-linking can be destroyed by removing cross-linking calcium ions in a phosphate buffer solution, including HPO_4^{2-} ions.

References:

[1] Y.L.Li, D.Maciel, J.Rodrigues, X.Y.Shi, H.Tomas, Chemical Reviews, 115 (2015) 8564–8608.
[2] K.Y.Lee, D.J. Mooney, Progress in Polymer Science, 37 (2012) 106–126.

Application of metal-organic Co/Ni for removal of heavy metals

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Abstract:
Metal-organic frameworks are a group of high-porosity materials that had been studying for enormous applications. One of the applications of MOFs is metal adsorption. Today, with increasing the population and the growth of technology and industry, the entry of various chemical and microbial contaminants such as toxic substances, heavy metals and etc.[1]into the ecosystem creates new health problems and important health hazards for humans and other creatures.

In the two past decades, several methods have been used to remove heavy metals from water, including ion exchange, membrane filtration, chemical deposition, and adsorption. Due to the effectiveness of absorption method, economic value, flexibility of design and reversibility, absorption techniques are currently one of the technologies used to remove heavy metals. According to the literature, one of the most important features of a good absorbent is its ability to be select. Several factors such as electrostatic interactions, covalent interactions, pore size and shape, etc. can be effective on absorption selectivity.[2]

In order to achieve the purpose of designing metal-metal frameworks with the ability to absorb and selectable metal contaminants, a metal-organic framework with the formula of $[CoNi\ (\mu_3\text{-tp})_2(\mu_2\text{-pyz})_2]$ containing nickel and cobalt metal ions and Cobalt and two types of terephthalic acid and pyrazine connectors.

In this paper, the adsorption behavior of the title framework was investigated for removal of heavy metal ions and, according to ICP data, copper ions have a high uptake by this MOF.

References:
[1] O'Keeffe, M. Chem. Soc. Rev. 38 (2009) 1215.

[2] M.A. Barakat, Arab. J. Chem. 4 (2011) 361–377.

Energy decomposition analysis of F-M bonds in F_2M (M=O, S, Se) compounds

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Abstract:
The energy decomposition analysis (EDA) is a powerful method for a quantitative interpretation of chemical bonds in terms of four major expressions. The instantaneous interaction energy ΔE_{int} between two fragments A and B in a molecule A–B is partitioned in four terms, namely, (1) the quasi-classical electrostatic interaction $\Delta E_{\mathrm{elstat}}$ between the fragments, (2) the repulsive exchange (Pauli) interaction $\Delta E_{\mathrm{Pauli}}$ between electrons of the two fragments having same spin, (3) the orbital interaction ΔE_{orb}, which comes from the orbital relaxation and the orbital mixing between the fragments and (4) dispersion energy. In this work, the nature of F-M bonds in F_2M (M=O, S, Se) compounds have been investigated at BP86-D3/TZ2P//M06/def2−TZVPP level of theory with C_{2v} symmetry constraints by using the program package ADF2013.01. The calculated values for the orbital interactions ΔE_{orb} can be used as an indicator for the best description of the F-M interactions. Those EDA calculations which give the smallest ΔE_{orb} value indicate which fragments are the best choices for describing the bonding situation, because the least alteration of the electronic charge distribution is required to yield the electronic structure of the molecule [1]. The data in Table 1 illustrate that fragmentation of (c) gives the smallest ΔE_{orb} value for F_2O, F_2S and F_2Se. The latter fragments show that the $(F)_2$ has has $s^2\, p_\sigma^1\, p_{\pi\perp}^2\, p_{\pi\parallel}^2$ orbital occupations and O, S and Se atoms have $s^2\, p_\sigma^1\, p_{\pi\perp}^1\, p_{\pi\parallel}^2$ orbital occupations (See Table 1).

Table 1. EDA (BP86-D3/TZ2P) with six different partitioning schemes (a)–(f). Energies are given in $\mathrm{kcalmol^{-1}}$. The most favorable partitioning scheme (c) yielding the smallest ΔE_{orb} value is given in Bola and Italics.

	Partition scheme	(a)	(b)	***(c)***	(d)	(e)	(f)
	Electronic state of E (E=O, S, Se) atom	$s^2 p_\sigma^2 p_{\pi\perp}^1 p_{\pi\parallel}^1$	$s^2 p_\sigma^1 p_{\pi\perp}^2 p_{\pi\parallel}^1$	$\boldsymbol{s^2 p_\sigma^1 p_{\pi\perp}^1 p_{\pi\parallel}^2}$	$s^1 p_\sigma^2 p_{\pi\perp}^2 p_{\pi\parallel}^1$	$s^1 p_\sigma^2 p_{\pi\perp}^1 p_{\pi\parallel}^2$	$s^1 p_\sigma^1 p_{\pi\perp}^2 p_{\pi\parallel}^2$
F_2O	ΔE_{int}	-2317.44	-2317.44	***-2317.44***	-2662.22	-2662.23	-2662.23
	$\Delta E_{\mathrm{Pauli}}$	1064.12	1012.97	***1048.43***	963.03	996.82	947.59
	$\Delta E_{\mathrm{elstat}}$	-318.29	-239.24	***-364.09***	-257.04	-381.26	-303.29
	ΔE_{orb}	-3063.30	-3091.20	***-3001.82***	-3368.24	-3277.83	-3306.56
F_2S	ΔE_{int}	-2382.05	-2382.06	***-2382.03***	-2620.21	-2620.17	-2620.18
	$\Delta E_{\mathrm{Pauli}}$	1425.38	1363.79	***1401.29***	1332.03	1364.41	1308.47
	$\Delta E_{\mathrm{elstat}}$	-486.96	-378.80	***-521.85***	-416.10	-555.36	-451.23
	ΔE_{orb}	-3320.54	-3367.11	***-3261.52***	-3536.20	-3429.28	-3477.47
F_2Se	ΔE_{int}	-2383.33	-2383.34	***-2383.30***	-2634.63	-2634.59	-2634.60
	$\Delta E_{\mathrm{Pauli}}$	1241.74	1191.68	***1222.41***	1186.31	1210.19	1164.84
	$\Delta E_{\mathrm{elstat}}$	-459.17	-371.85	***-495.92***	-404.06	-522.56	-441.55
	ΔE_{orb}	-3165.97	-3203.25	***-3109.87***	-3416.95	-3322.20	-3357.96

Reference:

[1] R. Tonner, G. Frenking, Chem. Eur. J. 14 (2008) 3260 – 3272.

Preparation and Characterization of Polycaprolactone/*x*% Cu-MOF Nanofibers

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Abstract:

Nowadays, porous compounds especially polymeric nanofibers mats have been the subject of intense research in biological applications such as wound dressing, drug delivery, and tissue engineering [1-2]. MOFs are porous crystalline structures consisting of metal ions (or metal clusters) linked through organic linkers [3]. The main objective of the present work is the fabrication of fibrous composites from blending the Cu-MOF with poly(caprolactone) by electrospinning technique. The as-prepared compounds were characterisized by various techniques including FT-IR, PXRD, EDS mapping, SEM, and TEM.

Polycaprolactone/*x*%Cu-MOF nanofibers by a two-step method including a hydrothermal and electrospinning process for the preparation of Cu-MOFs and PCL/*x*%Cu-MOF nanocomposites. The results of FT-IR, XRD, and EDS mapping were confirmed the incorporation of Cu-MOF into polycaprolactone matrix. TEM and SEM images showed that the fabricated compounds have nanofiberous morphology. Figure **1** depicts the SEM images of PCL and PCL/*20*%Cu-MOF nanocomposites. The SEM images revealed that PCL fibers have continuous and cylindrical shape (Figure **1**a).Figure **1**b shows that the morphology of PCL nanofibers wasn't changed during composite preparation.

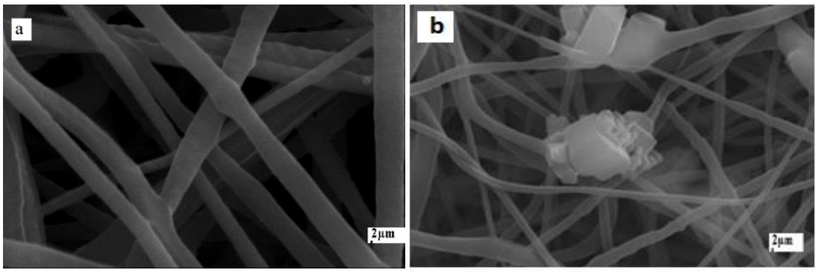

Fig. 1. SEM images of (a) pure PCL and (b) PCL/*20*%Cu-MOFs nanocomposite.

References

[1] A.M. Al-Enizi, M.M. Zagho, A.A. Elzatahry, Nanomaterials, 8 (2018) 259
[2] L. Weng, J. Xie, Current pharmaceutical design, 21 (2015) 1944
[3] K.A. Rieger, N.P. Birch, J.D. Schiffman, Journal of Materials Chemistry B, 1 (2013) 4531.
[4] J.L.C. Rowsell, O.M. Yaghi, Microporous and Mesoporous Materials, 73 3 (2004).

Investigation of anti-bacterial property of Fe-MIL88(NH$_2$) and MIL-53(Al)

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Abstract:

Increasing antibiotic resistance of microorganisms is one of the major societal challenges today and great efforts have been devoted to combat or mitigate the huge dependence on conventional antibiotics by finding alternative antimicrobial treatments. The extraordinary resistance to conventional antibiotic treatments particularly of biofilms grown on solid substrates not only in the medical area (surgeon’s tools, implants) but also in a number of technical applications (underwater optics, ship hulls) and has driven research towards the development of novel coatings with superior antimicrobial properties

Metal–organic frameworks (MOFs) are highly ordered structures composed of metal centers and organic linker molecules. The possibility to combine multiple functionalities within one framework makes MOFs an ideal system for designing a periodic arrangement of functional molecular subunits.

Fe-MIL-88NH$_2$ was synthesized using 2-aminoterephthalic acid and $FeCl_3.6H_2O$ as the precursors. $FeCl_3.6H_2O$ and of 2-aminoterephthalic acid were dissolved in DMF, and then acetic acid was added to the solution. The mixed solution was placed in an oil bath at 120 ˚C and after cooling to room temperature, the particles were isolated by centrifugation and washed with hot ethanol to remove the extra reactants. Finally, the brownish crystal sediment was dried at a gentle temperature in the oven. MIL-53(Al) was synthesized using $Al(NO_3)_3.9H_2O$ and terephthalic acid were dissolved in deionized water and placed in a thermal furnace. A soft white sediment was separated by centrifugation, which was then washed with deionized water twice and dried at room temperature

In his paper, we investigated about anti-bacterial, anti-oxidan and anticancer properties of Fe-MIL88(NH$_2$) for the first time**.** Fe-MIL-88(NH$_2$) synthesized from therephtalic acid and $FeCl_3.6H_2O$ in presence of DMF in oil bath. MIL-53(Al) also synthesized from therephtalic acid and $Al(NO_3).9H_2O$ in presence of water in furnace.Results shows that anti-bacterial activity of this compound upon both *E.Coli* and *Pseudomonas* stains is stronger than tetracycline and kanamycin antibiotic.

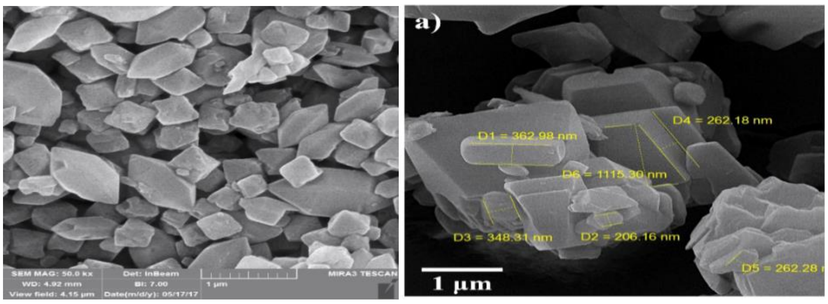

Fig.1 SEM image of Fe-MIL-88(NH

References:

[1] J.Juan-Alcaniz, Delft University of Technology, (2013).

[2] O.Barbosa, C.Ortiz, A.Berenguer-Murcia, R.Torres, R.C.Rodrigues and R.Fernandez-Lafuente, Biotechnol. Adv., 33(5) (2015) 435-456.

[3] Y.Chen, V.Lykourinou, C.Vetromile, T.Hoang, L.J.Ming, R.W.Larsen and S.Ma, J. Am. Chem. Soc., 134(32) (2015) 13188-13191.

[4] Y.Chen, S.Han, X.Li, Z.Zhang and S.Ma, Inorg. Chem., 53(19) (2014) 10006-10008.

[5] Y.Cui, B.Li, H.He, W.Zhou, B.Chen and G.Qian, Acc. Chem. Res., 49(3) (2016) 483-493.

[6] D.N.Tran, and K.J.Balkus Jr, ACS Catal., 1(8) (2011) 956-968.

[7] M.Ebrahimi, S.Hosseinkhani, A.Heydari, and J.Akbari, Biomacromolecular Journal, 1(1) (2015) 104-112.

[8] M.Ebrahimi, S.Hosseinkhani, A.Heydari, R.A.Khavari-Nejad and J.Akbari, Photochem. Photobiol. Sci., 11(5) (2010) 828-834.

Design of $Zn_{1-x}Cu_xO$ nanocomposite Ag-doped as an efficient antibacterial agent

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Abstract:

In this paper, we reported the preparation of the binary and ternary Nano-composite metal oxide and doping of Ag nanoparticles by using sol-gel and impregnation methods, respectively. Figure 1a showed the presence of peaks in related to ZnO, CuO and Ag nanoparticles which proved the formation of $Zn_{1-x}Cu_xO(Ag)$ nanocomposite. Fig. 1b shows FESEM analysis of $Zn_{1-x}Cu_xO(Ag)$ in relation with nanoparticles. Hydrazine was used as reduction for conversion of Ag cation to Ag nanoparticles. In addition, polyethylene glycol was used as stabilizer of nanoparticles [1,2]. These nanaoparticles were characterized by XRD, FT-IR and FESEM. The antibacterial and antifungal effects of these hybrid materials were investigated against E. coli, Salmonella. E, Staphylococcus. a, Bacillus subtilis and Cndida Kefyr [3].

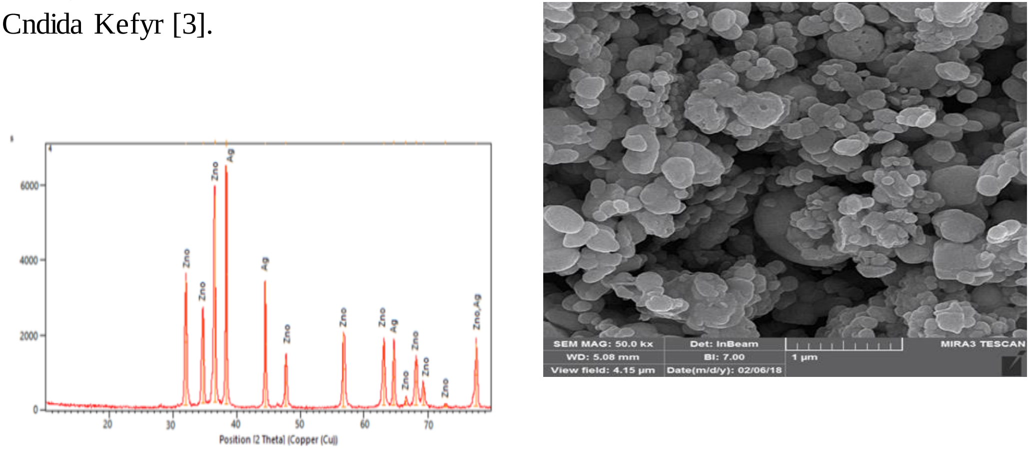

Fig. 1. a) XRD pattern of $Zn_{1-x}Cu_xO(Ag)$, **b)** FESEM analysis of $Zn_{1-x}Cu_xO(Ag)$

References:

[1] L. Zhang, Y. Jiang, Y. Ding, N. Daskalakis, L. Jeuken, M. Povey, D. W. York. coli. Nanoparticle Research, 12(5) (2010) 1625-1636.

[2] S. Shrivastava, M. Jyung wo lungue,Journal of Nanotechnol, 25 (2010) 103-125.

[3] K. M.Yu, B. Leung, Q.Guo, W. M Lau, And J. Yang. Nanotechnology, 22(11) (2011) 115603.

Selective and Sensitive Electrochemical-Sensor for Determination of Dichromate Anion Based on Modified Mesoporous Silica Nanomaterial

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Abstract:

Nanotechnology has great potential for application in the field of chemical and electrochemical sensors. Particularly, hybrid nanomaterials due to their unique characteristics have recently been recognized as promising systems in this branch of modern chemistry. In this paper, the channels of mesoporous silica (SBA-15) has been modified by the aluminum complex of 8-hydroxyquinoline according to the method described in the literature [1]. The synthesized nanomaterial (SBA-AlQ) shows a remarkable fluorescence emission at 486 nm, which is quenched in the presence of dichromate anion. In addition, the UV-vis absorption spectrum of SBA-AlQ upon the addition of dichromate onion indicates a specific isosbestic point at 210 nm, confirming the presence of a stable complex with a certain stoichiometric ratio between SBA-AlQ and dichromate anion. These results indicate that this fluorescence nanomaterial can be used as a chemosensor for detecting anion dichromate in aqueous solutions. In addition, due to the selective interaction with dichromate anions, it can be used as a sensing material in a new electrochemical sensor. Accordingly, the carbon paste electrode was made by combining 5% multi-walled carbon nanotubes (MWNTs), 55% graphite powder, 20% ionic liquid and 20% SBA-AlQ. This sensor worked well with the Nernstian response of -28.6±0.3 mV decade-1 of dichromate anion in a wide dynamic concentration range of 1.0×10^{-6}-1.0×10^{-1} M. The electrode also has a relatively short response time (about 23 s) and produces stable responses for more than 8 weeks.

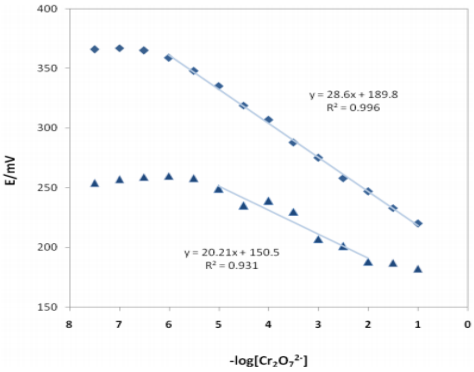

Fig. 1 The calibration curves of the $Cr_2O_7^{2-}$ sensors (traditional electrode and new proposed electrode)

References:

[1] A. Badiei, H. Goldooz, G.M. Ziarani, Appl. Surf. Sci. 257 (2011) 4912–4918.

A Highly Selective and Sensitive Fluorescent Chemo-Sensor for Detecting Lu^{3+} Ion Based on Mesoporous Silica Nanomaterial

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Abstract:

A novel Lu^{3+} sensitive fluorescent chemo-sensor for the selective detection of Lu^{3+} ion was developed using 8-hydroxyquinoline functionalized mesoporous silica with highly ordered structure (LUS-Q). The ordered porous structure of LUS-Q is still preserved after the post grafting procedure [1-2]. Both UV-vis and fluorescence spectroscopic studies indicated that the synthesized sensor showed good selectivity toward Lu^{3+} ion over other ions, most probably due to the presence of the fluorophore moiety at its surface and the forming of stable complex between the LUS-Q and LU^{3+}. The emission intensity of the Lu^{3+}-bound mesoporous material increases with an increase in concentrations of Lu^{3+} ion. The enhancement of fluorescence is attributed to the strong covalent binding of Lu^{3+} ion. The linear response range of Lu^{3+} chemo-sensor was from 1.6×10^{-7} to 1.0×10^{-5} mol L^{-1}. The sensor has a detection limit of 8.2×10^{-8} mol L^{-1} and the pH range which the proposed chemo-sensor can be applied was 3.3–8.3.

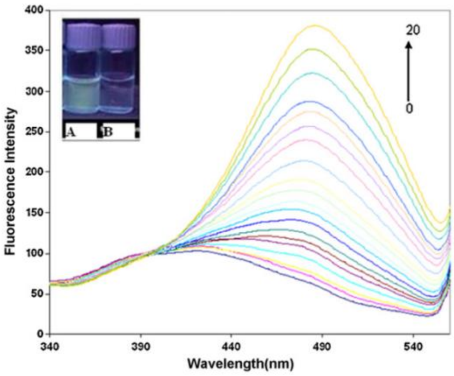

Fig.1. Emission spectra of the proposed chemosensor in the presence of varying concentration of Lu^{3+} ions

References:

[1] A. Badiei, H. Goldooz, G. Mohammadi Ziarani, A. Abbasi, J. Colloid. Interface. Sci., 357 (2011) 63–69.

[2] M. Hosseini, M. R. Ganjali, Z. Rafiei-Sarmazdeh, F. Faridbod and et al., Anal. Chim. Acta, 771(2013) 95-101.

Selective oxidation of sulfides to sulfoxides with *tert*-BuOOH catalyzed by oxovanadium (IV) asymmetrical tetradentate Schiff base complex

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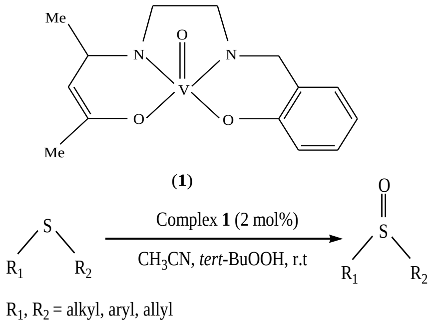
Abstract:

Sulfoxides have a wide range of applications in synthesis of chemically useful and biologically active molecules such as drugs, flavors, germicides, as well as activation of enzymes [1]. Investigation of environmentally friendly catalytic systems for oxidation of sulfides with high activity and selectivity has become the subject of interest to researchers. In this regard, the Schiff base transition metal complexes are attractive oxidation catalysts due to their easy synthesis and their chemical and thermal stability. Among different metal Schiff base complexes, special attention has been paid to oxovanadium(IV) Schiff base complexes because of their structural features, catalytic activity, and biological roles in a variety of biochemical processes [2].

In this work, asymmetrical tetradentate Schiff base ligand was prepared according to published procedure [3] and metallated with VO(acac)$_2$ by refluxing ethanolic solution of Schiff base ligand and VO(acac)$_2$ in 1:1 molar ratio to obtain complex **1**. The prepared complex **1** was characterized by FT-IR, UV-vis, ^{1}H NMR spectra and CHN analysis. Then, the synthesized complex **1** successfully used as a new homogeneous catalyst for selective oxidation of sulfides to sulfoxides with *tert*-BuOOH (TBHP) as oxidant at room temperature (Scheme 1). Good to high yields of products and mild reaction conditions can be mentioned as advantages of this protocol for oxidation of sulfides to sulfoxides.



Scheme 1: Selective oxidation of sulfides to sulfoxides catalyzed by complex **1**

References:

[1] B. Li, a. Liu, L.N. He, Z.Z. Yang, J. Gao, K.H. Chen, Green Chemistry. 14 (2012) 130-135.
[2] R. Ando, T. Yagyu, M. Maeda, Inorganica Chimica Acta. 357 (2004) 2237-2244.
[3] G. Grivani, S. Husseinzadeh Baghan, M. Vakili, A. Dehno Khalaji, V. Tahmasebi, V. Eigner, M. Dusek, Journal of Molecular Structure, , 1082 (2015) 91-96.

Absorption of Fenitrothion organophosphorus pesticide using UIO-66 metal-organic framework

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Abstract:

Several research works have been paid on the synthesis of metal organic framework and investigating their absorption and degradation properties. These porous compounds have attracted a great of attention in the last 10 years, due to the large size of their cavities, their high surface area, the selective absorption of small molecules and the light or magnetic responses in the presence of guest molecules [1]. In this study, the absorption properties of the UIO-66 MOF were investigated by using organophosphorus Pesticide [2]. Studies showed that prepared sample enhanced the absorption of organophosphorus Pesticide compare to carbon active. FESEM, XRD, BET, FTIR, NMR analysis were used to characterize the synthesized UIO-66 MOF. The MOF enabled facile absorption fenitrothion in water/dichloromethane under ambient conditions (90% after 24 h at pH10).

References:

[1] M. Kandiah, M. H. Nilsen, S. Usseglio, Jakobsen, S. U. Olsbye, M. Tilset, K. P. Lillerud, Chemistry of Materials, 24 (2010) 6632-6640.

[2 X. Zhu, B. Li, J. Yang, Li, Y. W. Zhao, J. Shi, J. Gu, ACS applied materials & interfaces. 1 (2014) 223-231.

Preparation and investigation of electromagnetic wave absorption of hybrid nanocomposites of $Ba_{.5}Sr_{.5}6Fe_2O_3$/MWCNT/PANI

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Abstract:
In this study, the wave absorption properties of ferrite based nanocomposite were investigated by using strontium and barium. This nanoparticle has been prepared by variety of methods and different commercial surfactants previously, in the present work the nanocomposite can be conveniently prepared by inexpensive materials. To enhance the absorption of magnetic waves, carbon nanotubes and polyaniline in the presence of magnetic nanoparticles were used [1-2]. After the Barium strontium ferrite nanoparticle were prepared by sol-gel method, radar absorption properties were enhanced by activated carbon nanotubes and polyaniline. The characteristics of the nanocomposites were investigated by FESEM, XRD, VSM and FTIR analysis and microwave absorption at 8-18 GHz. The best absorbance was observed in -45 dB at the X-band range for $Ba_{.5}Sr_{.5}6Fe_2O_3$/MWCNT/PANI sample (4% polyaniline – 96% a mixture of barium ferrite and strontium ferrite) while the weight ratio of the powder was 50% with 5 mm thickness. In the X-band range the absorbance increased from -5.8 dB to -20 dB for $Ba_{.5}Sr_{.5}6Fe_2O_3$/MWCNT/PANI sample by in-situ method (a mixture of barium ferrite/ nanotube and strontium ferrite / nanotube) with an increase in thickness from 1.8 to 6 mm.

References:
[1] W. H. Hayt, J. A. Buck, Engineering electromagnetics. 6 (1981).
[2] S. Ruan, B. Xu, H. Suo, F. Wu, S. Xiang, M. Zhao, (2000).

Preparation of ferrite based nanostructure and investigation on electromagnetic properties

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Abstract:
Camouflaging weapons, especially airplanes, helicopters, and drones, is inevitable. Radar camouflage means hiding a weapon from different types of radars that are done in a variety of ways that the reduction of the radar cross section or the use of radar absorbing materials are the most important methods [1-2]. In this research, Barium strontium hexaferrite nanostructure was synthesized by sol-gel method. The characterization of nanoparticles was performed by SEM, XRD, FTIR, and VSM analyzes. Absorption properties of the nanoparticles were investigated by Vector Network Analyzer at 8-12 GHz. The best absorbance was observed in -16 dB at the X-band range while the weight ratio of the powder was 20% and in 2 mm thickness.

Table 1. Samples of Barium strontium ferrite synthesized by sol-gel method.

	$Fe(NO_3)_3.9H_2O$ (mol)	$Ba(NO_3)_2$ (mol)	$Sr(NO_3)_2$ (mol)	Citric acid (Molar ratio with metal cations)	900 °C (min)	1000°C (min)
1	1	0/083	0/12	1:1	90	-
2	1	0/083	0/1	1:1	80	-
3	1	0/16	0/16	2:1	70	-
4	1	0/083	0/16	1:1	-	90

References:
[1] D. C. Jenn, American Inst. of Aeronautics. (1995).
[2] A. Wu, X. Yang, H. Yang, J. Alloy. Compd. 513 (2012) 193-201.

Synthesis and characterization of metal–organic frameworks Based on Zr^{+4} and benzene 1,4-dicarboxylic acid by reflux method for removal of methylene blue and methyl red

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Abstract:

Metal-Organic Frameworks (MOFs) give an alternative promising way to substitute these limitations due to their strong catalytic site, porosity, high specific surface area, easy separation, and reusable properties [1]. In this work, we reported the synthesis of MOFs based on zirconium (IV) and H_2BDC linker (H_2BDC = benzene 1,4-dicarboxylic acid) by reflux method. Reflux reaction at 100 ºC was found to be the optimum method that was indicated by most crystalline product compared to the simulated pattern in XRD analysis. The formation of the framework was characterized by FTIR analysis. The high thermal stability was related to the high oxidation state of Zr (IV), which give a significant covalent character to the Zr-O bond [2]. The pore volume and Brunauer−Emmett−Teller surface area of the prepared sample calculated 0.27 cm^3/g and 360 m^2/g, respectively. Finally, the photocatalytic performance of prepared MOF was investigated by photodegradation of methylene blue and methyl red dyes.

References:

[1] G. Maurin, C. Serre, A. Cooper, G. Férey, Chemical Society Reviews. 11 (2017) 3104-3107.
[2] I. Larasati, D. Winarni, F. R. Putri, Q. A. Hanif, W. W. Lestari, In IOP Conference Series: Materials Science and Engineering. 214 (2017) 1-12.

Synthesis of Co_3O_4 nanostructures and evaluation of their thermocatalytic activity in heat absorption and decomposition of ammonium perchlorate

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Abstract:
Metal oxide nanoparticles exhibiting interesting optical and electrical properties that can be grown efficiently as powder nanostructures are used extensively for variety of applications in catalysis, sensors, and environmental remediation and optoelectronic devices [1]. Nano-sized Co_3O_4 has a wide range of applications in various fields of industry including anode materials for rechargeable Li-ion batteries [2], gas sensors, solid state sensors, ceramic pigments, heterogeneous catalysts, rotatable magnets, electrochromic devices, magnetic materials and in energy storage [3]. Ammonium perchlorate (AP) is the most common oxidizer agent in composite solid propellants. The thermal decomposition characteristics influence the combustion behaviour of the propellant. The activation energy, reaction rate, high-temperature decomposition (HTD) and pyrolysis temperature of the thermal decomposition of AP are related to the properties of solid propellants, especially the heat absorption and combustion rate[1]. Among various catalysts, Co_3O_4 nanostructures have attracted a great deal of attention in both fundamental researches and technical applications because of their outstanding catalytic, electrical conductivity, chemical stability, low cost, and other properties. In this study, semi-spherical Co_3O_4 nanostructures were successfully synthesized using a facile sol-gel synthetic route at 100 °C under refluxing conditions and characterized by XRD, FTIR, SEM and TEM. The results showed that the Co_3O_4 nanoparticles were in pure face centered cubic (FCC) crystal phase and composed of many semi-spheres of diameter about 20 nm which are assembled and they formed micro-sphere morphology. Thermocatalytic properties of Co_3O_4 nanostructures investigated on thermal decomposition of AP using DSC curves. The results reveal that adding 1% of Co_3O_4 nanostructures to AP, decreases the temperature of HTD amount 92 °C (425 °C to 331 °C) and increases the heat absorption amount 889 J g^{-1} (redox decomposition of AP). Two major mechanisms have been proposed for the thermal decomposition of AP in the presence of Co_3O_4 nanostructures, first: electron transfer from perchlorate ion to ammonium ion, Second: proton transfer from ammonium ion to perchlorate ion.

References:

[1] Z. Yu, L. Chen, L. Lu, X. Yang, X. Wang, Chinese J. Catal. 30 (2009) 19–23.
[2] S.H. Hong, J.S. Bae, H.J. Ahn, Met. Mater. Int. 2 (2008) 229–232.
[3] Y. Liu, X. Zhang, Electrochim. Acta. 54 (2009) 4180–4185.

Synthesis of $[Ag(C_{15}H_{12}N_3O)]NO_3$ and $[Zn(C_{15}H_{12}N_3O)]Cl_2$ complexes and investigation of their anti-tumor properties

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Abstract:

Transition metal complexes with potential biological activity are the focus of extensive investigations and occupy many key positions in biological processes [1]. Metal-based drugs are traditionally undervalued by the pharmaceutical industry, which is dominated by organic chemistry. Nevertheless, a number of coordinated compounds have been applied in the therapy of various diseases [2], e.g., historically salvarsan against syphilis, gold complexes against arthritis, bismuth compounds as antiulcer drugs, or platinum compounds against cancer [3]. In this research, two new complexes: $[Ag(C_{15}H_{12}N_3O)]NO_3$ and $[Zn(C_{15}H_{12}N_3O)]Cl_2$ with the NO-donor bidentate Schiff base ligands obtained from inserted condensation of 4-Pyridinecarboxylic acid hydrazide with the Cinnamaldehyde in a 1:1 molar ratio were synthesized. Characterizations of the complexes were carried out by elemental analyses, FTIR, ^1H NMR, ^{13}C NMR and UV–Visible spectroscopic studies. These new compounds, after 72 hours, show excellent anti-tumor activity against HeLa (human cervix carcinoma) and LNCaP (Lymph Node Carcinoma of the Prostate) cancer cells. The 50% and 90% inhibitory doses (IC_{50} and IC_{90}) values, which are the compounds concentrations lethal for 50% and 90% of the tumor cells, were determined both in control and in compounds concentrations lethal in compounds-treated cultures. The corresponding IC_{50} and IC_{90} values are shown in Table 1. The results are completely new and provide new views for using of the mentioned inorganic complexes in chemotherapy.

Table 1: 72-h IC_{50} and IC_{90} values obtained for synthesized complexes against HeLa and LNCaP cancer cells.

Compound	Inhibitory	IC_{50}	IC_{90}
$C_{15}H_{13}N_3O$	0.001, 0.01, 1 M	-	-
$[Ag(C_{15}H_{12}N_3O)]NO_3$	0.0001, 0.001, 0.01 M	0.1 M	1 M
$[Zn(C_{15}H_{12}N_3O)]Cl_2$	0.0001, 0.001 M	0.01 M	-

References:

[1] A. Sigel, H. Sigel, Metal Ions in Biological Systems. (2004) 1-42.
[2] K.H. Thompson, C. Orvig, Dalton Trans. 6 (2006) 761-764.
[3] K. G. Germi, F. Shabani, A. Khodayari, J. World Appl. Sci. 18 (2012) 186-190.

Electrochemical Properties of Polyoxometalate− Graphene Oxide Hybrid Catalyst

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Abstract:

Polyoxometalates (POMs) are a large group of metal oxide clusters that possess rich structural diversity and unique chemical/physical properties, and may be widely applied in catalysis, medicine, magnets, (photo) electronic materials, and functional nanoscale systems [1]. Polyoxometalates (POMs) are composed of d-block transitional metal-oxide nanosized, anionic cluster structures and are prospective candidates for electrocatalysis due to their multiple redox properties [2, 3]. Graphene, consisting of a monolayer of sp^2 carbon atoms, is an attractive material in many research fields including electrocatalytic applications owing to its unique properties such as high surface area, outstanding electrical properties, and high mechanical and thermal properties [4, 5]. Graphene is a unique candidate for a POM support material to overcome problems of both low surface area and high solubility of POMs. Here we reported a new Polyoxometalate− Graphene Oxide hybrid materials and studied the Electrochemical properties of this hybrid cluster using experimental method. The electrochemical behavior of POMs in acidic media involves one or two electron reversible reductions to produce reduced POMs, or so-called heteropoly blues owing to their changed color, and further irreversible multielectron reduction with decomposition in the homogeneous state. These Polyoxometalate− Graphene Oxide hybrid materials were characterized by ^{1}H-NMR, FT-IR, UV-Vis spectroscopic methods and cyclic voltammetry.

References:

[1] H. Wu, H. K. Yang, W. Wang, **New** J. Chem. 40 (2016) 886-897.
[2] P. Jiménez-Lozano, A. Solé-Daura, G. Wipff, J. M. Poblet, A. Chaumont, J. J. Carbó, Inorg. Chem. 56 (2017) 4148−4156.
[3] H. N. Wang, M. Zhang, A. M. Zhang, F. C. Shen, X. K. Wang, S. N., Sun, Y. Q. Lan, ACS Appl. Mater. Interfaces, 10 (2018**)** 32265-32270.
[4] B. Qiu, M. Xing, J. Zhang, Chem. Soc. Rev. 47 (2018) 2165-2216.
[5] P. Solís-Fernández, M. Bissett, H. Ago, Chem. Soc. Rev. 46 (2017) 4572-4613.

Graphene oxide -Cu (II) catalyzed synthesis of triazoles from aryl iodides

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Abstract:

Copper-catalyzed azidee alkyne cycloaddition (CuAAC), also known as the “click reaction,” has become one of the most important reactions for the preparation of 1, 2, 3-triazoles [1]. Most of the reported CuAAC studies are on two component (organic azide and alkyne) reaction systems, especially in the synthesis of 1-aryl-1, 2, 3-triazoles. In this system, the organic azides need to be synthesized in advance, and the potential hazards of organic azides, especially in isolation or purification processing, can be problematic. Thus, it is desirable to develop an efficient one-pot methodology that uses aryl halides and sodium azide for direct cycloaddition with alkynes [2]. Graphene oxide based materials have found various applications including sensors, solar cells, catalysis, and gas storage [3, 4]. Covalent modification of graphene involves the reaction of functional molecules and the oxygenated groups on the GO surface such as carboxyl groups at the periphery, and epoxy, hydroxyl, and C=C groups in the basal plane of GO [5]. In this work, we wish to report the design and characterization of a Cu (II) complex supported on graphene oxide. The structural and chemical nature of the catalyst was characterized by a variety of techniques such FT- IR, UV-Vis, EDS, Raman and TG. The catalytic activity of Graphene Oxide−Cu^{II} (BAPTE) Cl_2 hybrid material was investigated in the three component reaction of sodium azide, phenylacetylene and benzyl halides and the corresponding triazoles were produced in good to excellent yield.

References:

[1] K. C. Mei, N. Rubio, P. M. Costa, H. Kafa, V. Abbate, , F. Festy, K. T. Al-Jamal, Chem. Commu. 51 (2015) 14981-14984.
[2] K. S. Chandrasekaran, A. Rentmeister, Biochemistry 58 (2018) 24-30.
[3] T. P. N. Tran, A. Thakur, D. X. Trinh, A. T. Dao, T. Taniike, Appl. Catal. Gen. 549 (2018) 60–67.
[4] V. B. Saptal, M. V. Saptal, R. S. Mane, T. Sasaki, B. M. Bhanage, ACS Omega. 4 (2019) 643–649.
[5] A. Saroja, B. R. Bhat, Ind. Eng. Chem. Res. 58 (2019), 590–601.

Nanocomposite of TiO_2 with functionalized graphene oxide nanosheets with PDI as efficient photocatalyst in visible light region

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Abstract:
Research into graphene oxide (GO) has been prospering in diverse areas due to their unique structural, optical, and electronic properties [1]. Functionalization of GO is the best way to obtain the desirable performance and improve its efficiency [2]. Herein an effective and facile approach for introducing photoactive and stable hybrid of graphene oxide (GO) and perylenediimide (PDI) was presented. For this purpose, we used three different methods such as (i) the amidation of GO and reaction between the amidated GO and perylene-3, 4, 9, 10-tetracarboxylic dianhydride (**GNP-1**), (ii) the conversion of carboxylic acid group of GO to acyl chlorides and the reaction between acylated GO and symmetric PDI (**GNP-2**), and (iii) amidation of GO and the reaction between amidated GO and asymmetric PDI (**GNP-3**). The studies on the stability and on the dispersibility of these hybrids showed that the **GNP-3** hybrid is more stable and dispersible than other hybrids. Also, non-using of hazardous materials such as thionyl chloride in third method (**GNP-3**) make it as a superior method. This hybrid considers as a sensitizer for photocatalytic process due to its stability in aqueous solution and visible light absorption. Then a series of GNP/TiO_2 nanocomposites with different percentage of GNP-3 were prepared, and the structure, morphology, and photocatalytic activity of these new materials were systematically investigated. This strategy can be extended to many other organic and inorganic semiconductors, which opens new possibilities for high-efficiency graphene-based solar energy conversion.

References:

[1] Roy-Mayhew, J. D.; Aksay, I. A., Chemical reviews. 114 (2014) 6323-6348.

[2] Stergiou, A.; Tagmatarchis, N., ACS applied materials & interfaces. 8 (2016), 21576-21584.

Synthesis and Crystal Structural of a Novel Lead (II) metal-organic system with hemidirected coordination sphere

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Abstract:

The design of crystal structures and control of molecular arrangements of coordination polymers has attracted much attention in recent years [1], The coordination chemistry of lead (II) with donor ligands has been investigated in the past decade and frequently discussed in regard to the coordination and stereoactivity of the valence shell lone electron pairs [2]. Herein we report the preparation and crystal structure of novel metal-organic lead (II) coordination polymer [Pb (4-ptsc)$_2$(OAc)$_2$]$_n$ and describe a simple synthetic sonochemical preparation of nano-structures of [Pb(4-ptsc)$_2$(OAc)$_2$]$_n$ coordination polymer. The composite was categorized by elemental analysis, scanning electron microscopy (SEM), FT-IR spectroscopy, powder X-ray diffraction (PXRD), and single crystal X-ray analysis. The coordination numbers of lead (II) centers are six with *hemidirected* coordination sphere. The adjoining chains are linked by π—π interactions of adjacent aromatic ligands rings and several other relatively weak interactions. As a result, weak interactions further enable the self-assembly of compound construction to formulate a 3D metal-organic coordination polymer.

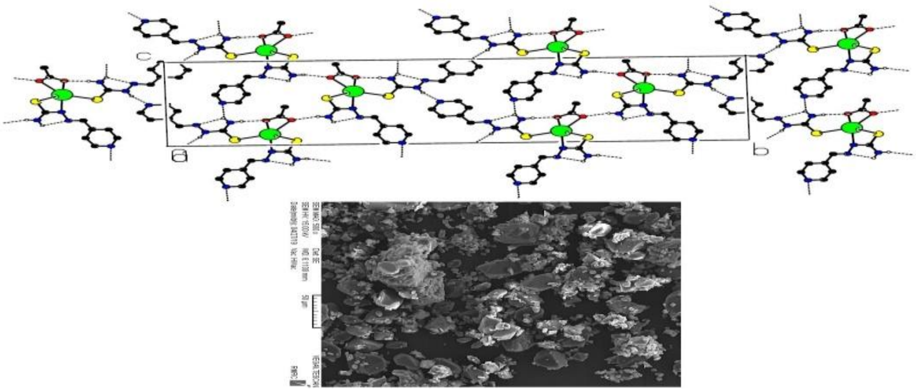

Fig. 1 The extended structure of complex and the morphology of the nano-structures.

References:

[1] D.Y. Du, J.S. Qin, S.L. Li, Z.M. Su, Y.Q. Lan, Chem. Soc. Rev. 43 (**2014**) 4615-4632.
[2] F.Y. Yi, D. Chen, M.K. Wu, L. Han, H.L. Jiang, Chem.Plus.Chem. 81 (**2016**) 675-690.

Magnetically separable nanocatalyst for selective oxidation of sulfides to sulfoxides

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Abstract:

A molybdenum complex, [MoO_2Cl_2 (DMSO) $_2$], was immobilized on Schiff base magnetic Fe_3O_4@SiO_2 nanoparticles by covalent linkage. First, superparamagnetic Fe_3O_4 nanoparticles were prepared by the coprecipitation method [1]. Secondly, the surface of Fe_3O_4 was encapsulated with silica in order to increase the functionality and stability of nanoparticles. Then, the Fe_3O_4 nanoparticles were surface-modified with 3-aminopropyltriethoxysilane (APTS) which introduced -NH_2 on to the surface of support [1]. After functionalization by APTS, free amino groups on the surface can react with many different carbonyl compounds to form Schiff base ligand. For preparation of Fe_3O_4@SiO_2/Schiff base, Fe_3O_4@SiO_2-NH_2 nanoparticles were reacted with dialdehyde and then reacted with the MoO_2Cl_2 (DMSO) $_2$ complex to synthesize Mo (VI) nanocatalyst.

The resulting nanocatalyst are used as an efficient and recyclable catalyst for the selective oxidation of sulfides to corresponding sulfoxides using urea hydrogen peroxide as the oxidant. The characterization of catalyst was carried out by means of TGA, SEM, TEM, VSM, elemental analysis, FT-IR and Raman microprobe techniques.

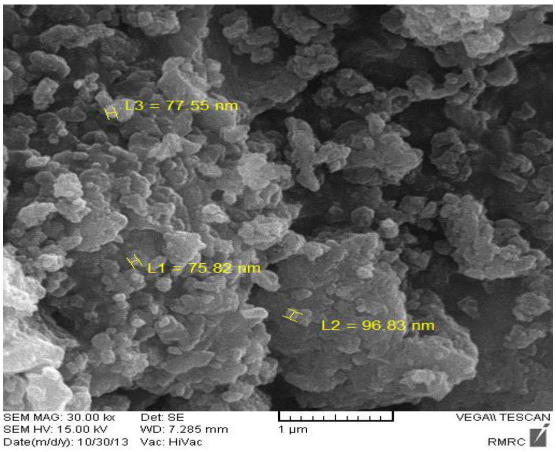

Fig. 1. SEM images of Mo(VI) nanocatalyst

References:

[1] M. Bagherzadeh, M.M. Haghdoost, A. Shahbazirad. J. Coord. Chem. 65 (2012) 591.

[2] M. Bagherzadeh, M. M. Haghdoost, F. Matlobi-Moghaddam, B. Koushki-Foroushani, S. Sarazdi, E. Payab. J. Coord. Chem. 66 (2013) 3025.

Synthesis and characterization of platinum compounds with ferrocenyl ligand

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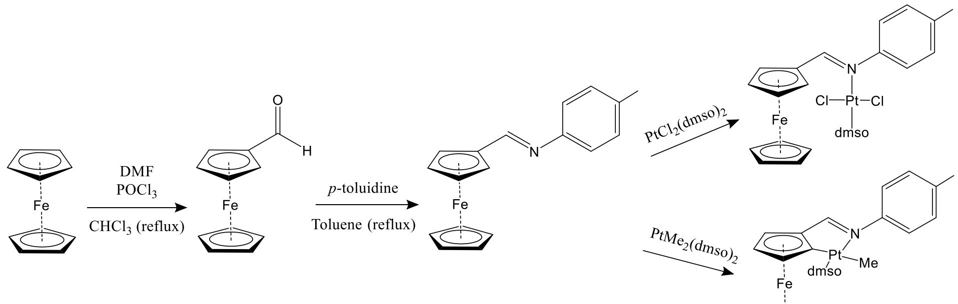
Abstract:

Platinum complexes are one of the most important compounds in cancer research and therapy. They target DNA molecules in cancerous cells and prevent these molecules from transcription and replication and thus result in cancer cell death. On the other hand, compounds having ferrocenyl moieties are widely used in several drugs including antiproliferative and antimalaria agents [1]; by combining these two promising compounds, platinum core and ferrocenyl moiety, we expect to build a stronger and more flexible antiproliferative drug [2]. In this project, we try to synthesis and investigate properties of a new series of platinum complexes with coordinated ferrocenyl imine ligand. We started from the ferrocene and it was transformed to its aldehyde and then to imine derivatives, finally combined with $Pt(Me)_2(dmso)_2$ and $Pt(Cl)_2(dmso)_2$ precursors (Scheme. 1). For biologic investigations of the new cyclometalated and monocoordinated platinum complexes, the Ligand-DNA binding via UV-Vis titration and also docking simulations were studied.The NMR spectra show formation of cyclometalated Pt(Me)(imine)(dmso) and monocoordinated $Pt(Cl)_2$(imine)(dmso) complexes. Experimental data from UV-Vis titration and docking simulations are in good agreement. In conclusion, some of the new Platinum complexes with coordinated / cyclometalated ferrocenyl imine ligand were synthetized. Their structures were identified by NMR spectra. Based on DNA titration and docking simulations, highest docking score to ct-DNA was for cyclometalated Pt(Cl)(imine)(dmso).



Scheme. 1. Prepared of $Pt(Me)_2(dmso)_2$ and $Pt(Cl)_2(dmso)_2$ precursors

References:

[1] M. Patra, G. Gasser, Nature reviews Chemistry. (2017) 0066.
[2] S. Pérez, C. López, A. Caubet, X. Solans, M. Font-Bardia, Eur. J. Chem. 10 (2008) 1599

Study on the reactivity of organoplatinum complexes with chelating 1, 2-bis(diphenylphosphino)ethane in presence of air

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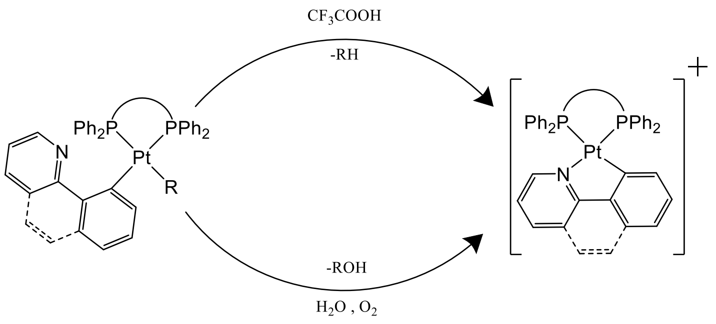
Abstract:

The Metal – Carbon bonds are among the strongest sigma bonds in organometallic complexes. Activation of these bonds with harsh conditions and reagents were common [1], but under mild conditions was unprecedent. In this work we suggest a straight forward reaction to activate these strong bonds (Scheme.1). Platinum complexes Pt(dppe)(R)(C^N) (dppe=bis(diphenylphosphino)ethane, R=Me or *p*-tollyl, C^N=2-phenylpyridne or benzo[*h*]quinoline) were synthesized and reacted in presence of air in different solvents such as: benzene, acetonitrile, dmso, acetone, ethanol, water/acetone and methanol. Mechanistic studies employed by Gaussian09 with B3LYP method and LANL2DZ basis set for Platinum atom and 6-31G (d) basis set for the rest of atoms.

Also similar reaction with acid reagent were carried out before, NMR spectra and Crystal structure of the products obtained. We compared NMR spectra of the resulting complex with previous work and it was revealed that the signals of the R group on Platinum complex are not present and also these data showed C^N chelate is closed. DFT calculation proposed the probable mechanism of this transformation. [2]

In conclusion, by using the milder condition we activate strong Pt – C bond. NMR spectra confirms formation of the products and DFT calculations proposed probable mechanism of this transformation. Also this process yields the ROH byproduct.



Scheme.1. suggest a straight forward reaction to activate these strong bonds

References:

[1] M. G. Haghighi, M. Nabavizadeh, M. Rashidi, M. Kubicki. Dalton Trans. 42 (2013) 13369.

[2] W. Liu, A. Sberegaeva, R. Nielsen, W. Goddard, A. Vedernikov, J. Am. Chem. Soc. 136 (2014) 2335.

Synthesis, Characterization and Biological evaluation of novel thiosemicarbazide and thiosemicarbazone functionalized calix[4]arene ligands and related transition metal complexes

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Abstract:

Calixarenes as the third generation of supramolecular hosts have attracted considerable attention among common molecules due to their easy synthesis from p-tertbutylphenol and formaldehyde via base-catalyzed condensation [1,2]. The flexibility of calixarene frame and capability of upper rim and lower rim for different functionalization make them an ideal candidate for use as coordinating ligand to different metal centers. With this regard, couple of the most important functional groups which can be introduced on calixarenes molecule are thiosemicarbazide and thiosemicarbazone with effective complexation capability [3], anti-cancer [4], antiviral and anti-bacterial [5] activities. we herein synthesized novel thiosemicarbazide **L1** and thiosemicarbazone **L2** functionalized calix[4]arene as ligand and their corresponding transition metal complexes for the first time. The synthesized compounds were characterized by FT-IR, ^{1}HNMR and ESI-Mass spectroscopy, elemental analysis and the structure of **L2** were studied by single-crystal diffraction method. coumponds **L1** and **L2** act as four-coordinated and six-coordinated ligand respectively (fig. 1). The compounds were evaluated for their antimicrobial activity, biocompatibility and anticancer activity in a panel of human breast cancer and bone cancer cell lines.

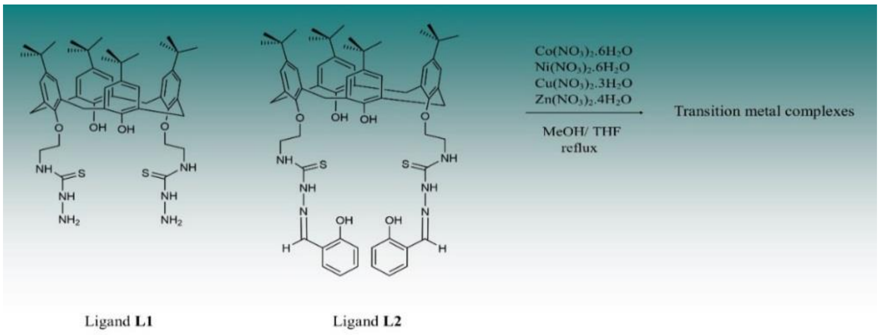

Fig. 1. L_1 and L_2

References:

[1] B. Bensenane, Z. Asfari, C. Platas-Iglesias, D. Esteban-Gómez, F. Djafri, M. Elhabiri, L. J. Charbonnière, Dalton Trans. 45 (2016) 15211-15224.
[2] T. Klejch, J. Slavíček, O. Hudeček, V. Eigner, N.A. Gutierrez, P. Cuřínová, P. Lhoták, New J. Chem. 40 (2016) 7935-7942.
[3] M. Gaber, T.A. Fayed, M.M. El-Gamil, G.M.A. El-Reash, J. Mol. Struct. 1151 (2018) 56-72.
[4] Ş.G. Küçükgüzel, G.P. Coşkun. Med. Chem. 16 (2016) 1288-1300.
[5] M. Molnar, M. Tomić, V. Pavić, Pharm. Chem. J. 51 (2018) 1078-1081.

Synthesis of UiO-66 based on $ZrOCl_2.8H_2O$ and TiO_2@UiO-66 Composite and photodegradation of Rhodamine-B

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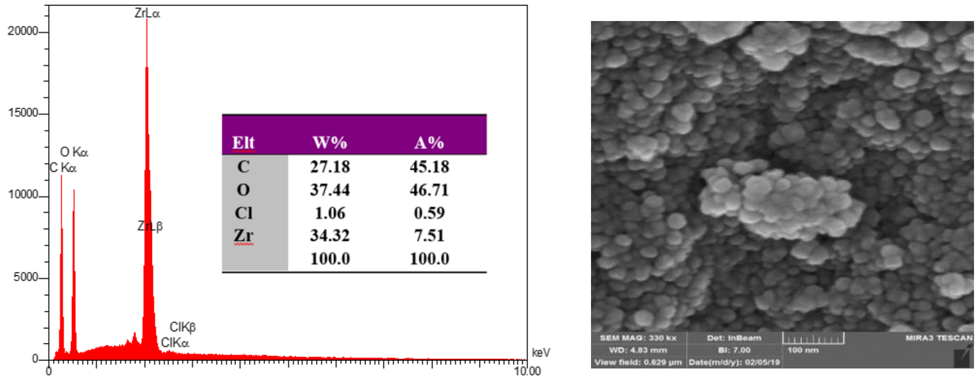
Abstract:

The organic-metal compounds are a new generation of Nano-adsorbents with high absorption capacity, due to the unique features, various methods of synthesis, the ability to adjust pore size, low density, high biocompatibility, high mechanical and thermal stability [1]. In this work, UiO-66 based on $ZroCl_2.8H_2O$ was synthesized and its photocatalytic properties were investigated [2]. The use of the less acidic $ZrOCl_2·8H_2O$ as the precursor seemed to be a suitable alternative to $ZrCl_4·xH_2O$, avoiding possible reproducibility issues as a consequence of the high hygroscopic character of $ZrCl_4$. $ZrOCl_2·8H_2O$ allowed the formation of good quality UiO-66 submicronic particles. In 70 minutes, UiO-66 destroyed 85% of Rhodamine-B under UV light irradiation.



Elt	W%	A%
C	27.18	45.18
O	37.44	46.71
Cl	1.06	0.59
Zr	34.32	7.51
	100.0	100.0

Fig 1. SEM and EDX of UIO-66 based on $ZroCl_2.8H_2O$.

References:

[1] S. Biswas, P. Van Der Voort, European Journal of Inorganic Chemistry. 12 (2013) 2154-2160.

[2] F. Ragon, P. Horcajada, H. Chevreau, Y. K. Hwang, U. H. Lee, S. R. Miller, C. Serre, Inorganic chemistry. 53 (2014) 2491-2500.

Preparation of magnetic chitosan/reduced graphene oxide nanocomposite for the removal of zinc and lead ions from water

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Abstract:
Nowadays, heavy metals contaminating water are considered as serious global concerns due to their deleterious environmental effects and not being biodegradable [1]. Among these toxic ions, zinc and lead species originated from diverse industries such as mining, metals, batteries, etc., could result in brain tissue damage, kidney failure and anemia. So far, different methods like membrane filtration, ion-exchange, adsorption, chemical deposition, advanced electrochemical oxidation processes and so on, have been used to reduce the amount of heavy metals in water. In this regard, using an in-expensive and biodegradable sorbent beseems a promising strategy which was reported on carbon, zeolite, metal oxides etc., in the past years [2,3]. In this work, we prepared a magnetic nanocomposite of chitosan-reduced graphene oxide (thiourea was used as reducing agent) to remove zinc and lead ions from simulated contaminated water. The structural properties of the as-synthesized nanocomposite was analyzed by XRD, FT-IR, FE-SEM, EDX, TEM and Raman spectroscopy characterization methods. The effects of some parameters such as pH, contact time and initial ion concentration were investigated on the Pb^{2+} and Zn^{2+} ions removal. The equilibrium and kinetic studies showed that lead and zinc adsorption followed Freundlich isotherm and pseudo-second order kinetic models. Moreover, the maximum adsorption capacities were estimated 169.58 and 421.78 mg/g for Pb^{2+} and Zn^{2+}, respectively.

References:

[1] M. Anbia, N. Mohammadi, K. Mohammadi, J. Hazard. Mater. 176 (2010) 965-972.
[2] C.F. Carolin, P.S. Kumar, A. Saravanan, G.J. Joshiba, M. Naushad, J. Environ. Chem. Eng. 5 (2017) 2782-2799.
[3] Q. Liang, H. Luo, J. Geng, J. Chen, Chem. Eng. J. 338 (2018) 62-71.

Cadmium and chromium adsorption from water using Fe_3O_4@SiO_2@ nano-chitosan/graphene oxide composite

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Abstract:

Heavy metals are the most toxic pollutants which enter the environment by diffusion through various industries and considered as a serious threat to human health due to the indissolubility and carcinogenic properties [1]. During past years, some techniques have been developed to remove heavy metal ions from water and wastewater such as ion-exchange, reverse osmosis, adsorption, photocatalytic degradation, membrane filtration, etc. The adsorption technique is used as a cost-effective and high-efficiency method. In recent decades, a variety of adsorbents including different polymers such as cellulose, chitosan, and carbonaceous matters like graphene oxide, as well as minerals as metal oxides, have attracted particular attention because of their unique properties [2,3]. In this study, we synthesized Fe_3O_4@SiO_2@ nano-chitosan/graphene oxide composite to remove Cr^{3+} and Cd^{2+} ions from contaminated waters. Chemical and morphological features of the prepared adsorbent were analyzed by Fourier transform infrared and Raman spectroscopies, scanning and transmission electron microscopies and X-ray powder diffraction technique. The results showed that the adsorption kinetic and isotherm data well fitted the pseudo-second-order and Freundlich models, respectively for cadmium ions with a maximum adsorption capacity of ca. 314.44 mg/g. Initial investigation was also carried out for the chromium adsorption which confirmed the high efficiency of the removal process for Cr^{3+} ions; the experiments will be completed. It is believed that the nanocomposite with surface functional groups such as OH, COOH, and NH_2 representing superior chemical properties, can be utilized as a promising candidate to remove toxic heavy metal ions especially cadmium and chromium from water.

References:

[1] C.F. Carolin, P.S. Kumar, A. Saravanan, G.J. Joshiba, M. Naushad, J. Environ. Chem. Eng. 5 (2017) 2782-2799.

[2] D. Ko, J.S. Lee, H.A. Patel, M.H. Jakobsen, Y. Hwang, C.T. Yavuz, H.C.B. Hansen, H.R. Andersen, J. Hazard. Mater. 332 (2017) 140-148.

[3] M. Anbia, N. Mohammadi, K. Mohammadi, J. Hazard. Mater. 176 (2010) 965-972.

Green synthesis of silver nanoparticles using C. verum extract

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Abstract:

A number of approaches are available for the synthesis of silver nanoparticles for example, reduction in solutions, chemical and photochemical reactions in reverse micelles, thermal decomposition of silver compounds, radiation assisted, electrochemical, sonochemical, microwave assisted process and recently via green chemistry route [1]. Greener syntheses of nanoparticles also provide advancement over other methods as they are simple, one step, cost-effective, environment friendly and relatively reproducible and often results in more stable materials [2]. Traditional drugs available now for oral or injectable administration are not always manufactured as the optimal formulation for each product. Products containing proteins or nucleic acids require a more innovative type of carrier system to enhance their efficacy and protect them from unwanted degradation. It is notable that the efficiency of most drug delivery systems is directly related to particle size. Due to their small size and large surface area, drug nanoparticles show increased solubility and thus enhanced bioavailability, additional ability to cross the blood brain barrier (BBB), enter the pulmonary system and be absorbed through the tight junctions of endothelial cells of the skin. Specifically, nanoparticles made from natural and synthetic polymers have received more attention because they can be customized for targeted delivery of drugs, improve bioavailability, and provide a controlled release of medication [3]. Because of antimicrobial properties and potential application of silver ions in medicine, in this research we have synthesized silver nanoparticles using Cinnamomum verum extract and characterized them using UV-Vis spectroscopy and scanning electron microscopy. Figure 1 shows SEM image of green synthesized silver nanoparticles using C. verum extact, size of these nanoparticles are in the range of 40.3- 81 nanometersand an UV-Vis peak in shows the formation of Ag NPs in figure 2.

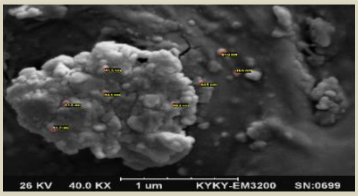

Fig.1. SEM image of green synthesized AgNPs

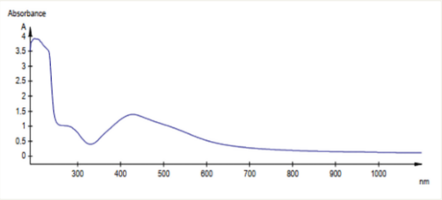

Fig.2. UV-Vis image of green synthesized AgNPs

References:

[1] A. Singh, D. Jain, M. K. Upadhyay, N. Khandelwal, H. N. Verma, 5 (2010) 483-489.

[2] S. Ahmed, S. M. Ahmad, B. Lal, Journal of Radiation Research and Applied Sciences. 6 (2016) 1-7.

[3] A.A. Syed, R. A. Saleh, J. Saudi Pharm. 26 (2018) 64–70.

Study on reactivity of organoplatinum complexes with electrophilic fluorinating reagents

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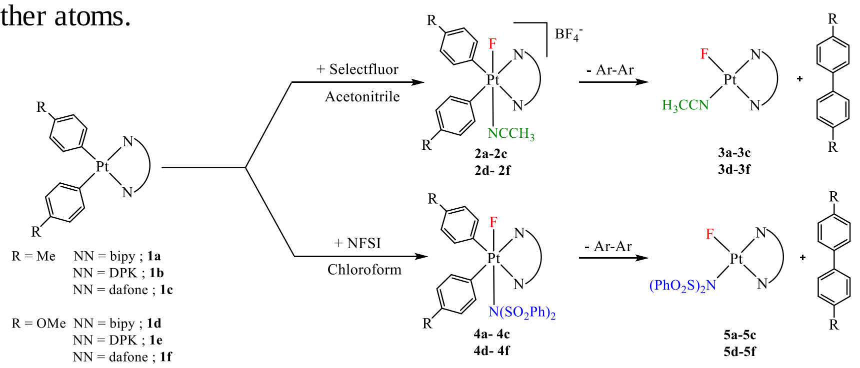
Abstract:

In recent years, C-H functionalization and aryl-aryl coupling reactions have great interest and are a valuable tool in organic synthesis. Among the many catalytic systems, palladium as a super-efficient metal has been reported in numerous transformations. However, these chemical reactivities with other group 10 metals are so limited [1], although platinum (II) complexes have great potential for activation of various inactivated C-H bonds that is the first step for their functionalization process [2]. One of the most important reasons for ignoring the platinum (II) complexes in these transformations is the reluctance of them to further reductive elimination (Red.El.) reactions to extrude the functionalized groups. Thus, introducing new methodology for increasing reductive elimination tendency of platinum complexes could be appreciated. Herein, the reactivity of diarylplatinum (II) complexes with two user friendly electrophilic reagents, NFSI (*N*-Fluorobenzenesulfonimide) and Selectfluor (*N*-Chloromethyl-*N′*-fluorotriethylenediammonium bis (tetrafluoroborate)) was studied (Scheme. 1). The resulted fluoro-Pt (IV) complexes are in dilemma between Ar-Ar and Ar-F Red.El. Reaction; however, they choose Pt (II) complex formation pathway through aryl-aryl Red.El. reaction and release the biaryl product. All complexes were fully characterized by ^{1}H and ^{19}F-NMR spectroscopy. Single crystal of **2a** was grown from a concentrated CH_2Cl_2 solution by slow diffusion of n-Hexane. Moreover, density functional calculations were performed with the program suite Gaussian03 using the B3LYP level of theory. The LANL2DZ basis set was chosen to describe Pt and the 6-31G (d) basis set was used for other atoms.



Scheme.1. the reactivity of diarylplatinum (II) complexes with two user friendly electrophilic reagents

References:

[1] McKeown, B. A., et.al. *Journal of the American Chemical Society*. 133 (2011) 19131.
[2] Labinger, *J. A., Chem. Rev*. 117 (2017) 8483.

Synthesis, Crystal Structure, Crystal Enginering and Theoretical Calculations of Some New Re(I)-tricarbonyl Complexes with Acenaphthequinonediimine Ligands

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Abstract:

Tricarbonyl rhenium(I) complexes of the type *fac*-Re(diimine)$(CO)_3Cl$ carrying polypyridyls such as *o*-phenanthroline or 2,2'-bipyridine ligands have been extensively studied for many years due to their exceptionally rich photophysical and photocatalytic properties [1]. These complexes possess relatively long-lived excited states which are of metal-to-ligand charge transfer (MLCT) character; they have been incorporated into a variety of π-conjugated oligomeric or polymeric systems [2]. We introduced new diimine derivatives with strong π-acceptor moieties namely BIAN which is bis (imino) acenaphthequinone instead of polypyridyls in Re $(CO)_3$ core to form Re$(CO)_3$(BIAN)Cl complexes.

In this study, first we synthesized new Zn complexes of acnaphthequinoneimine ligands and then the BIAN ligand was extracted from its Zn complex for synthesis of new Re $(CO)_3$ complexes. The new Re $(CO)_3$ complexes were investigated by UV-VIS, FT-IR and ^{1}H-NMR spectroscopic methods. Theoretical calculations were used by GAUSSIAN09, AOMix6.88 to study the electronic structure and NBO software to pursue the new intra- and intermolecular interactions such as n→π*.

References:

[1] E. Kianfar, U. Monkowius, E. Portenkirchner, G. Knör,. Z. Naturforsch B, 69 (2014) 691-698.
[2] W. K., Chan, C. S. Hui, K. Y. K. Man, K. W. Cheng, H. L. Wong, N. Zhu, A. B. Djurišić, Coord. Chem. Rev. 249 (2005) 1351-1359.

The effect of Mg atom on proton affinities of CH_3CONHO Ligand; A theoretical study

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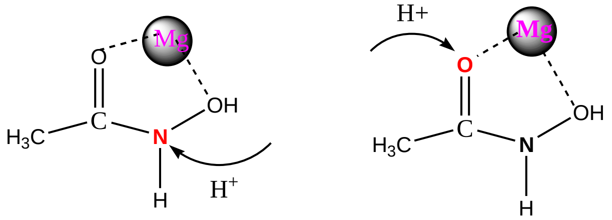
Abstract:
A theoretical study on protonation of CH_3CONHO Ligand in the presence of Mg atom has been reported. The gas-phase protonation energies (PA1) were computed using density functional theory (DFT) calculation. The proton affinity of a monobasic neutral ligand (related to the acidity) at 0 K is defined as the negative of the electronic energy difference between HL+ and L together with a correction for the difference in zero point energies. Two species CH_3CO (H+)NOH and CH_3CON(H+)OH can be considered in protonation of the above ligand. In order to understand the effect of Mg atom on protonation of CH_3CONHO Ligand which connect to OH group of this ligand (Fig. 1), the values of PA1 for two species before and after connection of Mg atom were calculated. The connection of Mg atom to OH group of this ligand has a decreasing effect on PA1 of two species.



$CH_3CON(H^+)OH$ $CH_3CO(H^+)NOH$

Fig. 1. Two species $CH_3C\mathbf{O}$ (H^+) NOH and $CH_3CO\mathbf{N}(H^+)OH$ in the presence of Mg atom

References:
[1] S. Salehzadeh, A. Shooshatri, M. Bayat, Dalton Trans. (2009) 2865.
[2] S. Salehzadeh, M. Bayat, M. Hashemi, J. Phys. Chem. A 112 (2008) 4090.
[3] Nepal, B.; Scheiner, S. Chem. Phys. 456 (2015) 34−40.
[4] H. Albright, P. S. Riehl, C. Christopher, M. Jolene, P. Reid, R. Jacob, L, Lindsey, A. Karp, M. P. Zimmerman, M. S. Sigman, and C. S. Schindler, J. Am. Chem. Soc. 141 (2019) 1690-1700.

Theoretical study on the non-covalent interaction between CH_3NO and PO_3H in the presence of Mg atom

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Abstract:

The non-covalent interactions between CH_3NO and PO_3H in the presence and in the absence of Mg atom were investigated using density functional theory (DFT) calculations. Firstly, the P…O and P…N interactions between NO group of CH_3NO and P atom of PO_3H were investigated. In this regard, the values of the interaction energies of these complexes were calculated. Then above interactions in the presence of Mg atom which coordinate to the O atoms of PO_3H were investigated. The obtained results showed that interaction energies between CH_3NO and PO_3H increase after coordinating the Mg atom to the O atoms of PO_3H molecule (Fig. 1). Also in order to understand the nature of the above interactions in these complexes, Bader's theory of atoms in molecules (AIM) and natural bond orbital (NBO) have been used.

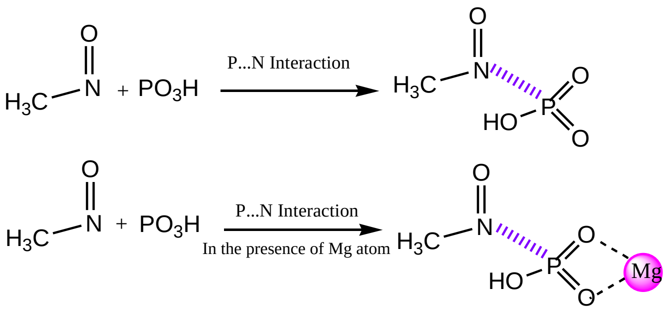

Fig.1. The P…N interaction between CH_3NO and PO_3H in the presence and in the absence of Mg atom

References:

[1] S. Scheiner, J. Chem. Phys. 134 (2011) 164313.
[2] S. Scheiner, Acc. Chem. Res. 46 (2013) 280–288.
[3] S. Scheiner, J. Chem. Phys. 134 (2011) 094315.
[4] B. Nepal, B. Scheiner, Chem. Phys. 456 (2015) 34–40.

Oxidative amidation of benzyl alcohol, benzaldhyde, benzoic acid styrene and phenyl acetylene catalyzed by HKUST-1

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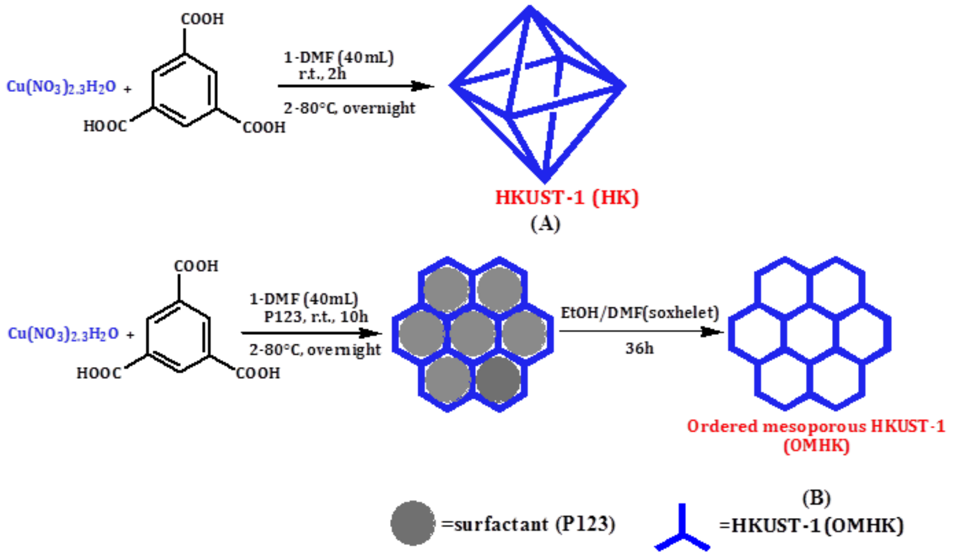
Abstract:

HKUST-1-Cu synthesized in the presence and absence of P-123 through the solvothermal method (Scheme. 1). After characterization using some different microscopic and spectroscopic techniques such as XRD, FT-IR, SEM, ICP, BET and TEM its catalytic activity was investigated in the oxidative coupling of benzyl alcohol, benzaldhyde, benzoic acid, styrene and phenyl acetylene with N,N-dialkylformamides for the preparation of N,N-dimethylformamides. Different derivatives of tertiary amides were synthesized in moderate to good yields in the presence of just ~0.28 mol% of this catalytic system. Reusability of the synthesized catalysts was examined and catalysts were reusable for 8 times without a significant decrease in optimized conditions [1, 2].



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Scheme.1. synthesized of HKUST-1-Cu

References:

[1] (a) J. M. Humphrey, A. R. Chamberlin, Chem. Rev. 97 (1997) 2243; (b) J. W. Bode, Curr. Opin. Drug. Discovery Dev. 9 (2006) 765; (c) T. Cupido, J. Tulla-Puche, J. Spengler, F. Albericio, Curr. Opin. Drug. Discovery Dev. 10 (2007) 768; (d) C.L. Allen, J.M.J. Williams, Chem. Soc. Rev., 40 (2011) 3405.

[2] (a) C.A.G.N. Montalbeti, Tetrahedron, 61 (2005) 10827; (b) E. Valeur, M. Bradley, Chem. Soc. Rev. 38 (2009) 606; (c) R.M. Al-Zoubi, O. Marion, D.G. Hall, Angew. Chem. Int. Ed. 47 (2008) 2876; (d) K.V.N.S. Srinivas, B. Das, J. Org. Chem. 68 (2003) 1165.

Synthesis and characterization of Ni (II) complex with an asymmetric tridentate Schiff base ligand and investigation of biological activitiy

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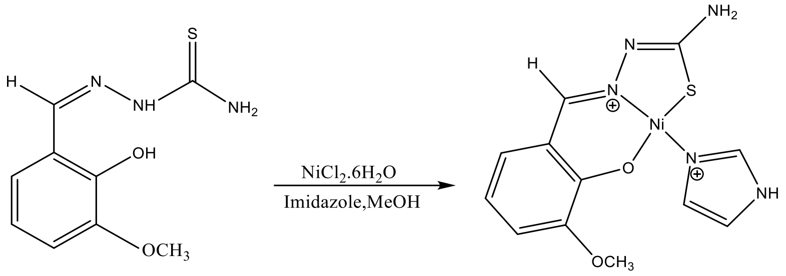
Abstract:

Schiff bases are flexible compounds that are easily synthesized from the condensation of an amino compound with carbonyl compounds and these interesting class of compounds having an azomethine linkage(C=N)[1]. Heterocyclic Schiff base ligands containing nitrogen, sulfur, and oxygen donor atoms, and their transition metal complexes are of great interest as simple structural models of the biological system due to the presence of multifunctional groups [2]. Schiff bases and their metal complexes have been shown to be promising leads for both synthetic and structural research due to their relatively simple synthesis and structural diversity and have been widely investigated, due to their incredible chemical properties and applications in various areas. Over the past few years, there have been many reports on their applications as homogeneous and heterogeneous catalysis and antibacterial, antifungal and antitumor activities[3,4].A new Ni(II) complex with 2-(2-hydroxy-3-methoxybenzylidene)hydrazine -1-carbothioamide (HL) in the presence of imidazole has been prepared (scheme 1). This complex was characterized by chemical analysis, ^{1}H NMR, UV–Vis and FT-IR spectroscopy. The synthesized ligand and the metal complex were screened for their antibacterial activity against two-gram positive bacteria (*Staphylococcus aureus* and *Bacillus subtilis*) and two-gram negative bacteria (*Escherichia coli* and *Klebsiella pneumonia*). The results revealed that the metal complex has shown pronounced activity than the free ligand[5].



Scheme. 1. A new Ni(II) complex with (HL)

References:

[1]M. Shakir, S. Hanif, M.A. Sherwani, O. Mohammad, M. Azam, S.I. Al-Resayes, J. Photochem. Photobiol. B: Biology. 157 (2016) 39–56.
[2] R. Alizadeh, M. Afzal, F. Arjmand, Spectrochim. Acta - Part A. 131 (2014) 625–635.
[3] Y.Yu, D.S.Kovacevic, A.R. Siafakas, P.J.Jansson, C.Stefani, D.B. Lovejoy, P.C.Sharpe, P.V.Bernhardt and D.R.Richadson, J. Med. Chem. 52 (2009) 5271-5294.
[4]D.S.Kalinowski, P.Quach and D.R.Richardson, Future Med. Chem. 6 (2009) 1143-1151.
[5] T. Rosu, E. Pahontu, C. Maxim, R.Georgescu, A. Gulea. Polyhedron. 30 (2011) 154-162.

Novel Synthesis M-DABCO MOF by solvothermal method

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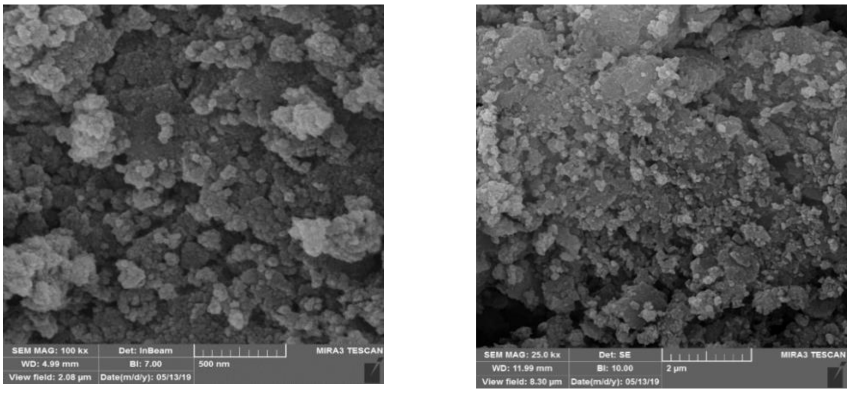
Abstract:
The synthesis and characterization of M-DABCO serie (M = Zr) of MOF with metal salt $ZrCl_4$ is described. Mixing of terephthalic acid (H_2BDC) and 1,4-diazabicyclo [2.2.2] octane (DABCO) with metal salt $ZrCl_4$ of mixed ligand systems to synthesize microporous MOF materials [1]. M-DABCO Synthesized were identified and characterized by fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron micrograph (SEM), Nuclear magnetic resonance (NMR) and BET.



Scheme. 1. SEM of M-DABCO (M=Zr).

References:
[1] S. Chaemchuen, K. Zhou, N. A. Kabir, Y. Chen, X. Ke, G. Van Tendeloo, F. Verpoort, Microporous and Mesoporous Materials. 201 (2015) 277-285.

Synthesis and chromotropism study of a copper complexes containing hemilabile tridentate and pseudo halide ligands

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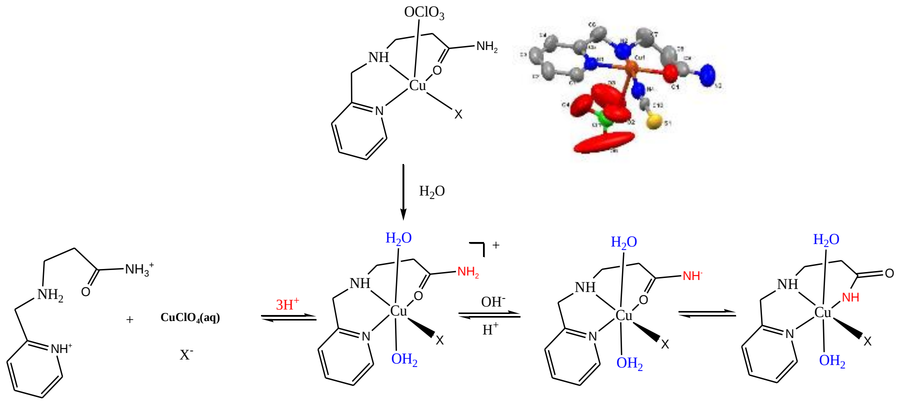
Abstract:

There is an interesting interchange between oxygen and nitrogen binding of amide group to metal ions in coordination compounds. Metal ions have tendency to interact only weakly with the oxygen atom of the carbonyl moiety of the amide group but it is strengthened if it is attached to an anchoring group with coordinating atom(s) so that a chelate ring can form that stabilizes the resultant complex due to chelate effect. However, the deprotonated amide nitrogen is a much stronger metal binding site; a condition that turn into more favorable at higher pH. Using appropriate metal ion, this phenomenon appears with distinct color change due to change in ligand field strength around the metal ion [1]. The reversible change in color of a substance under differing physical or chemical conditions such as pH and solvent, temperature, ion is called chromotropism [2]. In this work we prepared two copper(II) complexes with the general formula of [Cu(L)(X)](ClO4), where L =3-((pyridin-2ylmethyl)amino)propanamide, X= N_3^-, SCN^- were synthesized and characterized by elemental analyses, IR, UV-Vis spectroscopy techniques, molar conductance measurements and X-ray crystal analysis. The chromotropism (halo-, solvato- and ionochromism) of both complexes were studied using visible absorption spectroscopy. The complexes are found to be soluble in water and organic solvents and displayed reversible halochromism due to the flexible and sensitive nature of the amide group with changing pH values (Scheme 1). The complexes were ionochromic and exhibited high-sensitive and selective towards CN^- and N_3^- anions in presence of other halide and pseudo-halide ions.



Scheme 1. Interconversion of The complex triggered by acid and base (pH = 2.1-10)

References:

[1] L. Rostami, H. Golchoubian. Inorganica Chimica Acta. 462 (2017) 215–222.

[2] H. Golchoubian, A. Heidarain, E. Rezaee, F. Nicolò. Dyes and Pigments. 104 (2014) 175-184.

Synthesis, Characterization, and Electrocatalytic Activity of a New Polypyridyl Osmium (II) Complex

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Abstract:
The evidence that increased levels of atmospheric CO_2 are responsible for the rise in global temperature is overwhelming. The atmospheric CO_2 was measured to be 407 ppm in 2017, whereas it was 315 ppm in 1955 [1]. The utilization of CO_2 as a feedstock to produce the chemicals not only contributes to alleviating global climate changes caused by increasing CO_2 emissions, but also results in a great challenge in discovering new opportunities for the catalytic and industrial development. Several technologies have been studied to convert CO_2 to the value added chemicals and fuel such as methanol or CO as a renewable source [2, 3]. Among the most widely studied methods to CO_2 transformation, the efficient and selective electrochemical reduction is very important. A number of group VIII transition metal complexes (Fe, Ru, and Os) have been reported as the electrocatalysts for the CO_2 reduction [4, 5]. The detailed mechanistic insight required to design new electrocatalysts which run at low overvoltages with high selectivity of the desired product.

Here in, we report the synthesis and characterization of a new polypyridyl osmium (II) complex, $[Os\,(DMF)_2(tmp)_2](BF_4)_2$, by elemental analysis, spectroscopic techniques, and cyclic voltammetry. Moreover, the electrocatalytic activity of this complex was examined towards the CO_2 reduction to CO using cyclic voltammetry. The effect of the different parameters such as concentration of the electrocatalyst, temperature, and scan rate was investigated on the catalytic activity of the Os (II) complex. Further, DFT calculations were used to confirm the suggested electrocatalytic cycle for the conversion of CO_2 to CO.

References:
[1] R .J. Dixit, C. B. Majumder, J. CO_2 Util. 26 (2018) 80–92.
[2] R. Francke, B. Schille, M. Roemelt, Chem. Rev. 118 (2018) 4631−4701.
[3] M. Muratori, H. Kheshgi, B. Mignone, L. Clarke, H. McJeon, J. Edmonds, Int. J. Greenh. Gas Control 57 (2017) 34–41.
[4] M. Daryanavard, H. Hadadzadeh, M. Weil, H. Farrokhpour, J. CO_2 Util. 17 (2017) 80–89.
[5] C. D. Windle, R. N. Perutz, Coord. Chem. Rev. 256 (2012) 2562–2570.

Thermal behavior and antimicrobial activity of some new zinc (II), cadmium (II) and mercury (II) nitrate complexes

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Abstract:

Metal complexes with Schiff-bases as ligands play an important part in the development of coordination chemistry. The ability of different metal ions to arrange the coordinating ligands in different orientations is the reason for the development of different assembly structures [1]. Transition metal complexes of Schiff-base ligands find applications as models for metal enzymes, catalysts and modifiers in materials chemistry [2]. Schiff-bases and their biologically-active complexes have often been used as radiopharmaceuticals for cancer targeting, agrochemicals, as model systems for biological macromolecules, as catalysts and as dioxygen carriers [3].

In this research, a new N_4-Schiff base ligand (L) (L = obtained by condensation reaction between 2-nitrocinammaldehyde and triethylenetetraamine) were synthesized and characterized by FT/IR, ^{1}H and ^{13}C NMR, UV–visible, thermal analyses, and molar conductivity measurements. Thereafter, some new Zn (II), Cd (II) and Hg(II) nitrate complexes of the ligand have been prepared both in bulk and in nanostructure sizes under ultrasonic irradiation confirmed by XRD and SEM. Antibacterial/antifungal activities of the compounds were screened by the disk diffusion method against the Gram-negative bacteria and the Gram-positive bacteria. Also, the zinc and cadmium complexes were used as a precursor for the preparation of zinc and cadmium oxide nanoparticles.

References:

[1] N.S. Venkataramanan, G. Kuppuraj, S. Rajagopal. Coord. Chem. Rev. 249 (2005) 1249.
[2] M. Montazerozohori, S.A. Musavi, J. Coord. Chem. 61 (2008) 393
[3] M. Montazerozohori, H. Mohammadi, A. Masoudiasl, J. Iran. Chem. Soc. 14 (2017) 297.

Crystal structure and Hirshfeld surface analysis of [(S-)(C_6H_5)CH(CH_3)NP(S)NH(S)-(–)CH(CH_3)(C_6H_5)]$_2$,H_2O

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Abstract:

The cyclic compound [S-(–)-(C_6H_5)CH(CH_3)NP(S)NH(S)-(–)-CH(CH_3)(C_6H_5)]$_2$,H_2O, or $C_{32}H_{38}N_4P_2S_2$,H_2O is a member of a class of molecules that may be used for extraction of metals. The literature shows many studies of the bidentate phosphorus ligands HN [P (E) R2]$_2$ (E: O, S) [1] and RN [P (E) R2]$_2$ [2]. The title compound was characterized in the solid state by IR and X-ray crystallography and in the solution with calculation of the specific optical rotation. The compound crystallizes in the chiral space group $P2_12_12_1$ and the asymmetric unit of the structure consists of four symmetry-independent cyclodiphosphazanes and four water (H_2O) molecules.

In the molecular structure, each phosphorus atom is bonded to one sulfur and three nitrogen atoms. The P–N bond distances in the ring are longer than the P–N_H distances, and the P–S distances are in the range of 1.9376 (9) to 1.9434 (9) Å. These geometric parameters are in agreement with those observed in related compounds [3]. In the crystal structure, molecules are linked through N–H…O_W hydrogen bonds in a tape arrangement along the c axis (O_W is the oxygen of H_2O molecule). This pattern includes an $R_2^1(8)$ graph-set motif, formed through (NH…)(NH…)O_W grouping. The prevalence of these interactions is illustrated by an analysis of the three-dimensional Hirshfeld surface (HS) and by two-dimensional fingerprint plots (FP) for one of the cyclodiphosphazane molecules in the asymmetric unit. The relative contributions of different interactions in the HS are: H…H 69.0%, C…H/H…C 17.4% and S…H/H…S 10.6%.

References:

[1] A. Cristurean, S. Irisli, D. Marginean, C. Rat, A. Silvestru, Polyhedron, 27 (2008) 2143–2150.
[2] N. Peulecke, B. R. Aluri, A. Wöhl, A. Spannenberg, M. H. Al-Hazmi, Acta Cryst. 65 (2009) 1084.
[3] A. Alamdar, M. Pourayoubi, A. Saneei, M. Dušek, M. Kučeráková, M. S. Henriques, Acta Cryst. 71 (2015) 824–833.

Synthesis of a new azulene based ligand and its complexation with Gold (I) center

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Abstract:

Nonalternant hydrocarbons, consisting of organic conjugated hydrocarbons with odd membered carbon cycles, exhibit chemical and physical properties different from alternant hydrocarbons. Among the nonalternant hydrocarbons, azulene and its derivatives has received considerable attention from both a theoretical and experimental point of view [1]. Although azulene is an isomer of naphthalene and like naphthalene has a bicyclic unsaturated structure, it differs greatly in its properties from aromatic molecules built up from six membered rings. It has a blue color, large dipole moment and the best known example of a molecule that does not obey Kasha's Rule [2]. In this work the azulene derivative **1** has been prepared from reaction of 6-methyl azulene with B_2Pin_2[Bis(pinacolato) diboron]and then C-C bond coupling of **1** and 2-bromo pyridine in the presence of Palladium catalyst [$PdCl_2(PPh_3)_2$] affords the new azulene ligand **2**. Ligand **2** characterized using 1&2D NMR spectroscopy. Ligand **2** characterized using 1&2D NMR spectroscopy.

Reaction of Gold (I) complex AuCl (SMe_2) with two equivalent of **2** yields the the Gold (I) complex **3** (fig. 1).

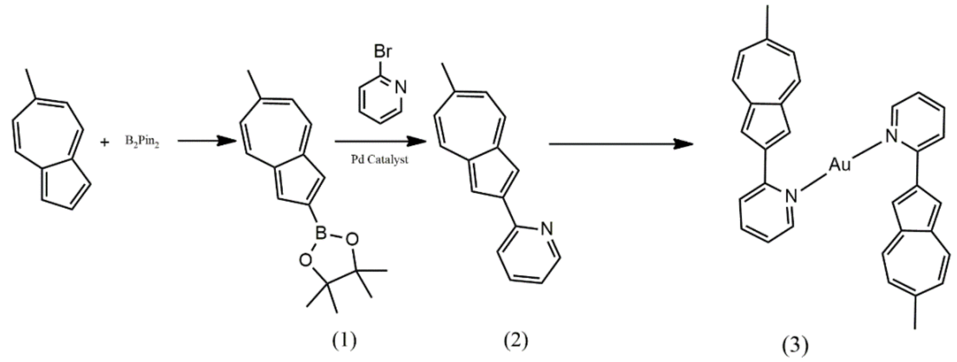

Fig.1. Synthesized of Gold(I) complex **3**

References:

[1] S. Jamali, N. Mousavi, M. Bagherzadeh, R. Kia and H. Samouei, Dalton Trans. 46(2017) 11327-11334

[2] J. I. Selco, T. Brooks, M. Chang, and M. T. Trieu, J. Org. Chem. 59 (1994) 429-433.

Porous nanorods as catalyst for one-pot synthesis and oxidation of tricyclic dihydropyrimidine derivatives in aqueous medium

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Abstract:

At the beginning of the new century, it is widely accredited that the development of efficient, practical and environmentally friendly methods of synthesis has been recognized as one of the most important topics of modern organic synthesis [1]. As the biggest pollution problem in many synthetic organic processes is with organic solvents, the development of efficient synthetic methodologies for organic reactions in the presence of non-toxic solvents is an important challenge. It is known that water is a non-flammable, non-hazardous, non-toxic, uniquely redox-stable and inexpensive green solvent. Therefore, using water as the reaction medium has gained considerable interest [2].

In recent years, much attention has been devoted towards dihydropyrimidine (DHPM) derivatives as the most important classes of tricyclic compounds, due to their significant therapeutic and biological activities, such as antiviral, antibacterial, anti-inflammatory, anti-hypertensive, anti-tubercular, anti-malarial, cytotoxic, and DNA-topoisomerase activities [3-6].

Thus, it is necessary to further develop an efficient and convenient method to construct this type of heterocyclic compounds. Based on our ongoing efforts in exploring environmentally benign syntheses, herein we report an efficient and green procedure for the synthesis of dihydropyrimidine derivatives in presence of [Porous manganese oxide nanorods (PMN) in water.

$$\text{Imidazole} + \text{ArCH}_2\text{O} + \begin{matrix}\text{Ethylacetoacetate}\\ \text{or}\\ \text{Malononitrile}\end{matrix} \xrightarrow[\text{Water, rt}]{\text{PMN}} \text{Dihydropyrimidine} \xrightarrow{\text{Oxidant}} \text{Oxidized product}$$

Facile synthesis of DHPM was achieved by using Porous manganese oxide nanorods under very mild conditions. The product was then oxidized to the desired compound. Further manipulation of this reaction is currently under way in our laboratory.

References:

[1] T. H. Istvan, T. A. Paul, Chem. Rev. 107 (2007) 2167.
[2] S. Chitra, N. Paul, S. Muthusbramanian, P. Manisankar, Green Chem. 13 (2011) 2777.
[3] L.E. Overman, M.H. Rabinowitz, P.A. Renhowe, J. Am. Chem. Soc. 117 (1995) 2657.
[4] A.R. Trivedi, V.R. Bhuva, B.H. Dholariya, D.K. Dodiya, V.B. Kataria, V.H. Shah, Bioorg. Med. Chem. Lett. 20 (2010) 6100
[5] B.R.P. Kumar, G. Sankar, R.B.N. Baig, S. Chandrashekaran, Eur. J. Med. Chem. 44 (2009) 4192.
[6] O. Alam, S.A. Khan, N. Siddiqui, W. Ahsan, S.P. Verma, S.J. Gilani, Eur. J. Med. Chem. 45 (2010) 5113.

Introducing the coordination polymer of lead (II) with PbO_4S environment

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Abstract:

Coordination polymers have been emerging as a topical research field in crystal engineering, solid-state chemistry, and materials science and they have attracted an enormous interest among chemists due to their novel physical and chemical properties [1]. These compounds are relevant to many fields such as organic and inorganic chemistry, biochemistry, materials science, electrochemistry, and pharmacology [2]. In this work, the Pb(II) complex of 2-mercaptoethenol (L), [Pb(2-mercaptoethenol)(μ-OAc)]n, was synthesize. The compound was identified by elemental analysis, FT-IR, ^{1}H NMR spectroscopy and single-crystal X-Ray diffraction. X-ray analysis revealed an 1D-coordination polymer extending by the acetato bridges. The complex cores on the chains are containing the lead (II) atom with rare PbO_4S environment and hemidirected arrangement. In the crystal structure of complex (figure 1), the lead atom is coordinated by one OS-donor ligand and two bridging acetato ligands, O2- and O-donor, with coordination number of five. The ligand acts as bidentate NS-donor and forms a five-membered non-planar chelate ring. The dihedral angles between mean planes through the four- and five-membered chelate rings is 87.32°, confirming that the acetato and ligand have perpendicular direction to each others. In the crystal structure the polymeric chain was formed by briddging the acetato ligands with coordination mode of “(O,µ-O)”. In the structural network of the complex, there are C–H···O and O–H···O hydrogen bonds which are appeared between adjacent chains to extend the 1D coordination polymer into 3D.

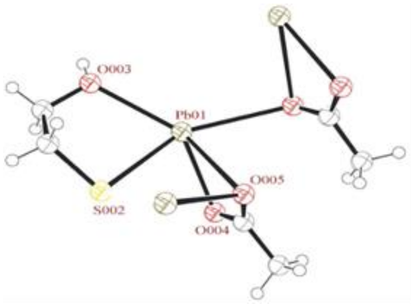

Fig 1. ORTEP-III diagram of the molecular structure of complex.

References:

[1] K. Biradha, M. Sarkar and L. Rajput, Chemical Communications. (2006) 4169-4179.

[2] K.M. Fromm, Coordination Chemistry Reviews, (2008) 856-885.

Dinuclear Zn (II) and tetranuclear Co(II) complexes of a N_2O_2 Schiff base ligand: Synthesis, crystal structure and spectral characterization

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Abstract:

Salpr-type ligands (R–CH=N–$(CH_2)_2$–N=CH–R) and their metal complexes have been extensively investigated in modern coordination chemistry for several decades [1,2]. In this study, we design, synthesis and characterize of two new complexes of Co(II) (**1**) and Zn(II) (**2**) with H_2**L** by elemental analysis, FT-IR spectra, UV-Vis spectra and X-ray crystallography. The X-ray crystal structures of the complexes **1** and **2** contain four and two metal ions, respectively, which are inter-connected through μ-phenolato and μ-acetato bridges. The crystal structures of the complexes are shown in Fig. 1.

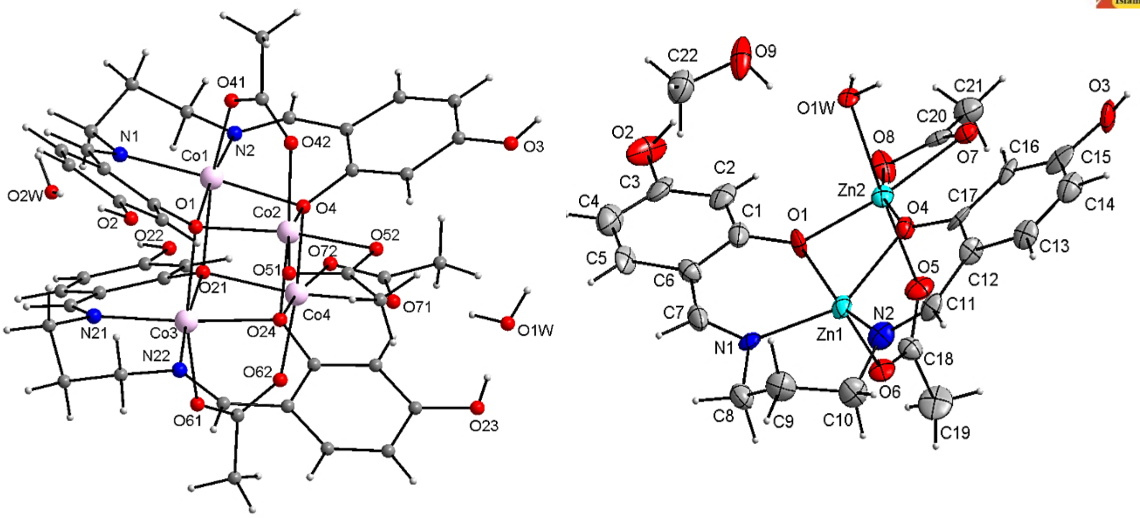

Fig. 1. View of the molecular structures of **1** and **2**.

References:

[1] (a) W.K. Dong, X.Y. Zhang, M.M. Zhao, G. Li, X.Y. Dong, Chinese J. Inorg. Chem. 30 (2014) 710.

[2] (a) S.T. Zhang, T.R. Li, B.D. Wang, Z.Y. Yang, J. Liu, Z.Y. Wang, W.K. Dong, Dalton Trans. 43 (2014) 2713.

Double complex formation of naphthadiaza-crown macrocycle bearing two pyridine side arms with ZnTPP

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Abstract:

During the last two decades, zinc metalloporphyrins (ZnTPPs) have been studied, inspired by several novel applications in different fields, namely solar energy harvesting, optoelectronics, sensors, and photodynamic therapy species [1]. Meanwhile, the interactions of donor molecules, as axial ligands of metalloporphyrin, with metalloporphyrins either in their ground or excited states can intensely influence of their UV/Vis and fluorescence spectra, redox properties, wherein the structure is crucial in understanding all the above-mentioned applications for ZnTPPs [1, 2].

After our recent successful synthesis of complex of ZnTPP with the aza-crown macrocycles bearing pyridine moiety (**ZnTPP$_{benz}$**) [2], herein we describe synthesis and spectroscopic results for a new double-complex of ZnTPP, axially ligated with naphthdiaza-crown macrocycle having two pyridine side arms (**ZnTPP$_{naph}$**).

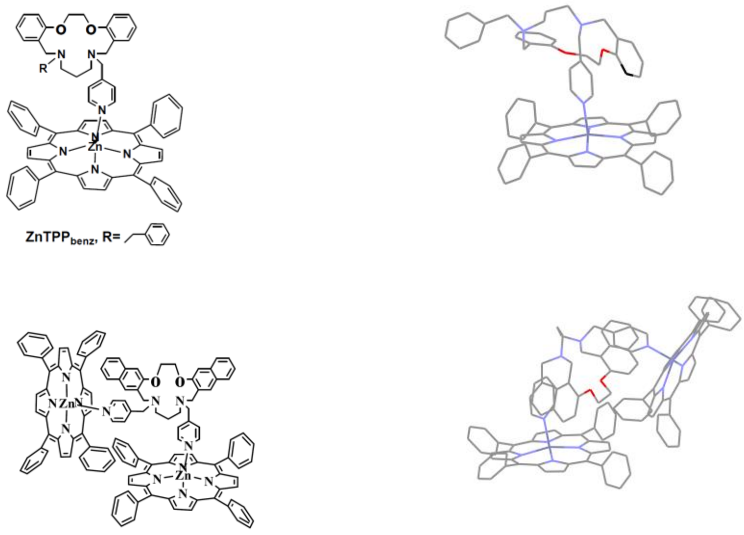

Fig. 1. The molecular and crystal structure of **ZnTPP$_{benz}$**^{2} (top) and **ZnTPP$_{naph}$** (down)

References:

[1] Z. Denden, K. Ezzayani, Eric Saint-Aman, F. Loiseau, S. Najmudin, C. Bonifácio, J.-C. Daran, H. Nasri, Eur. J. Inorg. Chem. (2015) 2596–2610 and the references cited therein.

[2] B. Ghanbari, L.Shahhoseini, M. Kubicki, Polyhedron, 133 (2017) 419–432.

Interaction and Diffusion of Li and Li+ with Defective Graphene

A comparative DFT study

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Abstract: Graphene is a substance with notable properties and uncommon thermal, optical and mechanical characteristics. The very high specific surface of graphene makes this material as an ideal support for catalysts and gas sensors [1]. It is a single layer of carbon atoms that arranged in aromatic rings, forming a honeycomb like structure. Graphene is a semimetal [2], a densely packed two-dimensional (2D) sheet of sp2-hybridized carbon system, owing to its special structural and notable properties [3-7] has become important in the field of material science and has numerous potential applications [8−9] .We investigated the defected graphene for diffusion Li and Li+.in this defected central C6 was removed and one crown of C6 unit saturated with 6H atoms were used. The resulting structure can be described to that of the molecule without its central C6 atoms is C90 H30. The properties and reaction these cases on graphene quantum dot sheet were studied by means of first principles based on density functional theory. We analyzed the thermodynamic and structural properties of this defected graphene, and compared interaction between single Li and Li+ and this defect. Finally diffusion and scanning of these cases were performed. All DFT calculations performed using Gaussian 09 package at the M062X/6-31G* computational level of theory. The diffusion barrier values, show the advantage of doped graphene for use in LiBs with respect to pure graphene. Examples of applications of these defects include supercapacitors, batteries, sensors, fuel cells, solar cells, and photocatalyst.

References:

[1] O. Leenaerts, P. Partoes, F.M. Peeters,, Phys. ReV B 77 (2008) 125416.
[2] A.H. Castro Neto et al. ReV. Mod. Phys., 81(2009) 109-162.
[3] D. S. L. Abergel, V. Apalkov, J. BerasheVich, T. Ziegler, Adv. Phys. 59 (2010) 261−482.
[4] M. J. Allen, V. C. Tung, R. B. Kaner, Chem. ReV. 110 (2010) 132−145.
[5] M. F. Craciun, S. Russo, M. Yamamoto, S. Tarucha, Nano Today, 6 (2011) 42−60.
[6] C. N. R. Rao, K. Biswas, K. S. Subrahmanyam, Govindaraj. Chem. 19 (2009) 2457− 2469.
[7] V.Singh, D. Joung, L. Zhai, S. Das, S. Khondaker, Mater. Sci. 59 (2011) 1178−1271.
[8] Z. K. Liu, J. H. Li, Z. H. Sun, G. A. Tai, S. P. Lau, F. Yan, ACS Nano, 6 (2012) 810−818.
[9] Y. P. Dan, Y. Lu, N. J. Kybert, Z. T. Luo, A. T. C. Johnson, Nano Lett.9 (2009) 1472−1475.

Effect of Electric Field on Defected Graphene Quantum Dot: A DFT Study

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Abstract: Graphene quantum dots (GQDs) [1-4] are a few atoms thick graphene and their size is less than 30 nm. GQDs possess excellent features such as large diameter, high surface area, and good surface grafting using conjugated π-π network and other physical properties [5]. These properties include highly tunable photoluminescence, remarkable UV-blocking property, good biocompatibility, unique spin property, and high photo stability. It possesses a wide range of applications in ion detection, bio-imaging, photo catalysts, photo detectors, electrochemical luminescence, optical sensors and photovoltaic devices [6, 7].

Doping of graphene and GQDs with heteroatoms has led to improve their catalytic activities towards oxidation-reduction reactions which are a requisite for energy storage or conversion. We designed a porous graphene and doped them with N. in this defected central C_6 was deleted and one crown of C_6 unit saturated with 3N atoms were used. The resulting structure can be described to that of the molecule without its central C_6 atoms is $C_{87}H_{24}N_3$. we analyzed the interaction energy and properties of Helium on defective graphene sheet in present of electric field were investigated by means of first-principles based on density functional theory. All DFT calculations performed using Gaussian 09 package at the M062X/6-31G* computational level of theory. Our results show that the He optimized energy value on doped graphene and band gap decreased when electric field rises.

References:
[1] J. Zhang, F. –X. Xiao, J. Mater. Chem. A 5 (2017) 23681-23693.
[2] A.E. Fatimy, R, K.M. Daniels, D.K. Gaskill,P. Barbara, Nat.Nanotechnol. 11 (2016) 335-338.
[3] N.M. Freitag, L.A. Chizhova, P. Nemes-Incze, C.R. Woods, Nano Lett. 16 (2016) 5798-5805.
[4] C. Gutiérrez, L. Brown, C.-J. Kim, J. Park, A.N. Pasupathy, Nat. Phys. 12 (2016) 1069-1075.
[5] N. Li, A. Than, C. Sun, J. Tian, J. Chen, K, ACS Nano 10 (2016) 11475-11482
[6] N. Zhang, M.-Q. Yang, S.Q. Liu, Y.G. Sun, Y.-J. Xu, Chem. Rev. 115 (2015) 10307-10377.
[7] Y. Zhao, X. Wu, S. Sun, L. Ma, L. Zhang, Carbon 124 (2017) 342-347.

Synthesis, Characterization and Photoluminescence Investigation of a New Arylplatinum (II) Complex Containing N_2S_2 Donor Atoms

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Abstract:

Organometallic compounds containing metal-carbon bonds have many applications in biochemistry. One of the most important elements in organometallic chemistry is platinum, because it makes a wide range of organometallic compounds that are kinetically inert to provide them to be isolated and characterized. The importance of platinum(II) and palladium(II) complexes with square-planar geometry have been increased after finding of the anti-tumor activity of *cis*-dichlorodiammineplatinum(II) [1]. Also, organoplatinum complexes are oxidized or reduced easily by two-electron transfer between the two essential oxidation states and so the oxidative addition and reductive elimination reactions perform easily in these complexes. Since, the main geometry for +2 and +4 oxidation state are square planar and octahedral, respectively [2]. In this research, we reported synthesis and structural characterization of a new arylplatinum (II) complex containing N_2S_2 donor atoms. In order to synthesize of this complex, $[(p\text{-}MeC_6H_4)_2Pt\,(SMe_2)_2]$ was used as starting material and was synthesized by the reaction of $[PtCl_2\,(SMe_2)_2]$ and *para*-tolyllithium. The new platinum complex containing N_2S_2 chelating ligand was synthesized by the reaction of *cis*-$[Pt\,(p\text{-}MeC_6H_4)_2(SMe_2)_2]$ and chelating ligand in a 1:1 molar ratio. This reaction was performed in chloroform and stirred for 72 h. Then the solvent was evaporated and an orange precipitate obtained and washed with n-hexane and diethylether. The complex was characterized by FT-IR, ^{1}H NMR, UV-Vis spectroscopies, elemental analysis and molar conductance. Emission behavior of this complex was studied by fluorescence spectroscopy.

References:

[1] B. Rosenberg, L. Van Camp, E.B. Grinley, A.J. Thomson, J. Biol. Chem. 242 (1967) 1347-1352.

[2] F.R. Hartly, The Chemistry of Platinum and Palladium, Applied Science, London. (1973).

Synthesis, Characterization and Crystal Structure Determination of Iron(III) Complexes: [Fe(5,5'-dmbipy)$_2$Cl$_2$]Cl, [Fe(5,5'-dmbipy)$_2$Cl$_2$][FeCl4] and [Fe(5,5'-dmbipy)$_2$Cl$_2$]ClO$_4$

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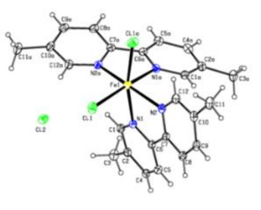
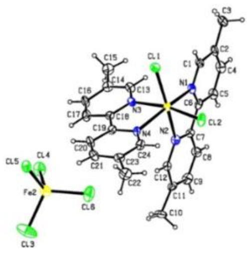
Abstract:

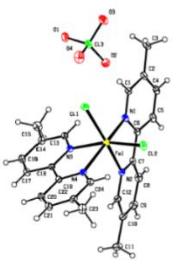
Bipyridine and analogous ligands such as phenanthroline are commonly used in the formation of different complexes with a general variety of transition metals [1]. Studies of these transition metal complexes are important in understanding electron transfer processes, mixed valence complexes, magnetic coupling and magnetic transitions [2]. Although bipyridine coordination to iron has been widely investigated, most complexes are iron (II) complexes, little attention has been paid to bipyridine iron (III) complexes [3-5]. In order to expand this field, [Fe(5,5'-dmbipy)$_2$Cl$_2$]Cl complex (1), [Fe(5,5'-dmbipy)$_2$Cl$_2$][FeCl$_4$] complex (2) and [Fe(5,5'-dmbipy)$_2$Cl$_2$]ClO$_4$ complex (3) (5,5'-dmbipy is 5,5'-dimethyl-2,2'-bipyridine) were prepared from reaction of FeCl$_3$.6H2O with 5,5'-dimethyl-2,2'-bipyridine in methanol, hydrochloric acid 0.1 M and sodium perchlorate respectively. These complexes were characterized by elemental analysis, IR, UV-Vis and ^{1}H-NMR spectroscopy and their structures were studied by single-crystal diffraction method. In these complexes, Fe^{III} ion is six-coordinated in a distorted octahedral environment.



Complex 1



Complex 2



Complex 3

References:

[1] E. C. Constable, Adv. Inorg. Chem. 34 (1989) 1.
[2] E. C. Constable, & P. J. Steel, Coord. Chem. Rev. 93 (1989) 205.
[3] V. Amani, N. Safari, H. R. Khavasi, Polyhedron, 26 (2007) 4257.
[4] V. Amani, N. Safari, H. R. Khavasi, & Mirzaei, P. Polyhedron, 26 (2007) 4908.
[5] Farsheed Shahbazi-Raz, Vahid Amani, Ehsan Bahojb Noruzi, Nasser Safari, Roman Boca, Ján Titiš, Behrouz Notash

Synthesis, characterization, crystal structure and Hirshfeld surface analysis of 4'-furyl-2, 2’:6’, 2’’-terpyridine complex of Ni(II): a new precursor toward the formation of nickel oxide nanoparticles

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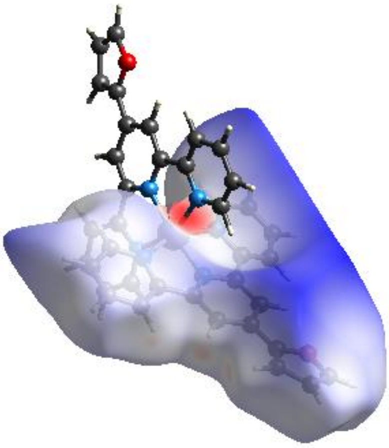
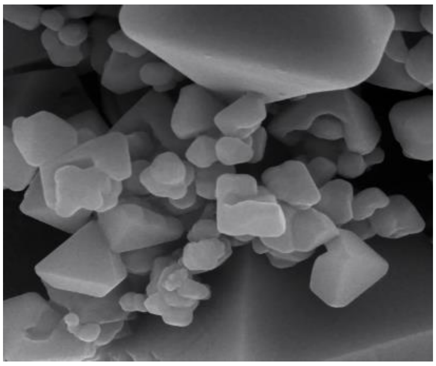
Abstract:

The coordination chemistry of 2, 2′:6′, 2″-terpyridine derivatives is of particular interest due to their applications such as catalyst, biochemistry, anticancer agents and nanoscience [1,2]. Herein, we report the preparation and characterization of a new complex [Ni (ftpy)2](PF6)2 (1) (ftpy = 4'-(furan-2-yl)-2,2':6',2''-terpyridine) which has been characterized by elemental analysis, FTIR and X-ray crystallography. The X-ray crystal structure of 1 shows that nickel (II) ion is hexa-coordinated by six nitrogen atoms from two ftpy ligands with N6 coordination sphere, displaying a distorted octahedral arrangement. Hirshfeld surface analysis and two-dimensional fingerprint maps were used for 1 which indicate the N…H, H…F and H…H interactions. Thermal properties of 1 were also investigated. On the other hand, nickel(II) oxide nanoparticles were prepared by simple calcination of complex 1 at 600 °C in air. The resulting nanostructures have been characterized using XRD, FESEM and EDX which show the purity of the resulting nanoparticles. Notably, the average particle size using Scherrer’s equation is calculated to be about 27 nm.





References:

[1] H. Hofmeier, U.S. Schubert, Chem. Soc. Rev. 33 (2004) 373.
[2] L.L. Cai, Y.T. Hua, Y. Li, K. Wang, X.Q. Zhang, G. Muller, X. M. Li, G.X. Wang, Inorg. Chim. Acta 489 (2019) 85.

Labile interactions effects in self-assembly of new Cu (II) metal-organic coordination system

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Abstract:

Metal-organic coordination systems have attracted considerable attention in recent years for their various applications [1]. These materials are built from metal ions (or metallic clusters) and organic ligands. They have great potential due to their ease of processability, flexibility, structural diversity, and geometrical control [2]. The components in coordination compounds mainly exist in a solid state. In solution, small units create building blocks through coordination interactions and weak forces, such as hydrogen bonding, π-π stacking, and van der Waals interactions. Based on these labile interactions, coordination sestems then grow through self-assembly processes [3]. In the present work, we investigate the coordination behaviors of new of Cu(II) coordination systems with pyridin-2-isonicotinohydrazide multifunctional ligand. The arrangement of metal-ligands produces quadric nuclear square ring. The adjacent frameworks connected by strong hydrogen bonding interactions and other labile interactions of adjacent aromatic rings. We describe a simple sonochemical synthesis method for a nano-structure of this compound and its use in the preparation of copper oxide nano-particles.

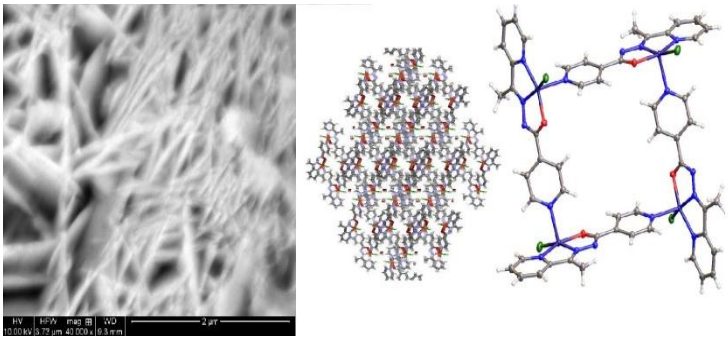

Fig. 1 from right: Discrete structure – 3D structure via labile interactions -morphology of the nano-structures.

References:

[1] J.R. Li, J. Sculley, H.C. Zhou, Chem. Rev. 112 (2011) 869.
[2] R.A. Bilbeisi, J.-C. Olsen, L. J. Charbonnière, A.Trabolsi, Inorg.Chim. Acta. 79 (2014) 417.
[3] M.D. Ward, P.R. Raithby, Chem. Soc. Rev. 42 (2013) 1619.

A reliable and efficient method for synthesis of hydroxyapatite-chitosan nanocomposite

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Abstract:

Inorganic-organic nanocomposites have attracted increasing attention as promising material for medical applications [1]. Hydroxyapatite (HA) as the main inorganic constituent of bone is one of the most relevant inorganic phase of nanocomposites. Several studies have investigated the synthesis of hybrid HA/polymer materials. Among them, composite prepared from HA and chitosan (CS) has advantages due to its biocompatibility, biodegradability and bioactivity [2]. Although several methods including coprecipitation, sol–gel, hydrothermal and emulsion have been reported for the synthesis of HA-CS nanocomposite, still remains a great demand for the introduction of efficient, simple and practical method with controlled manufacturing conditions which enables an accurate control of nanocomposite properties such as size, geometry, morphology, homogeneity and surface area. Among the mentioned methods, coprecipitation is a simple, economical and industrially viable technique but the most common drawback of this technique is formation of agglomerated precipitate. To overcome the problem of agglomeration we have suggested a new combined sonochemical-coprecipitation method for synthesis of HA-CS nanocomposite since the ultrasound irradiation has proven to be a beneficial technique to prevent agglomeration arises from acoustic cavitation phenomenon [3]. In this work, we have successfully synthesized HA-CS nanocomposite by sonochemical-coprecipitation method under controlled conditions. The prepared HA-CS nanocomposite was characterized by the Fourier Transform Infrared (FTIR) spectroscopy, the X-Ray Diffraction (XRD), thermogravimetric analysis (TGA), scanning electron microscopy (SEM) and the particle size analysis. The characterization results confirmed that this technique leads to a more reliable production of HA-CS nanocomposite with more uniform particle size and higher morphological homogeneity.

References:

[1] C. Sanchez, B. Julián, P. Belleville, M. Popall, J. Mater. Chem., 15 (2005) 3559–3592.
[2] S. Dorozhkin, J. Funct. Biomater, 6 (2015) 708–832.
[3] V.K. Patel, J.D. Sen, H.U. Pate, C.N. Patel, J. Chem. Pharm. Res., 2 (2010) 573-580.

Synthesis and characterization of pH-sensitive curcumin loaded onto the surface of Ni-Cu-Zn Fe_2O_4 nanoparticles modified by pluronic P123 for controlled drug release

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Abstract:

Over the past few decades, magnetic nanoparticles have been considered by many researchers due to their unique physicochemical, magnetic and optical properties and extensive applications in the field of biomedical (such as magnetic resonance imaging (MRI), drug delivery system and magnetic hyperthermia), etc [1]. Most of the magnetic nanoparticles are made up of iron oxide, such as magnetite (Fe_3O_4), maghemite (γ-Fe_2O_3), hematite (α-Fe_2O_3) and ceramic spinel ferrites with a structure MFe_2O_4 that M containing some metals such as Cu, Mn, Cd, Ni, Zn, Ca [2]. However, in this work, we have tried to examine the effect of different metal ions (Cu^{2+} and Ni^{2+}) with different ratios on the size, morphology and magnetic properties of ferrite spinel ($Ni_xCu_{0.2-x}$) $Zn_{0.8}Fe_2O_4$ nanoparticles. We used two methods of gel auto-combustion and microwave for producing spinel ferrite nanoparticles. Pluronic stabilized magnetic nanoparticles (PSMNPs) were producted by introducing amphiphilic tri-block co-polymer, Pluronic P123 onto the surface of hydrophobic magnetic nanoparticles (HMNPs) and evaluated their efficacity for delivery of hydrophobic anti-cancer agent, curcumin (CUR) [3]. The CUR@PSMNPs are well characterized for their structural, morphological, magnetic properties by various characterization techniques such as the XRD, SEM, IR, EDX, UV–Vis, VSM and TEM analysis. The MTT test showed that both curcumin and CUR@PSMNPs with different values of IC_{50} significantly reduced the proliferation of 4T1 cells. These results indicated that the CUR@PSMNP formula is convenient to producing cytotoxic tumors, that is probably due to increased bioavailability of the drug to the target site.

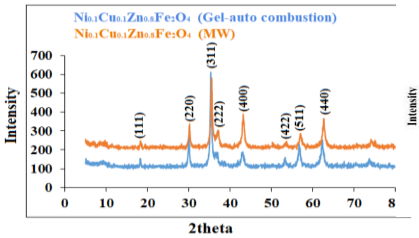

Fig.1 XRD pattern of CUR@PSMNPs

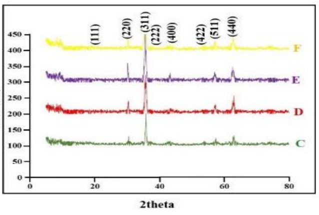

Fig.2 The XRD

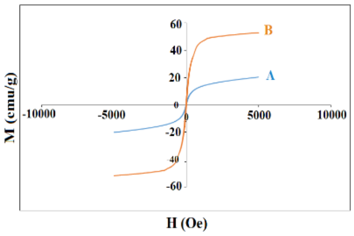

Fig.3 The VSM of CUR@PSMNPs

References:

[1] H. Thi, T. Thanh, D.H. Nguyen Tran, L.G. Bach, H. Vu-Quang, D.C. Nguyen, K.D. Park, and D.H. Nguyen, 2019. Pharmaceutics, 11(3), p.120.

[2] L.H. Nie, F.H. Bai, M.F. Liu, J. Ning, B.T. Chen, and Z.Y. Wu, 2016. Integrated Ferroelectrics, 168(1), pp.183-194.

[3] K.C. Barick, , S.L. Gawali, A. Sarkar, A. Kunwar, K.I. Priyadarsini, and P.A. Hassan, 2016. RSC Advances, 6(101), pp.98674-98681.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Synthesis and characterization of a new dione by Mannich reaction method containing Thiophene moiety with related macrocyclic ligands and complexes

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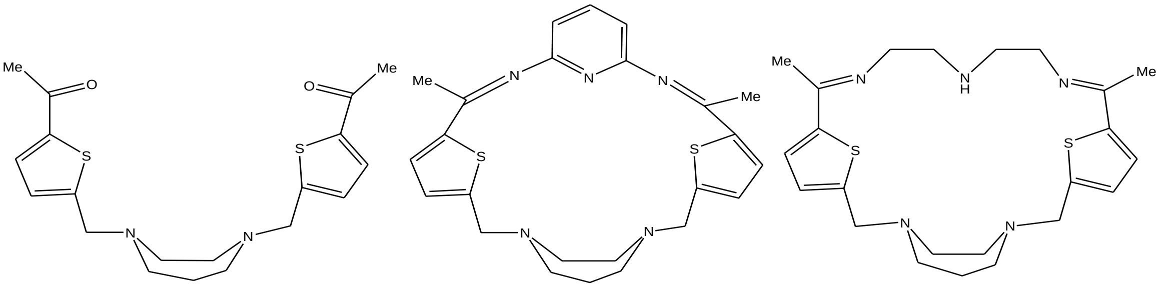
Abstract:
The importance of the Mannich reaction relates to the fact that the products of this reaction, known as Mannich bases, the reaction provides a good method for C-C bond formation. It essentially consists of the condensation of an aldehyde (mostly formaldehyde) and an amine with a substrate possessing acidic hydrogen [1].

Thiophene is a heterocyclic compound consist of sulfur atom, it is aromatic as indicated by its extensive substitution reactions [2].

In this work a new diketone has prepared by using 2-Acetyle thiophene and Homopiperazine by Mannich reaction method (1) and related ligands were obtained by condensation of synthesized dione with 2, 6-diamino pyridine (2) or Bis(2-aminoethyl) amine (3). Mn^{2+} and Zn^{2+} complexes of these ligands were syntesised by using of perchlorate salts of these ions. The ketone and related ligands and complexes were investigated by elemental analysis, IR spectroscopy, ^{1}H and ^{13}CNMR and Mass analysis.



(1)

(2)

(3)

Fig.1. structure of dione(1) and macrocyclic ligands(2, 3)

References:

[1] Cordova, A.; Watanabe, S.-I.; Tanaka, F.; Notz, W.; Barbas, C. F., Journal of the American Chemical Society. 124 (9) (2002) 1866–1867.

[2] J. Roncali, Chem. Rev. 92 (4) (1992) 711–738.

Effect of electric field on Interaction of Na+, Li+ with Defected silicene sheet: DFT study

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Abstract: Silicene as an equivalent of graphene has recently obtained volatile studies due to its many amazing remarkable properties such as topological insulating state, the realization of the quantum spin Hall effect, ultra-high carrier mobility and the existence of the Dirac cone [1-3]. Silicene could be synthesized and provided using perfect semiconductor techniques, but defects are almost obvious during the fabrication process, and their existence strongly affects thermodynamic and electronic properties of two-dimensional materials [4, 5]. In this contribution, we performed calculations to investigate the effect of absent and present of vertical electric field on interaction energy of Na+, Li+ with defected silicene sheet. For this reason, we have examined theoretically the creation of silicene sheet and their defected silicene (divacancies = missing two atom) structures with Li and Na ions. Calculations were carried out within the framework of density functional theory (DFT) using a local density approximation scheme, as implemented in the Dmol3 package. The generalized-gradient approximation (GGA) for the exchange correlation functional with the parametrization of Perdew − Burke − Ernzerhof (PBE) was used [6, 7]. The double numerical plus polarization (DNP) basis set, 4.4 basis file and Monkhorst-Pack k-point mesh of (6×6×1) and (4×4) supercell. To avoid interactions of the silicene sheet with its periodic images, a vacuum gap of 60 Å in the z direction was used. According to the gained results for defected silicene structures with Li and Na ions, our calculations show that vertical electric field can impact on interaction energy values structures of silicene and it could be worthwhile strategy for applications of these defects include sensors, batteries, supercapacitors, solar cells and fuel cells.

References:

[1] D. Jose, & A. Datta, Acc. Chem. Res, 47 (2014) 593–602.
[2] C. C. Liu, W. Feng, & Y. Yao, Phys. Rev. Lett. 107 (2011) 076802.
[3] Z.-G. Shao, X.-S. Ye, L. Yang, & C.-L. Wang, J. Appl. Phys, 114 (2013) 093712.
[4] Z.Y.Ni, Nano. Lett, 2012, 12.
[5] G. Brumfiel, Nature, 495 (2013) 152–153.
[6] J. Soler, J. Phys.: Condens. Matter, 14 (2002) 2745.
[7] J. Perdew, Phys. Rev. Lett, 77 (1996) 3865.

A theoretical study for the Quantum Capacitance Effect of Electric Field on Defective Silicene

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Abstract: Supercapacitors are fully interested in recent years because of their distinctive features such as long life, rapid charging, high-power density, low cost, high power storage and faster release [1-3]. To obtain high capacitance for Supercapacitors, the choice on electrode materials is a key factor and limiting factor in the total capacity of Supercapacitors is their finite quantum capacitance [4]. Silicene is supposed to have potential application of supercapacitor [5].

In this study, we have investigated defects and electric field in Silicene sheet and then compared the effects of them on quantum capacitance. All our density functional theory (DFT) Calculations were carried out within the generalized-gradient approximation (GGA) for the exchange correlation functional with the parametrization of Perdew−Burke−Ernzerhof (PBE), as implemented in the Dmol3 package [6,7]. The double numerical plus polarization (DNP) basis set, 4.4 basis file and Monkhorst-Pack k-point mesh of (6×6×1) and (4×4) supercell. To avoid interactions of the silicene sheet with its periodic images, a vacuum gap of 60 Å in the z direction was used. We investigated the effect of absent and present of vertical electric field on defects silicene, in order to improve the quantum capacitance by the way of electric field. On the basis of these results, we expect these results stimulate the further experimental works on silicene and shed some light on silicene-based electrodes for the applications of supercapacitors.

References:

[1] M. Mousavikhoshdel, et.al, J. Phys. Chem. C 119 (2015) 26290-26295.
[2] L. L. Zhang, et.al, Energ. Environ. Sci. 5 (2012) 9618–9625.
[3] Y.-Z. Zhang et.al, Chemical Society Reviews, 44 (2015) 5181-5199.
[4] M. D. Stoller, et.al, Energ. Environ. Sci. 4 (2011) 4685-4689.
[5] Y. Shulga, et.al, J. Power Sources, 279 (2015) 722–730.
[6] J. Soler, J. Phys.: Condens. Matter, 14 (2002) 2745.
[7] J. Perdew, Phys. Rev. Lett, 77 (1996) 3865.

New dimethyltin(IV) complexes containing pyridyl ligands and halide or pseudohalide

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Abstract:

Organotin complexes have attracted much consideration attributable to their properties, structural chemistry and potential applications in numerous scientific areas. Among them, organotin (IV) compounds with nitrogen containing aromatic ligands are of particular interest over the last years. In general, the biocidal activity of organotin complexes is greatly influenced by the structure of the molecule and the coordination number of the tin atoms which can be predicted by Sn-N bond distance [1, 2]. It has been shown that some organotin (IV) carboxylates can be active against cancer cells where cisplatin is inactive for these resistive cancer cells [3]. Herein, we report the preparation and characterization of four new dimethyltin (IV) complexes having a series of substituted pyridyl ligands and halide or pesudohalide. The resulting complexes have been fully characterized using elemental analysis, IR and multinuclear (^{1}H, ^{13}C, ^{119}Sn) NMR spectroscopy. Moreover, the thermal properties of all products were investigated. *In vitro* anticancer activities of *trans*-[$SnMe_2Cl_2$ (*p*-PyCOOH) were tested against human breast carcinoma (MDA-MB-468) and glioblastoma multiforme (U-87MG) cell lines.

References:

[1] J. L. Williams, L. C. Lewis-Alleyne, M. Solomon, L. Nguyen, R. Johnson, J. Vital, P. Martin, Biomed. Res. Clin. Pract, 1 (2016) 7.
[2] B.Z. Momeni, F. Sefidabi, S. Khademi, N. Fathi, Appl. Organomet. Chem, 32 (2018) e4432.
[3] M.K. Amir, S. Khan, Zia-ur-Rehman, A. Shah, I.S. Butler, Inorg. Chim. Acta 423 (2014) 14.

Synthesis, characterization and docking studies of oxazolidine-based ligand and its cadmium complex

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Abstract:
POPME contains an oxazolidine moiety which is produced by the reaction of amino alcohols with carbonyl compounds or is accessible by other routes. These ring systems have been exploited successfully in medicinally valuable compounds and also as chiral auxiliaries in the synthesis of a variety of chiral compounds [1]. In this paper, we report the preparation and characterization of a ligand (POPME) and its cadmium complex, [Cd(POPME)Cl_2]. The compound was identified by elemental analysis, FT-IR and ^{1}H NMR spectroscopy. In the crystal structure of complex (figure 1), the cadmium atom is octahedraly coordinated by the $N_{2py}N_{amine}N_{imine}$-donor POPME and two chloride ions. In the crystal network of complex, there are C–H···O and C–H···Cl hydrogen bonds. In addition to these hydrogen bonds, the crystal packing features π–π stacking interactions between pyridine rings on adjacent ligands. In the structure of complex, POPME acts as tetradentate ligand and forms three five-membered chelate rings. The ligand has one chiral center (C11) and a new one (N3) is formed after coordination. The two chiral centers have the same enantiomeric form, however the crystals contain a racemic mixture of both R, R and S, S isomers. To predict any biological activities of POPME, interactions of this compound with ten macromolecular receptors were studied using Gold docking software [2]. Docking studies revealed that POPME can interact with bio macromolecules (BRAF kinase, CatB, DNA gyrase, HDAC7, rHA, RNR, TrxR, TS, Top II and B-DNA) and the best predicted protein target for this is HDAC7 (Figure 2).

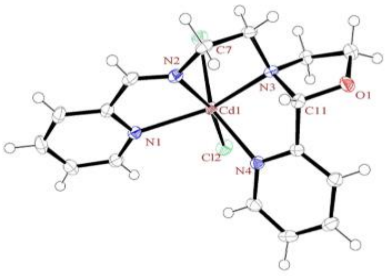

Fig.1. The ORTEP-III diagram of complex.

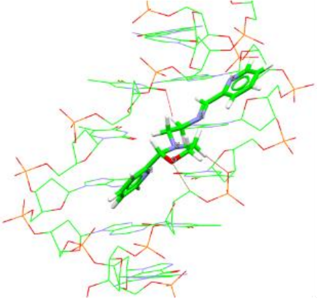

Fig. 2. Docking study results, showing the interaction between the POPME and B-DNA.

References:
[1] R.S. Gonçalves, et al., European journal of medicinal chemistry, (2010) 6095-6100.
[2] G. Jones, et al., Journal of molecular biology, (1997)727-748.

Laboratory inhibition effect of QIL on supramolecular formation of methane-water clathrate

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Abstract:

Gas hydrates or clathrates are crystalline non-stoichiometric structures consisting of gas and water. As a well-established examples of supramolecular chemistry, methane-water clathrate formation is a major failure in the oil and gas industry, due to hydrate formation in subsea infrastructure carrying natural gas. Practically, ionic liquids (ILs) are capable to act as thermodynamic inhibitor, whereas they can also delay the hydrate formation by slowing down the hydrate nucleation rate [1]. Although the literature data for imidazolium ILs- methane gas hydrates systems are available; however, fewer studies deal with quaternary ammonium based ionic liquid (QIL) [2].

In the present work, a comparative study of the effect of mono (TMAC, TPOH, and TPAB) and diammonium salts (TMPAEDA and TMDPEA) on inhabitation of water-methane hydrate formation is undertaken. Accurate reactor tests indicated a significant 1-2 K temperature drop for these QIL. According to the obtained experimental pressure-time curves in Fig. 1, the more hydrate-formation time, the more inhabitation effect of the QIL sample.

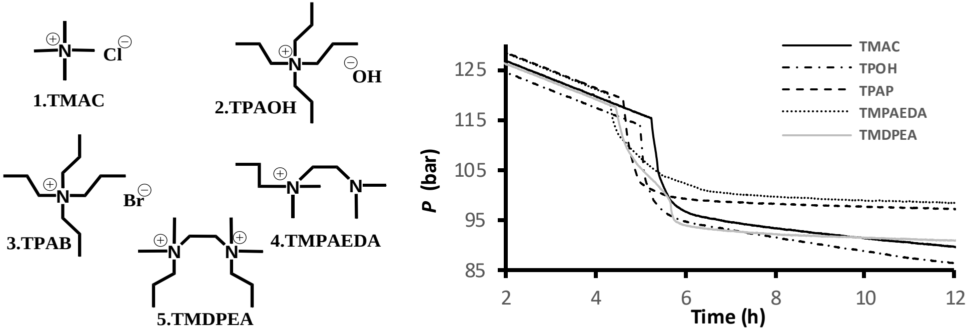

Fig. 1. QILs chemical structures applied in this work (left), their experimental *p*-time curves (right)

References:

[1] A. Perrin, O. M. Musa, J.W. Steed, Chem. Soc. Rev. 42 (2013) 1996–2015.
[2] M. S. Khan, B. Lal, L. K. Keong, I. Ahmed, Fuel. 236 (2019) 251–263.

Salicylic acid derivatives of epoxide for efficient synthesis of β- hydroxyl esters

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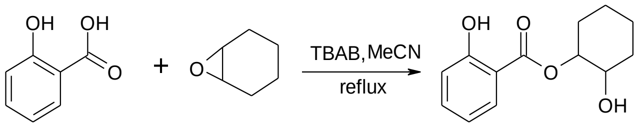
Abstract

Plants are a rich source of natural medicines. Indeed, people often fail to realize that many currently used drugs, including digitalis, quinine, taxol, the opiates codeine and morphine, and aspirin [a synthetic derivative of salicylic acid (SA)] are derived from plants**.** Salicylic acid is a kind of β-Hydroxy acid [1, 2]. This acid is crystalline and also non colored natures and also named as ortho hydroxyl benzoate acid. In over all, Salicylic acid is an herbal internal secretion the faunded in the plants and has important roles in: growth, photosynthesis, Tran's piration, absorpation and transfer of the materials, in view of saurce. The drugs divide to: natural, partly artificial and artificial. In order to production of the new partly artificial drugs. The accurate and valid changes should make on the composition of the natural material, and then, the result of this changes, could be considered [3].

In this study the reaction of Salicylic acid derivatives with the proper epoxid in the presence of Tetra butyl ammonium bromid (TBAB) in refluxing anhydrous Acetonitrile furnished β- hydroxyl esters of Salicylic acid derivatives (Scheme 1). The crud products were purified using column choromatography with proper solvent. The structure of synthesized compounds was confermed using ^{1}H-NMR, ^{13}C-NMR and IR spectroscopy.



Scheme 1: synthesis of β- hydroxyl ester

References:
[1] S. Hayat, A. Ahmad, M. N. Alyemeni, New York: Springer, 2013.
[2] S. K. Kohli, N. Handa, A. Sharma, V. Gautam, S. Arora, R. Bhardwaj, P.Ahmad, Protoplasma, 255 (2018) 11-24.
[3] M.N. Soltani Rad, S. Behrouz, Mol. Divers.17 (2013) 9-18.

Synthesis, characterization and structural studies of new palladium(II) complex including pyridinium ylides as the homogeneous catalyst for the Suzuki cross-coupling reaction

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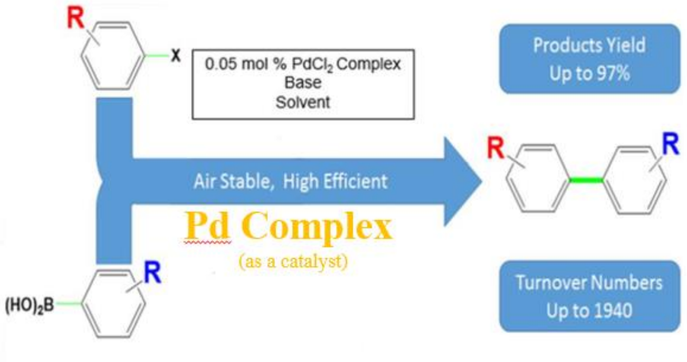
Abstract

Pyridinium ylides are important reagents in organic chemistry, especially in the synthesis of naturally occurring products with biological and pharmacological activities. These compounds have been used as reducing agents in coordination chemistry [1]. They can behave as ambidentate ligands, because the carbanion located at the Cα of the ylide is able to donate electron density to a transition metal [2,3]. This work reports the synthesis and catalytic properties of new palladium complex that prepared by reaction of new pyridinium ylides (**Y**) and $PdCl_2$. The reaction of pyridine with 2-Bromo-2'-acetonaphthone in acetone produces new pyridinium salt (**S**). The action of K_2CO_3 on **S** compound leads to a new type of stable ylide (**Y**). The reaction of **Y** with palladium(II) Chloride in dry dichloromethane as a solvent led to the formation of C-coordinated dimeric complex $[PdY_2Cl_2]$. The complex was characterized by spectroscopic methods (FT-IR, ^{13}C NMR, ^{1}H NMR). Also, this complex was applied in the Suzuki–Miyaura coupling reactions as an efficient catalyst. Various aryl halides were coupled with aryl boronic acids in DMF, under air atmosphere, in the presence of low-level of the homogeneous catalyst to afford the cross-coupled products in good to excellent yields.



References:

[1] G. Wittig, and D. Krauss, Liebigs Ann., 679 (1964) 34.
[2] S.J. Sabounchei, A. Sedghi, M. Bayat, M. Hosseinzadeh, A. Hashemi, A. Yousefi, R.W. Gable, J. Mol. Struct., 346 (2019) 346.
[3] S.J. Sabounchei, M.S. Hashemi, R. Karamian, S.H. Moazzami Farida, P. Gohari Derakhshandeh, R.W. Gable, K. Van Hecke, , J. Coord. Chem., 71 (2018) 3277.

UV-vis studies on the interaction of Zn(II) complex of propranolol drug with ct-DNA

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Abstract:

The investigations of interaction of metal complexes containing drugs as a ligand with DNA is very exciting and significant, not only in understanding the mechanism of interaction, but also for the design of new drugs [1]. In the present work, we studied the interaction of Zn(II) complex containing propranolol drug with ct-DNA. Electronic absorption spectroscopy is an effective technique to study the interaction between drug molecules and ct-DNA by monitoring possible changes in absorption intensity and position of the bands [2]. The changes in UV–vis absorption of above complex in the absence and presence of ct-DNA were examined (Fig. 1) in the Tris–HCl buffer solution (pH=7.4). Upon the increasing of the concentration of ct-DNA, the absorption band of above Zn(II) complex at 289 nm was influenced, resulting in hypochromicity and indicated that there is an attractive interaction between them. The value of intrinsic binding constant (K_b=4×10^4 M^{-1}) indicates that the Zn(II) complex binds to the ct-DNA with a high affinity.

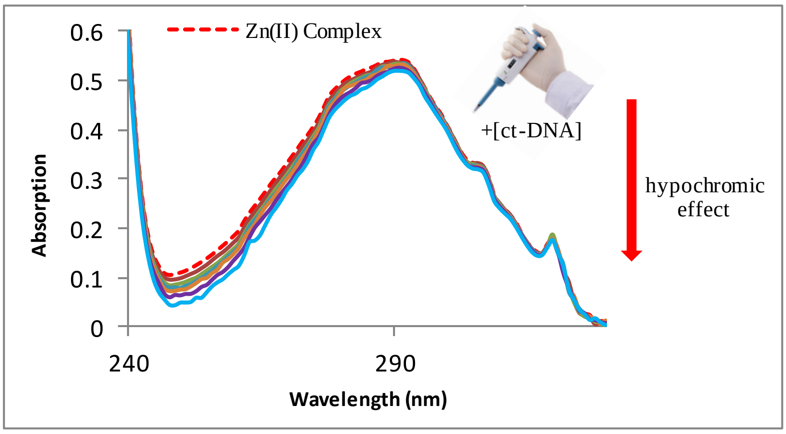

Fig. 1. UV-vis spectra of Zn(II) complex in the presence of ct-DNA at 298 K and pH 7.4 where in [Zn(II) complex]= 5.0×10^{-5} M and [DNA]= 0.0 to 9.0 × 10^{-5} M.

References:

[1] F. Hajibabaei, S. Salehzadeh, R. Golbedaghi, N. H.Moghadam, S. Sharifinia, S. Khazalpour, Z. Baghaeifar, Polyhedron, 162 (2019) 232-239.

[2] L. F. Tan, H. Chao, K. C. Zhen, J. J. Fei, F. Wang, Y. F. Zhou, L. N. Ji, Polyhedron, 26 (2007) 5458-5468.

Sonosynthesis and Characterization of ZrO_2@ZnO core-shell nanostructure and its application on photodegradation of wastewater-contained an Azo dye

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Abstract:

ZnO@ZrO_2 core-shell nanostructure (NS) was synthesized under ultrasonic irradiation by sol-gel method in two steps involving preparation of ZnO as core and the ZrO_2 shell layer was covered on ZnO for preparation of ZnO@ZrO_2 core-shell The synthesized ZnO@ZrO_2 core-shell NS was characterized by powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FESEM) and photoluminescence (PL) spectroscopy. Structural characterization by XRD confirmed the formation of monoclinic ZrO_2 and high crystalline wurtzite structured ZnO. The particle size of ZnO@ZrO_2 core-shell NS is in the range of 30-40 nm respectively. The photo-catalytic activities of the NPs were evaluated by the photo-degradation of a model dye, Congo red (CR). Compared with ZnO@ZrO_2 and ZrO_2, ZnO NPs, the ZnO@ZrO_2 core-shell exhibited the better photo-catalytic activity [1-3].

References:

[1] C. Karunakaran, R. Dhanalakshmi, P. Gomathisankar, Phenol-photodegradation on ZrO2 .92(2012) 201-206..

[2] S. Aghabeygi, , Z. Shrifi , N. Molahasani, Digest Journal of Nanomaterials and Biostructures 12, (2017). 81 – 89.

[3] S.S. Kanmani, K. Ramachandran, Synthesis and characterization of TiO_2/ZnO core/shell nanomaterials for solar cell applications, Renewable Energy 43 (2012)149-156.

Investigation of Sm^{3+} ion substitution in the hydroxyapatite-chitosan nanocomposite

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Abstract:

Hydroxyapatite (HA), the major component of hard tissue, has properties that include deodorization, protein adhesiveness, bioactivity, and biocompatibility [1]. An important and interesting property ofHA isits ability to undergoion-exchange but low mechanical strength and high packing density of hydroxyapatite lead to the limitation of its industrial application.As one of the methods to overcome these limitations, a recent study has attempted to utilize HA/chitosan nanocomposites [2].It is known that lanthanide ions have ability for substitution with the Ca^{2+} sites within HA, because of their similarities in ionic radii, donor atom requirements, and coordination geometries [3]. In this study hydroxyapatite-chitosan nanocomposite wasprepared and characterized by FTIR, SEM and BET analysisMoreover, itsion exchange properties and Sm^{3+} ion substitution in the were evaluated . Its ion exchange capacity (IEC) of prepared nanocomposite for Sm^{3+} was found to be 0.91meq.g^{-1}. Distribution coefficients (*K*d) values for Sm^{3+} ion was also determined. For this purpose batch experiments were carried out using synthetic hydroxyapatite-chitosan nanocomposite. Parameters that influence the substitution reaction such as contact time, temperature and pH of solution were investigated.The maximum sustitution was found at contact time of 8 h and 9 h, temperature of 25 ºC and pH of 7. The results indicated that the hydroxyapatite-chitosan nanocomposite used in this work proved to be effective material for substitution of Sm^{3+} ions in aqueous solutions.

References:

[1] ZamiriA, De S,. J Mech. Behav. Biomed. Mater. 4 (2011) 146–152.

[2] Patel PP, BuckleyC, Taylor BL, SahyounCC, Patel SD, Mont AJ, MaiL, Patel S, FreemanJW; J.Biomed. Mat. Res. 107 (2019) 732-741.

[3] Vidaud C, BourgeoisD, MeyerD, Chem. Res. Toxicol. 25 (2012) 1161-1175

DNA interaction studies a new complex of (1, 4-bis (3-aminopropyl) piperazine) Ni (II) perchlorate

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Abstract:

For a long time, ammonia and amines have been important ligands in the chemistry of coordination. Amines and others Nitrogen-containing compounds are one of the most abundant organic molecules and as amino acid components, peptides, proteins and alkaloids are important in biochemistry. Polyamines, in both solid state and soluble state, form stable complexes [1]. In this study, the new complex of (1, 4-bis (3-aminopropyl) piperazine)-perchlorato-Ni (II) perchlorate was synthesized (Fig 1). Binding interaction of this complex with calf thymus (CT) DNA was investigated by emission, absorption, FT-IR, measurement techniques. Upon addition of CT-DNA, changes were observed in the characteristic UV-Vis bands of the complex. It can be observed that with increasing amounts of Ni(II) complex added to the DNA solution the intensity of the absorption peak of DNA obviously decreased (hypochromism), and complex binds to CT-DNA in an intercalative mode [2] (Fig 2).

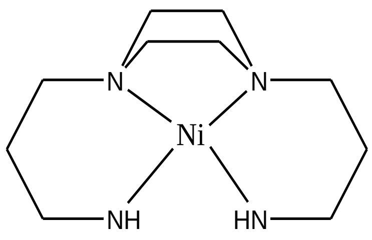

Fig .1. The structure of complex

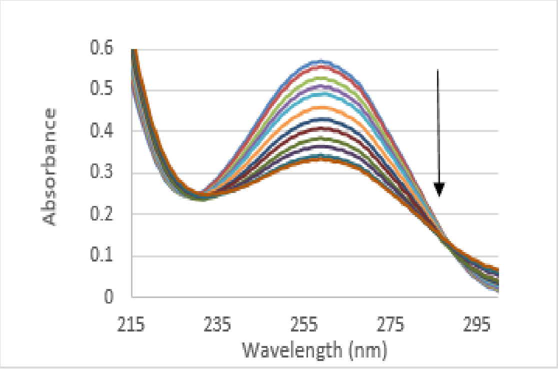

Fig. 2. Absorption spectra of complex in Tris-HCl buffer upon addition of calf thymus (CT)-DNA.

References:

[1] H. Keypour, M. Rezaeivala, L. Valencia, P. Pérez-Lourido, Polyhedron 27 (2008)3172.
[2] H. Hu, Y. Chen, H. Zhou, and Z. Pan, Synthesis, crystal structure, and DNA cleavage activity of a dinuclear nickel (II) complex with a macrocyclic ligand. Trans Met Chem 36 (2011) 395–402.

Solvent-Assisted Ligand Exchange (SALE) For Enhancement of the Capability of Epoxide Ring-Opening Reaction Catalysis Based on Three Amide-Functionalized Metal-Organic Frameworks

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Abstract:

Solvent-assisted ligand exchange (SALE) is a post synthesis method which has been assisted to confront this challenge by replacing functional groups together. N1, N3-di (pyridine-4-yl) malonamide linker (S) is one the pillar ligands which does not easily enter to the structure in order to synthesize MOFs compound. Therefore, to solve this issue , amide functionalized benzene-cored ligand derivatives were designed as linkers for manufacture of new 3D structures of $[Co(oba)(bpta)]\bullet(DMF)_2$ TMU-50, $[Co_2(oba)_2(bpfn)]\bullet(DMF)_{2.5}$ TMU-51 and one novel 2D $[Co(oba)(bpfb)]\bullet(DMF)_2$ TMU-49 , layered of compound via hydrothermal reaction. Moreover, their ability as catalysts were figured out in the methanolysis reaction of the epoxides. To increase the MOFs catalytic efficiency, we designed N1, N3-di (pyridine-4-yl) malonamide linkers (S) as a malonamide pillar ligand, which consists of an acidic hydrogen which is suitable for catalysis an epoxide ring-opening reaction that enhance the catalytic activity. Due to the synthesis the MOFs structure via this linker was not possible, we tried to design three new structures with incorporating different percentages of S linkers and exchange acylamide functional group was with malonamide via SALE pathway. The acylamide functional group was successfully replaced and produced daughter MOFs TMU-49S, TMU-50S and TMU-51S. PXRD and NMR spectroscopy confirmed that the S linker is incorporated to acylamide-MOFs structure. The obtained materials TMU-49S, TMU-50S and TMU-51S, are isostructural to their parent frameworks. The S spacer significantly improved the catalytic properties of MOFs compound in ring-opening reaction of epoxides and TMU-50S showed 98% catalytic efficiency after incorporated S linker. They can be recycled without any significant loss of the catalytic efficiency.

References:

[1] M. D. Allendorf, V. Stavila, CrystEngComm, 17(2) (2015) 229-246.
[2] Y. Cui, B. Li, H. He, W. Zhou, B. Chen, G. Acc. Chem. Res, 49(3) (2016) 483-493.

Synthesis of Two New Macrocycles Capable to Act as Linkers for Coordination Polymers

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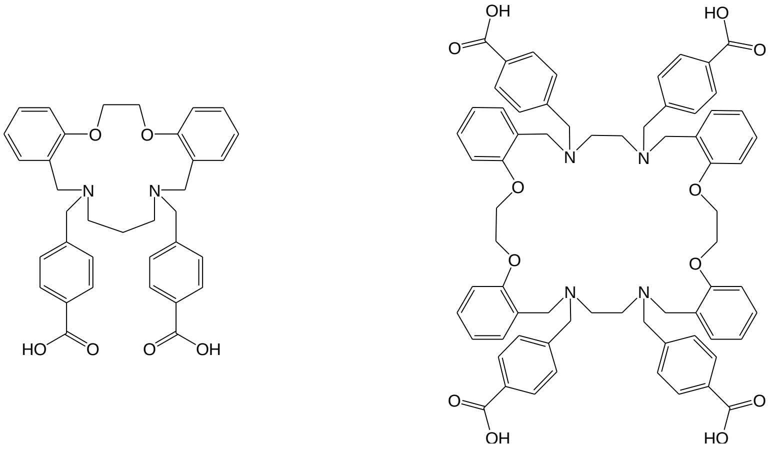
Abstract:

The design of coordination polymers (CPs) is essentially reliant on the type, number, and the position of the donor groups alongside the length and flexibility of the linker[1]. Thanks to their pre-organized entities together with central role in ligand field, employing organic linkers containing aza-crown macrocycles encourage the scientific community to synthesize new interesting coordination networks[2].

Recently, we reported new organic likers based on macrocyclic backbones bearing pyridine side arms as coordinating sites, whereas their ability to generate coordination CPs in the presence of metal ion nodes was also investigated[3]. Our subsequent observations[4,5] also indicated on various novel applications for these CPs. Here we report the synthesis of two new linkers **1** and **2** (Scheme 1) based on macrocyclic backbones bearing carboxylic coordinating sites, capable to act as new likers for upcoming CPs.



Scheme 1. The molecular structure of linkers **1** (left) and **2** (right)

References

[1] T. R. Cook, Y. Zheng, P. J. Stang, Chem. Rev. 113 (2013) 734.
[2] L. Yu, F. Li, -z. Wu, J.-y. Xie, J.-q. Li, S. J. Inorg. Biochem. 154 (2016) 89-102.
[3] B. Ghanbari, L. Shahhoseini, A. Owczarzak, M. Kubicki, R. Kia, P. R. Raithby, CrystEngComm, 20 (2018) 1783.
[4] B. Ghanbari, L. Shahhoseini, H. Hosseini, M. Bagherzadeh, A. Owczarzak, M. Kubicki, *J.* Organomet. Chem. 866 (2018) 72-78.
[5] L. Shahhoseini, R. Mohammadi, B. Ghanbari, S. Shahrokhian, Applied Surface Science, 478 (2019) 361–372.

Electrochemical Production of Syngas (CO + H_2) Using a Polypyridyl Osmium(II) Complex

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Abstract:
The growing concerns about energy crisis due to depletion of fossil fuels and the global warming caused by ever-increasing carbon dioxide (CO_2) level have encouraged the search for an economical process to produce useful chemicals from CO_2. Electrochemical reduction of CO_2 has drawn much attention from both researchers and industries for the past decades [1]. Up to now, a variety of homogeneous and heterogeneous transition metal catalysts have been reported for their ability to electrochemically or photochemically accelerate the reduction of CO_2 to CO [2,3]. CO itself can be used as a precursor compound for fuel synthesis processes, where CO and H_2 are mixed as synthesis gas (syngas) to form hydrocarbons such as methane or methanol in the well-known Fischer–Tropsch (FT) process [4,5]. Therefore, the sustainable syngas can be resulted in a greener chemical industry and the production of transported liquid fuels through the Fischer–Tropsch technology. The electrochemical conversion of CO_2 into syngas can be provided a carbon cycle, which decreases the greenhouse gas emissions and the world's demand for fuels.

Here, we report the facile synthesis and fully characterization of a new mononuclear Os(II) complex with phen-dione as a polypyridyl ligand. This Os(II) complex shows an outstanding electrocatalytic activity for CO_2 reduction in the presence of the weak acid as a hydrogen source to simultaneously produce H_2, and consequently syngas (CO + H_2). The compositions of the resulting syngas mixtures are controllable by controlling the reaction conditions. For example, an increase in the acid concentration results in a larger mole ratio of H_2:CO. The computational results using DFT are in agreement with the experimental results and confirm the proposed mechanisms.

References:

[1] R. Francke, B. Schille, M. Roemelt, Chem. Rev. 118 (2018) 4631–4701.

[2] J.-P. Du, A. Wilting, I. Siewert, Chem. Eur. J. 25 (2019) 5555–5564.

[3] B. M. Szyja, ChemElectroChem 5 (2018) 2105–2112.

[4] Y. H. Choi, Y. J. Jang, H. Park, W. Y. Kim, Y. H. Lee, S. H. Choi, J. S. Lee, Appl. Catal. B 202 (2017) 605–610.

[5] P. Huang, S. Ci, G. Wang, J. Jia, J. Xu, Z. Wen, J. CO_2 Util. 20 (2017) 27–33.

Synthesis and characterization of N_4O_2 macroacyclic Schiff-base ligand contaning piperazine moiety and its mononuclear Zn (II) complex

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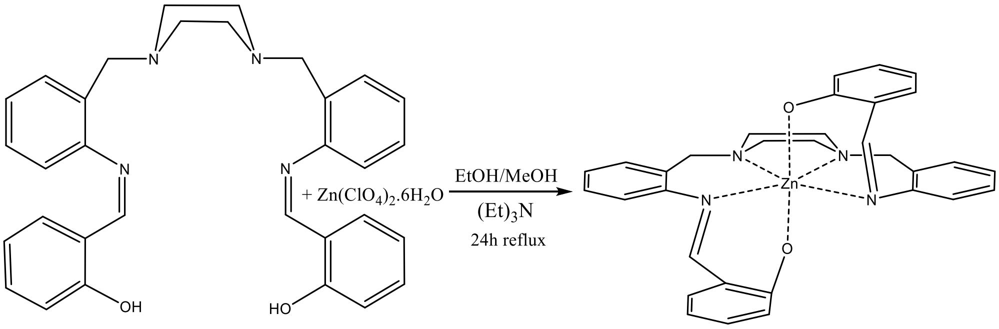
Abstract:

The polyamine 2,2'-(piperazine-1,4-diylbis(methylene))dianiline (A) was synthesized by the reaction of piperazine with 2-nitrobenzaldehyde. IR spectrum of polyamine A exhibit a $\nu(NH_2)$ vibration in 3347-3447 cm^{-1}. In the mass spectrum of polyamine A, presence of the peak at 296 m/z confirms the synthesis of polyamine. Macroacyclic Schiff-base ligand H_2L with the N_4O_2 donor system was synthesized from condensation of 2-hydroxybenzaldehyde with polyamine A. IR spectrum of ligand exhibited a ν(C=N) vibration in 1616 cm^{-1}. In the mass spectrum of ligand (H_2L) presence of a peak at 504 m/z confirms the synthesis of ligand. The elimination of C=O and NH_2 band in IR spectrum of ligand shows the ligand synthesis. The corresponding complex was synthesized from direct reaction of zinc (II) metal ion and ligand (H_2L) in the methanol solvent (Scheme 1). In the IR spectrum of the complex, ν(C=N) in the 1613 cm^{-1}, and also in mass spectrum of complex the presence of peak at 568 m/z confirms the synthesis of complex. The elemental analysis and ^1H and ^{13}C NMR confirm the synthesis of all compounds [1-2].



Scheme.1

Reference:

[1] M. Rezaeivala, H. Keypour, Coord. Chem. Rev. 280 (2014) 203.

[2] H. Keypour, M. Mahmoudabadi, A. Shooshtari, M. Bayat, M. Ghassemzadeh, L. Hosseinzadeh, F. Mohsenzadeh, K. Harms, Polyhedron 129 (2017) 189.

Synthesis, spectroscopic characterization and crystal structure of a new chiral amidophosphoester

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Abstract:

The chiral amidophosphoester families have found widespread use in the preparation of different classes of drugs, and for processing of biologically active compounds [1]. We report here the synthesis of single-enantiomer amidophosphoester $(C_6H_5O)_2P(O)[(R)\text{-}(+)\text{-}NHCH(CH_3)(C_6H_4\text{-}4\text{-}CH_3)]$ (I) and its characterization by IR, NMR, mass, optical rotation and single crystal X-ray diffraction. The compound crystallizes in monoclinic system with chiral space group $P2_1$. The asymmetric unit is composed of two independent molecules. The P atoms have a distorted tetrahedral $(O)_2P(O)(N)$ configuration. In the crystal, chiral one-dimensional hydrogen-bonded architecture, formed along b axis, is mediated by classical N—H…O(P) and weak C—H…O(P) hydrogen bonds. This architecture includes $D_1^1(2)$, $R_2^2(10)$, $C_2^2(8)$ and $C_2^1(8)$ graph-set motifs. In the IR spectrum, the band centered at 3174 cm^{-1} is attributed to the NH stretching frequency. The melting point of title structure (393 K) is a few lower than the closely related analogous compound $(C_6H_5O)_2P(O)[(R)\text{-}(+)NHCH(CH_3)(C_6H_5)]_2$ (408 K) [2]. The phosphorus signal appears at –0.07 ppm, in comparison with the signal at –0.81 ppm for this analogous compound noted [2]. The two diastereotopic phenyl groups reveal two sets of signals in ^{1}H- and ^{13}C{^{1}H}-NMR spectra. The specific optical rotation is measured as $[\alpha]_D^{20}$ = 51° (c 0.009, MeOH).

References:

[1] T. K. Warren, et al,Nature, 531(2016) 381–385.
[2] F. Sabbaghi, M. Pourayoubi, M. Nečas, K. Damodaran, Acta Cryst. C75 (2019) 77–84.

Synthesis and characterization of coordination polymers using Copper(II)-carboxylate disulfide

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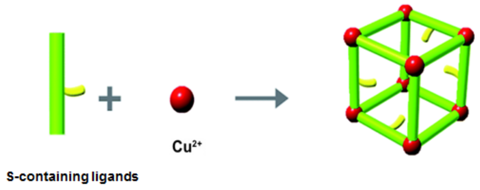
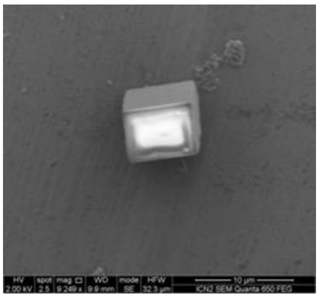
Abstract:

Two copper(II)-carboxylate disulfide coordination polymers $[Cu_2((O_2CPhS)_2)_2(DMF)_2]_n$ (**1**) and $Cu_2((O_2CPhS)_2)_2(4,4'\text{−dipyridyl})]_n$ (**2**) have been synthesized using the 4,4′-dithiodibenzoic acid $((SPhCO_2H)_2)$ and 4,4′−dipyridyl as ligands [1]. These two compounds were characterized by X-ray diffraction, IR, thermogravimetric analyses and SEM and then their porosity was determined by N_2 and CO_2 sorption. Compounds **1** and **2** are polymorphs with the presence, for both, of dinuclear paddle-wheel copper(II)-carboxylates. In compound **1**, the adjacent dimeric Cu_2 units are linked by two $(O_2CPhS)_2$ ligands generating a cyclic loop 1D chain, and in compound **2**, each pair of Cu(II) atoms is linked by four ligands to create 2D networks, that are 2-fold interpenetrated [2].

By using 4,4′−dipyridyl as a pillar ligand to extend 1D CPs to 2D network, the BET value was increased form 196 m^2/g in 1D network to 680 m^2/g in 2D structure.





References:

[1] O. Veselska, L. Cai, D. Podbevšek, G. Ledoux, N. Guillou, G. Pilet, A. Fateeva, A. Demessence, Inorg. Chem. 2018, 57 (2018) 2736–2743.
[2] H. B. Zhu, S.H. Gou, Coord. Chem. Rev. 255 (2011) 318–338.

A new ionic Schiff base co-polymer and its Metallo- polymers

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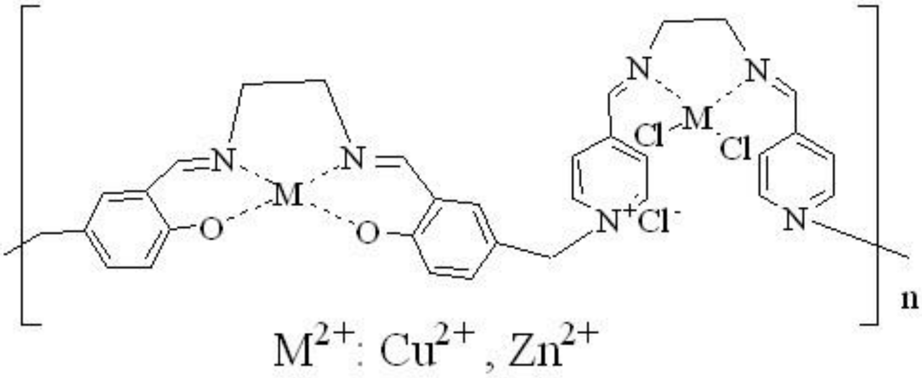
Abstract:

Schiff base polymers, also known as polyazomethines, have drawn attention of researchers to design thermally resistant and semiconductive materials. They are promising materials for other applications such as photorefractive holographic materials (PRHMs), solar cells (SCs), organic light emitting diodes (OLEDs) and organic field effect transistors (OFETs) [1]. They have thermal stability similar to that of polyamides and have been used as solid stationary phases for gas chromatography.

Polymeric ionic liquid electrolytes have received great attention for use in next-generation solid lithium ion batteries. However, most polymeric ionic liquid electrolytes require a high proportion of organic liquid plasticizer to improve the room temperature ionic conductivity. [2]. These types of compounds can be used for various applications, but the most widely known application to date is CO_2 cycloaddition reaction and as anticancer compounds.

In this study, a new ionic Schiff base copolymer and its Cu(II) and Zn(II) metallo-polymers were synthesized (Scheme 1) and characterized by different analytical and spectral methods. The GPC(gel permeation chromatography) has been used to determine the molecular weight of the synthesized polymers. The aim of this research is the studying of the solid state conductivity of the synthesized polymer in different temperatures and the variation of the conductivity by metalation.



Scheme 1. Ionic metallo-Schiff base co-polymers

References:

[1] N.Y.Baran, Journal of the Turkish Chemical Society, Section A: Chemistry, 5(2) 607-620.

[2] A.Wang, X.Liu, S.Wang, J.Chen, H.Xu, Q.Xing, & L.Zhang ,Electrochimica Acta, 276 (2018) 184-193.

Sonochemical Synthesis of a Novel Nanoscale Hg(II) Iodo-bridged Coordination Polymer with Thiosemicarbazide Derivative Ligand

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Abstract:

Infinite coordination polymers are constructed with metal ions and organic ligands as main elementary building blocks, linked by coordination bonds and other weak chemical bonds [1]. Research on coordination polymers has rapidly grown in recent years due to an increasing demand for functional materials with conducting, magnetic, nonlinear optical, porous, thermal, and fluorescence properties [2]. Nanometer-sized particles of metal coordination polymers are fascinating to explore, since their unique properties are controlled by the large number of surface molecules, which experience an entirely different environment than those in a bulk crystal. Controlling the growth of materials at the submicrometer scale is of central importance in the emerging field of nanotechnology [1]. As a continuation of the previous studies [1,2], in this work we extend our studies to investigate the interactions of universal bridging ligand(iodo anion) with Hg(II) ions in the presence of thiosemicarbazide derivative ligand (4-ptsc) and describe a simple synthetic sonochemical preparation of nano-structures of $[Hg(I_2)(4\text{-ptsc})]_n$ (1) metal-organic coordination polymer.

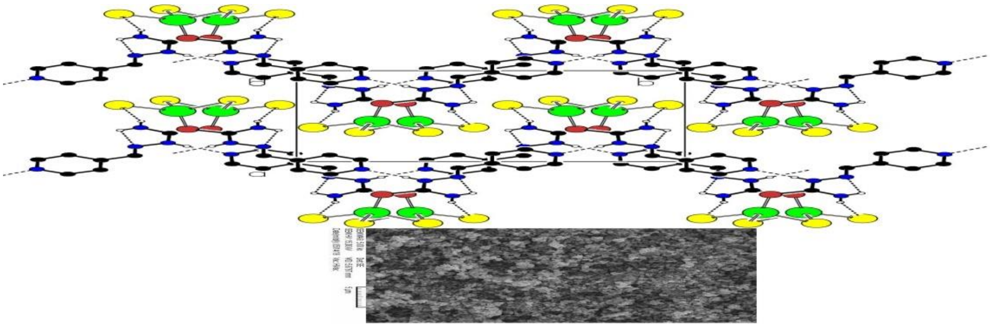

Fig. 1. Up: The structure of 1; Down: the morphology of nano structure of 1.

References:

[1] C.R. Kim, T. Uemura, S. Kitagawa, Chem. Soc. Rev., 45 (2016) 3828-3845.
[2] L. Zeng, X. Guo, C. He, C. Duan, ACS Catalysis, 6 (2016) 7935-7947.

Copper(II), Nickel(II), Cobalt(II) and Manganese(II) Complexes of Schiff Bases: Synthesis, Characterization, and Antibacterial Properties

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Abstract:

Schiff base ligands containing different donor atoms(like N,O,S,etc.) show a wide range of biological activities and are of special interest because of the variety of methods in which they are bonded to the transition-metal ions[1]. Schiff bases and their complexes have attracted considerable attention because of their usages in various biological fields[2], catalysis reactions[1], water photolysis[2] and etc.

Similarly,pyridine base ligands have also been used in many biochemical studies designed to develop molecular systems of biological and medicinal importance.[5,6] In our research, we describe the synthesis of four new mononuclear complexes of Cu(II), Ni(II), Co(II), Mn(II) containing the corresponding N-donor schiff base ligand. The structures of the ligand and its metal complexes were studied by elemental analyses, spectroscopic methods(FTIR, UV-vis, NMR). Their electrochemical properties were studied by cyclic voltammetry technique. Also antibacterial activities of the ligand and its complexes were tested against two Gram-negative bacteria Escherichia coli(ATCC 25922) and Pseudomonas aeruginosa(ATCC 9027) and two Gram-positive bacteria Staphylococcus aureus(ATCC6538) and Corynebacterium renale. The results exhibited suitable antibacterial properties for ligand and its complexes . The study has shown that complexation of ligand to metallic center lead to enhancement of antibacterial activity.

Refrences:

[1] L. Shi, W. J. Mao, H. L. Zhu, J. Coord. Chem. 62 (2009) 3471.
[2] S.Chandra, S. Parmar, Y. Kumar, Bioinorganic Chemistry and Applications (2009).

The competitive binding studies on the new Zn(II) complex of isoxsuprine drug with ct-DNA by fluorescent probes

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Abstract:

Methylene Blue (MB) is one of the sensitive fluorescent probes that bind to DNA via intercalation. On the other hand, Hoechst 33258 (HO) binds strongly to the minor grooves of ct-DNA [1]. Figure 1 shows the emission spectra of the MB with adding different amounts of the Zn(II) complex to DNA–MB system. As can be seen, upon the addition of Zn(II) complex the fluorescence intensity of MB increases, which is due to the intercalation of this complex to ct-DNA base pairs and displacing some MB from the DNA–MB system. Also, the effect of Zn(II) complex on DNA–HO system fluorescence intensity or the position of the emission of the DNA–HO system was negligible, indicating that Zn(II) complex cannot displace HO from the DNA–HO system [2].

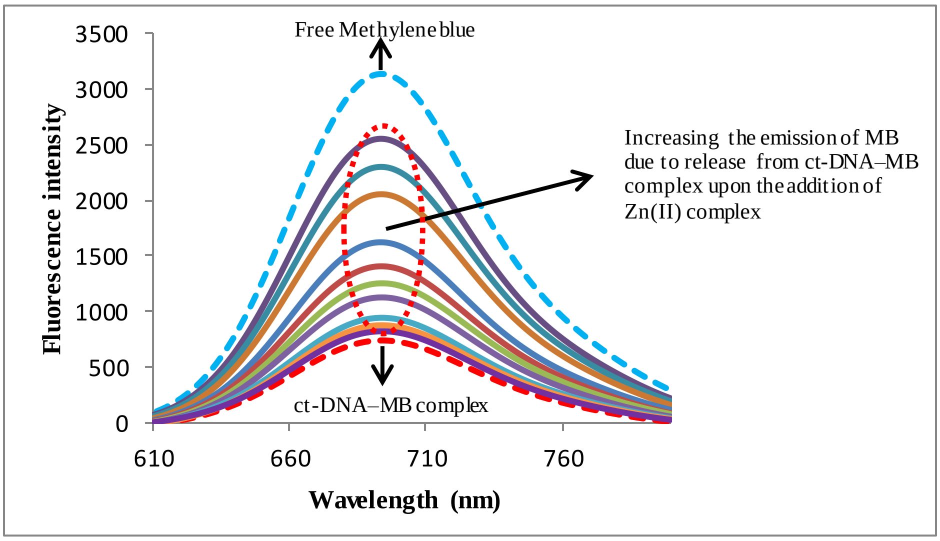

Fig. 1. The emission spectra of ct-DNA–MB system in the absence and the presence of Zn(II) complex at 298 K and pH 7.4.

References:

[1] E. Tuite, B. Norden, J. Am. Chem. Soc. 116 (1994) 7548–7556.

[2] F. Hajibabaei, S. Salehzadeh, R. Golbedaghi, N. H.Moghadam, S. Sharifinia, S. Khazalpour, Z. Baghaeifar, Polyhedron, 162 (2019) 232-239.

Synthesis, characterization and in vitro cytotoxic activities of chlorogenic acid loaded on γ-Fe_2O_3@SiO_2 nanoparticles

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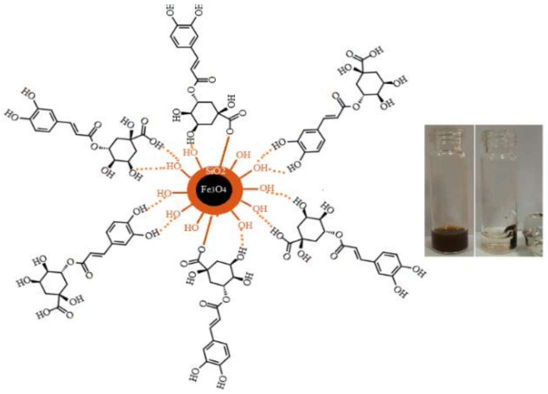
Abstract:

In recent years, nanoscale drug delivery systems have been remarkably interested. The use of magnetic nanoparticles (MNPs) in targeted drug delivery is according to their magnetism and simplicity of being manipulated by an external magnetic field which directly guides MNP drug-carriers to the exact region [1]. Chlorogenic acid (CGA) is phenolic compound generated via esterifying caffeic acid with (-)-quinic acid. Green coffee is a main natural resource of CGA [2].

In the current study, nanoparticles with anticancer features were synthesized through loading CGA on magnetic nanoparticles (MNPs). Firstly, the synthesis of Fe_3O_4 MNPs was carried out through chemical coprecipitation reaction and the silica was coated on Fe_3O_4 MNPs surface through the sol-gel procedure. Next, the chlorogenic acid was used to modify Fe_3O_4@SiO_2 MNPs surface. Characterization of γ-Fe_2O_3@SiO_2-CGA MNPs was performed using Fourier transform infrared spectroscopy (FT-IR) and transmission electron microscopy (TEM) that show effective coating of the MNPs with SiO_2 and chlorogenic acid (CGA) ligand and spherical shape of the nanoparticles with a mean diameter of 16 nm, respectively. The *in vitro* cytotoxic function of γ-Fe_2O_3@SiO_2-CGA MNPs and CGA against the human cancer cells (U-87 MG, A-2780, and A-549) using MTT colorimetric test indicated that the cytotoxicity of the nanoparticles was considerable more than free CGA.



References:

[1] K. Ulbrich, K.i. Holá, V. Šubr, A. Bakandritsos, J. Tucek, R. Zboril, Chemical reviews, 116 (2016) 5338.
[2] A. Farah, M. Monteiro, C.M. Donangelo, S. Lafay, The Journal of Nutrition, 138 (2008) 2309.

Photocatalyst Activity of $MgZrO_3$ Prepared by Sol-gel Method and Study Its Structure and Characteristics

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Abstract:

Magnisum zirconate forms the perovskite structure and possesses excellent mechanical, optical and electrical properties. The properties of $MgZrO_3$ (MZ) depend on the synthesis method employed. The most common method for powder synthesis is the solid mixing technique. Although the method is simple and inexpensive, wet chemical methods like sol-gel, hydrothermal routes and co-precipitation can improve cation homogeneity and reduce the temperatures required for phase formation. These methods also help produce more surface active powders that sinter better and thus produce higher density ceramics [1-2].

An aqueous solution of barium and zirconium was obtained by mixing 0.40 g $BaCl_2.2H_2O$ and 0.53 g $ZrOCl_2.8H_2O$ in deionized water. Then, a solution of NaOH added to them. Then powder calcination at 400°C for 2h. Ceramic was characterized by FT-IR, UV-vis spectroscopy and X-ray diffraction (XRD). XRD analysis reveal pure perovskite phase structure.

Parameters such as concentration of substrate, amount of photocatalyst, pH of the solution, temperature of reaction medium and time of irradiation of light for photocatalysis degradation of methylene blue (MB) and Eosin Y (EY) were investigated. When the pH increased to 10, the photodegradation of MB increased to 10% at the end of 30 min and when the pH decreased to 3, the photodegradation of EY increased to 92% at the end of 30 min.

References:

[1] M.L.Moreira, et al. Chemistry of Materials 20.16 (2008) 5381-5387.

[2] Celik, Erdal, et al. IEEE transactions on applied superconductivity 10.1 (2000) 1329-1332.

Synthesis of $CaZrO_3$ nanoceramics by a sol-gel method and Photocatalysis Applications

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Abstract:

Large scale solution routes to perovskite ceramics, such as the alkaline earth zirconates ($A^E ZrO_3$, A^E = Ca, Sr, Ba), titanates, and their binary systems are of interest for their temperature insensitive dielectric properties. These perovskites have reasonable permittivities, very low dielectric loss, as well as extremely small positive (CZ, SZ) or negative (BZ, CT, ST) temperature coefficients which allow them to have minimal changes in their capacitance as a function of temperature [1-2].

The $CaZrO_3$ nanoceramic was prepared by sol-gel method using the precursors of $CaCl_2.2H_2O$ and $ZrOCl_2.8H_2O$. In a typical procedure, 0.40 g of calcium chloride that was dissolved in 10 mL of deionized water added to zirconium oxychloride. Then, a solution of NaOH added to them. Solid gels were readily obtained at 60°C. Finally, so obtained precipitation was calcinated at 700°C for 2 h to prepare $CaZrO_3$ nanoceramic.

Ceramic was characterized by FT-IR, SEM, and X-ray diffraction (XRD). SEM shown uniform grain size. Parameters such as concentration of substrate, amount of photocatalyst, pH of the solution, temperature of reaction medium and time of irradiation of light for photocatalysis degradation of methylene blue (MB) and Eosin Y (EY) were investigated. Ceramic show the maximum adsorption at neutral pH hence the photodegradation also found maximum at neutral pH. When the pH increased to 10, the photodegradation of MB increased to 20% at the end of 30 min and when the pH decreased to 3, the photodegradation of EY increased to 50% at the end of 30 min.

References:

[1] R.C.Kell, E.E.Riches, P.Brigginshaw, G.C.E.Olds, A.J.Thomas, R.E.Mayo, D.F.Rendlf, Electronics Letters 6(19) (1970) 614-616.

[2] A.Fujishima, K.Honda, Nature, 238 (1972) 37.

^{31}P NMR study of the stoichiometry, stability and thermodynamic data for the complexation of several HgX_2 – *p*-Cyano acetylemethylentriparatolylphosphorane complexes in various Tetrahydrofuran - Dimethylsulfoxide mixtures

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Abstract: The unsymmetrical phosphorus ylide, (*p*-tolyl)$_3$P=CHCOC$_6$H$_4$(*p*-CN) (L) is shown to react with Hg(II) halides to form binuclear products **Fig. 1** with the composition $\{HgX_2[(p\text{-tolyl})_3P{=}CHCOC_6H_4(p\text{-CN})]\}_2$, where X = Cl, Br and I. ^{31}P NMR measurements were employed to monitor the stoichiometry and stability of HgX_2 complexes with phosphorus ylide in binary Tetrahydrofuran – Dimethylsulfoxide mixtures of varying composition. In all cases studied, the variation of ^{31}P chemical shift with the $[HgX_2]/[ylide]$ mole ratio indicated the formation of 1:1 complexes. The formation constants of the resulting complexes were evaluated from computer fitting of the mole ratio data to an equation that relates the observed chemical shifts to the formation constant. In all solvent mixtures used, the stabilities of the resulting 1:1 complexes varied in the order $HgCl_2 > HgBr_2 > HgI_2$. It was found that, in the case of all complexes, an increase in the percentage of Tetrahydrofuran in the solvent mixtures, significantly increased the stability of the complexes. The temperature dependence formation constant were used for the evaluation of the enthalpy and entropy values for the complexation reaction. It was concluded that in all complexes, except for Hg(II) halides, the resulting complex enthalpy is stabilized and the ΔH compensates the $T\Delta S$ contribution

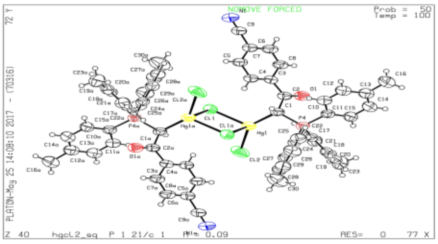

Fig. 1. ORTEP view of X-ray crystal structure of $[\mathbf{Y}\rightarrow HgCl_2]_2$

References:
[1] Y. Shen, Acc. Chem. Res. 31 (1998) 584.
[2] C. Puke, G. Erker, N. C. Aust, E. U. Wurthweine, R. Frohich, J. Am. Chem. Soc. 120 (1998) 4863.

Novel transition metal complexes of 5-methyl-5-(4-nitrophenyle)-hydantoin: Synthesis, characterization, theoretical study and anticancer and antioxidant studies

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Abstract:

New Ni(II), Pd(II) and Pt(II) complexes of 5-methyl-5-(4-nitrophenyle)-hydantoin **(L)** were synthesized and characterized. The new complexes were exactly determined by elemental analysis, FT-IR, ^{1}H NMR, ^{13}C NMR and Mass analysis. Resulting data, offered evidence for coordination of CO-ligand of hydantoin to the Ni(II), Pd(II) and Pt(II), as the metal center. Results from antioxidant activity assay of the compounds Pd(II) and Pt(II) showed their considerable radical scavenging abilities (IC_{50}: 0.15 to 0.23 mg mL^{-1}). Moreover, cytotoxic activity of the compounds Pd(II) and Pt(II) was tested against three different cancer cell lines including MCF-7 (breast), A549 (lung) and AGS (gastric) adenocarcinoma cells. The bonding situation between the [MCl_2] and L fragments in [$L\rightarrow PdCL_2\leftarrow L$] complexes, were carried out by NBO and energy-decomposition analysis (EDA), as well as its natural orbitals for chemical valence variation (EDA-NOCV). The results show that the M←O bond interaction energies (ΔE_{int}) of the L and MCl_2 fragments in 2-4 complexes are substantial and conform to the V-shaped trend for the transition metals of the first, second, and third row as Ni >Pt >Pd.

References:

[1] A. Bakalova, R. Buyukliev, I. Tcholakova, G. Momekov, S. Konstantinov, M. Karaivanova38 (2003) 627-632.
[2] H. Varbanov, A. Bakalova, R. Buyukliev, G. Momekov, R. Baykushev, 35 (2010) 457-461.

Study of photocatalytic application of nano mixed metal oxides $Ca_{0.01}Fe_{2.99}O_4/CaTiO_3$ functionalized by porphyrin

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Abstract:

The problem of water pollution and finding appropriate solutions to reduce them take a large part of the researches which was done to purify it, it turn, reduce the effects of damage on the other environments (atmosphere and soil). In this study, a novel mixed metal oxide contains calcium doped-magnetite ($Ca_{0.01}Fe_{2.99}O_4$) and calcium titanate ($CaTiO_3$) with different ratios (1:1, 1:2, 1:4 and 1:6) were synthesized via solovothermal method, which can be used new photocatalysts for degradation of methylene blue (MB). The molar ratio of 1:6 showed the best photocatalytic activity for degradation of MB. Therefore, mixed metal oxide synthesized with this molar ratio was functionalized by porphyrin to increase light absorption in visible region. Then the photocatalytic activity of TCPP@ $Ca_{0.01}Fe_{2.99}O_4/CaTiO_3$ was investigated by photodegradation of MB under visible light irradiation in various concentrations and contact times. Light absorption rate increased in the visible region by consolidation of porphyrin on surface of TCPP@$Ca_{0.01}Fe_{2.99}O_4/CaTiO_3$, which lead to increase in photocatalytic activity. All synthesized materials were characterized by using XRD, FESEM, VSM, FT-IR, DRS, EDS-mapping and TEM techniques. More significantly, the mixed metal oxides functionalized by porphyrin exhibited superparaferromagnetic property that is useful for efficient magnetic separation after 25-30 seconds[1-3].

References:

[1] D.Beydoun, R.Amal, G.Low, and S. McEvoy, “Journal of Nanoparticle Res, 1 (1999) 439–458.

[2] A.Houas, Appl. Catal. B Environ, 31 (2001) 145–157.

[3] X. Yang, J.Fu, C.Jin, J.Chen, and C.Liang, 5 (2010) 14279–14287.

21st Iranian Inorganic Chemistry Conference
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Methods for Improving Silica and Alumina Contents of Kaolin

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Abstract:

This study focus on chemical activation of kaolin under acid and alkaline conditions. For this purpose the metakaolin were prepared by calcination of a natural kaolin at 800 and 900 °C. This metakaolin was more reactive than the initial kaolin and then was utilized for acid and alkaline activation. The physical and chemical features of kaolin is related on external layer. Usually two methods are applied for improvement of kaolin which included physical and chemical methods. In physical method hydrothermal reaction is used [1]. In chemical method acids (HNO_3 ،HCl ،H_3PO_4 ،CH_3COOH) and alkaline (NaOH, KOH) are utilized [2]. In this study the extraction of aluminum and silicon was done by HF and NaOH. The kaolin contains Al_2O_3 (38%) and SiO_2 (45%). After calcination, the percentages of alumina and silica became, Al_2O_3 (41%), SiO_2 (54%). For reducing silica content and producing high alumina materials, metakaolin was leached by caustic soda (NaOH) solution. Silica solubility increased in high temperature so the reaction temperature increased to 100 °C. After this process (20 min) percentages of alumina and silica became, Al_2O_3 (46%), SiO_2 (48%). In order to increase the percentage of silica in kaolin, leaching process was done by HF diluted solution in a room temperature for 20 min on metakaolin, after that percentages of alumina and silica became, Al_2O_3 (35%), SiO_2 (61%). The XRD patterns of kaolin, metakaolin and leaching with NaOH were shown in Fig 1. a-c.

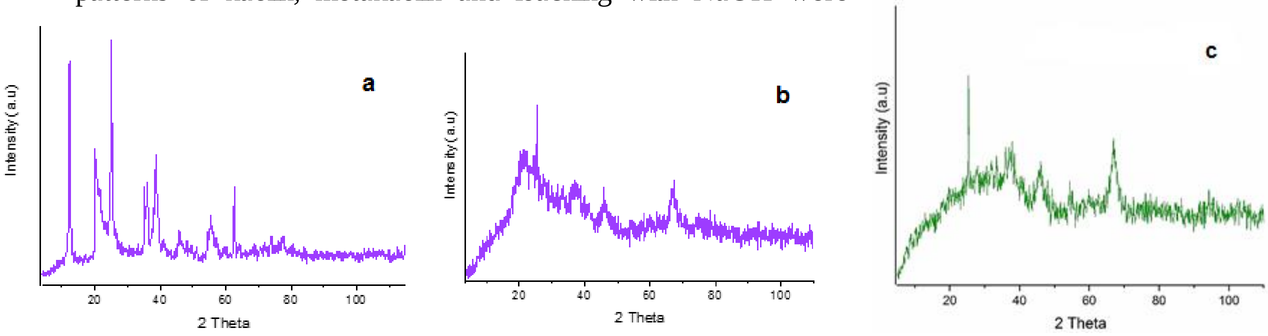

Fig.1

References:

[1] L.Heller-Kallai, "Developments in clay science: handbook of clay science," Thermally Modified Clay Minerals, Elsevier, Oxford, 2006.

[2] F. Hussin, M. K. Aroua, and W. M. A. W. Daud, Chemical Engineering Journal, 170 (1) (2011) 90-106.

Synthesis and Spectroscopic characterization of a new phosphoric triamide; $[2,3\text{-}F_2–C_6H_3C(O)NH]P(O)[N(CH_3)(C_6H_{11})]_2$ as an example of a compound with a second-order ^{13}C NMR spectrum

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Abstract:

Phosphoramids are suitable compounds for demonstrating the high capability of NMR spectroscopy in characterizing newly synthesized compounds [1-3]. In this study, we synthesized a new phosphoric triamide with formula $[2,3\text{-}F_2–C_6H_3C(O)NH]P(O)[N(CH_3)(C_6H_{11})]_2$ (**1**) and characterized by ^{1}H, ^{13}C{^{1}H}, ^{31}P{^{1}H} NMR and IR spectroscopy. The ^{31}P{^{1}H} NMR spectrum of this compound represents a singlet at chemical shift 25.01 ppm (Fig. 1) which indicates that the synthesized compound is pure. In the ^{13}C NMR spectrum of **1**, both two- and three-bond distance couplings with the phosphorus atom [^2J(P,C) and ^3J(P,C), respectively] is observed for corresponding carbon atoms of cyclohexyl rings and as expected, ^2J(P,C) = 4.6 Hz is greater than ^3J(P,C) = 1.7 and 3.6 Hz [i.e. ^2J(P,C) > ^3J(P,C)]. As shown in the experimental ^{13}C NMR spectrum in Fig. 2, the unsubstituted carbon atoms of the $2,3\text{-}F_2–C_6H_3–$ fragment (C-4, C-5 and C-6) give the second-order spectra that are attributed to the coupling with two fluorine atoms. Among these carbons, the carbon ortho to the fluorine (C-4) appears upfield which can be confirmed by comparing the predicted spectrum, calculated by the MestReNova software (Mnova) [4], and the experimental spectrum (Fig. 2). As Mnova failed to calculate the splitting for compound **1**, only the chemical shift information was used for building predicted spectrum. Hence, only singlet peaks are observed in the predicted spectrum.

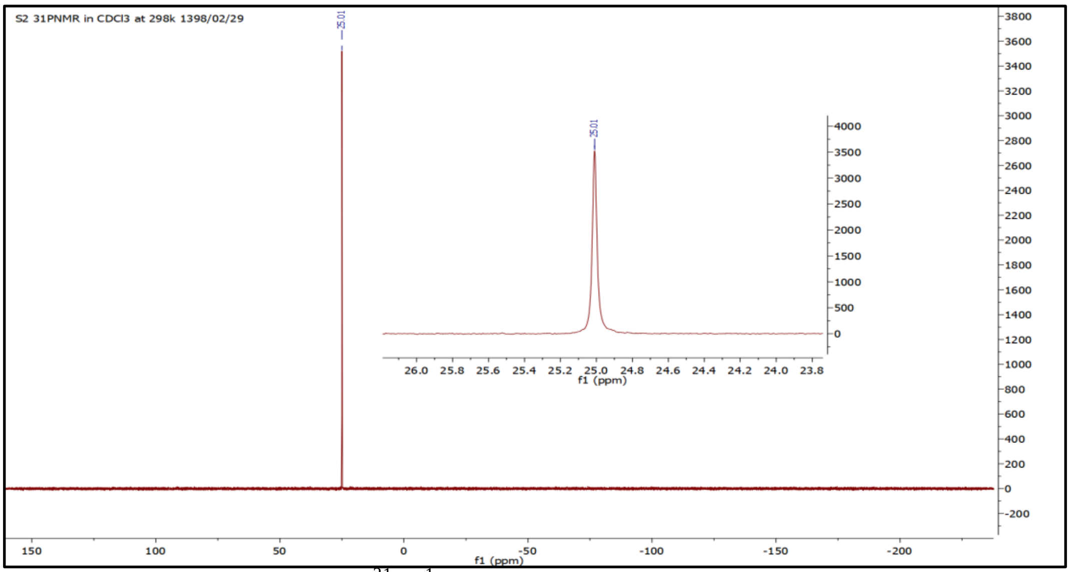

Fig. 1. The ^{31}P{^{1}H} NMR spectrum of compound **1**.

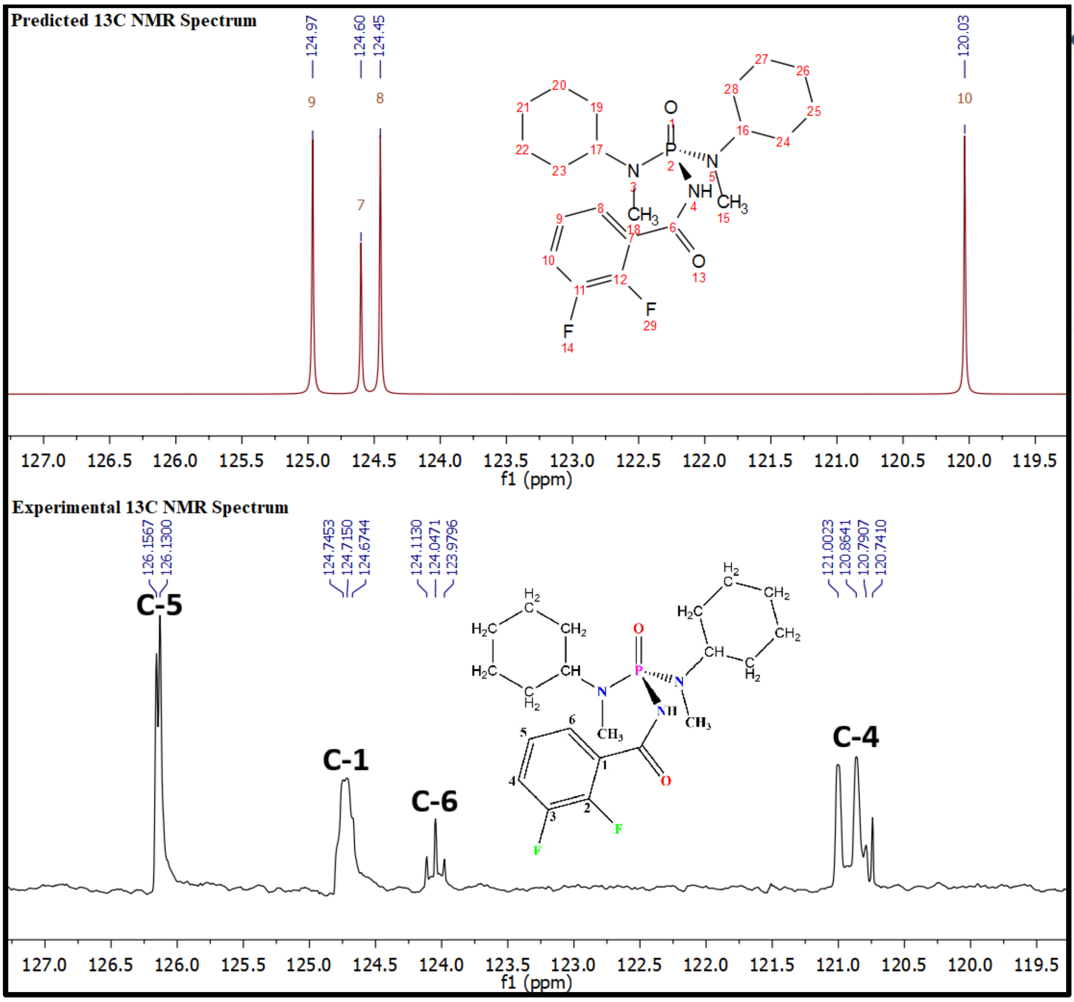

Fig. 2. A part of the ^{13}C NMR spectrum of compound **1**, belonging to four carbon atoms of the 2,3-F_2–C_6H_3– fragment. The experimental spectrum is shown below the predicted spectrum.

References:

[1] K. Gholivand, H. Mostaanzadeh, Z. Shariatinia, N. Oroujzadeh, Main Group Chemistry 5 (2006) 95-109.

[2] K. Gholivand, M. Pourayoubi, Z. Shariatinia, Polyhedron 26 (2007) 837-844.

[3] M. Pourayoubi, S. Shoghpour Bayraq, A. Tarahhomi, M. Nečas, K. Fejfarová, M. Dušek, Journal of Organometallic Chemistry 751 (2014) 508-518.

[4] [92] Mnova Suite, 11.0.4, Mestrelab Research, Santiago de Compostela, Spain, www.mestrelab.com, 2017.

Synthesis and spectroscopic characterization of two pairs of phosphoric triamide enantiomers

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Abstract:

Many chiral phosphorus compounds have been synthesized and used in different scientific domains such as medicine [1] and enantioselective catalysts [2], however few number of chiral phosphoric triamides were investigated [3]. In this study, two pairs of enantiomer phosphoric triamides, $CCl_3C(O)NHP(O)[(R)\text{-}(+)\text{-}NHCH(CH_3)(C_6H_4\text{-}4\text{-}CH_3)]_2$/$CCl_3C(O)NHP(O)[(S)\text{-}(–)\text{-}NHCH(CH_3)(C_6H_4\text{-}4\text{-}CH_3)]_2$, denoted (I)/(II), and $CCl_3C(O)NHP(O)[(R)\text{-}(+)\text{-}NHCH(C_2H_5)(C_6H_5)]_2$/$CCl_3C(O)NHP(O)[(S)\text{-}(–)NHCH(C_2H_5)(C_6H_5)]_2$, denoted (III)/(IV), have been synthesized and characterized by melting point, IR, NMR, mass. In the IR spectra of (I)/(II) and (III)/(IV), the bands centered at 3300 cm^{-1} for the first pair and at 3311/3307 cm^{-1} for the second pair are attributed to the NH_{amine} stretching frequencies. The mass spectra, in 70 eV experiments, of (I)/(II) and (III)/(IV) reveal the presence of the molecular ion peaks at m/z = 477 (considering one ^{37}Cl and two ^{35}Cl). For (I)/(II) and (III)/(IV), the ^{31}P signals appear at 4.30/4.24 ppm and 4.67/4.75 ppm, respectively. The signals of $N_{CP}H$, in ^{1}H NMR spectra, are observed at 9.29, 9.34, 9.55 and 9.42 ppm for (I) to (IV), respectively, all of them to be broad. The two chiral amine fragments in all of the compounds (I), (II), (III) and (IV) reveal two sets of signals in corresponding ^{1}H and ^{13}C NMR spectra. Typically,the two NH protons in each compound appear as two triplets. The triplet pattern is a result of vicinal H-H and geminal P-H couplings. In the ^{13}C NMR spectra of (I)/(II) and (III)/(IV), the carbon atom of the C(O) group appears as a singlet.

References:

[1] Gál, B., Bucher, C., Burns, N. Z. Mar. Drugs, 14 (2016) 206–217.

[2] Lu, Y., Nakatsuji, H., Okumura, Y., Yao, L., Iahihara, K.. J. Am. Chem. Soc. 140 (2018), 6039–6043.

[3] Eghbali Toularoud, M., Pourayoubi, M., Dušek, M., Eigner, V., Damodaran, K.. Acta Cryst. C. 74 (2018) 608–617.

Preparation of carbon nanotube enriched with $\{Mo_{154}\}$ for the hollow fiber-solid phase microextraction of naproxen in urine samples

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Abstract:

According to our experience from previous studies on the development of novel catalytic methods for oxidation of organic compounds in green media [1-3], we describe the preparation of CNT enriched with polyoxomolybdate $\{Mo_{154}\}$. $\{Mo_{154}\}$ was prepared by a one-step reaction at room temperature and characterized by FT-IR, XRD, Uv-Vis and TEM [4]. Based on chemical adsorption between $\{Mo_{154}\}$ and carboxylic acid groups in CNT, which were introduced to the CNTs by adding dilute nitric acid, $\{Mo_{154}\}$ was successfully located on the CNTs as the modifier. The hollow-fiber was used for the microextraction of the naproxen from urine sample under the optimized conditions as sensitive technique to determinate naproxen. After optimizing the reaction conditions, extraction of naproxen in the presence of hollow-fiber combined with fluorescence spectrophotometry was performed.

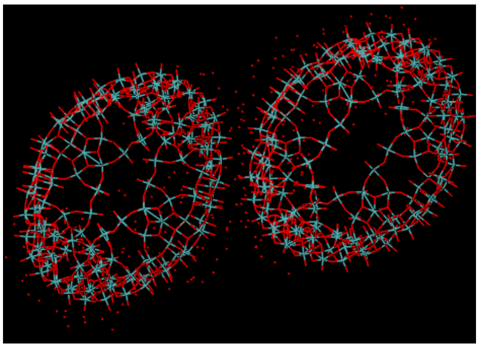

Fig. 1. Representation of the $\{Mo_{154}\}$-type giant-wheel anion

References:

[1] R. Haddad, Current Catalysis, 6 (2017) 97.
[2] R. Haddad, Current Catalysis, 5 (2016) 116.
[3] R. Haddad, M. Dusti , H. Abedi, A. Roostaie, Current Organic Synthesis, 15 (2018) 533-540.
[4] A. Muller, S. K. Das, V. P. Fedin, E. Krickemeyer, C. Beugholt, H. Bogge, M. Schamidtmann, B. Hauptfleisch. Z. Anorg. Allg. Chem. 625 (1999) 1187-1192.

Electrospun nanofiber with PAN and polyoxomolybdate as a new membrane for adsorption diethyl chlorophosphate(DCP)

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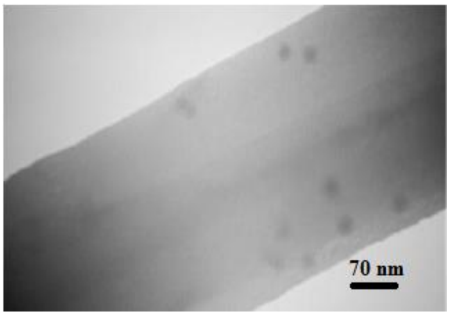
Abstract:

Chemical warfare agents (CWA) are some of the most nefarious weapons, and their possible use in terrorist attacks has led to growing interest in the development of reliable and accurate methods to absorb these lethal chemicals [1]. In this paper, we have prepared new membrane for adsorption of diethyl chlorophosphate (DCP) as a nerve-agent simulant and assess the possibility of using the nanofiber as protective membranes in face masks and warfare clothing [2]. Adsorption of DCP, was investigated on the surface of PAN nanofiber embedded with {Mo_{132}}. The result showed the role of modified PAN nanofiber with {Mo_{132}} on the effective adsorption of DCP, as a stimulant of nerve agents, and possesses a suitable candidate for protecting cloth. The surface morphology and other properties of the PAN/{Mo_{132}} nanofiber membrane are characterized by various techniques, including SEM, TEM, FT-IR, TGA and UV-vis spectroscopy. The leaching of {Mo_{132}} from the nanofiber was not observed, meaning that the catalyst had excellent stability and could be used as a heterogeneous structure against the adsorption of sulfur mustard stimulant at room temperature[3].



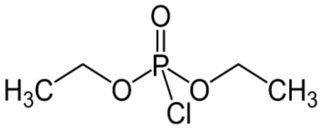


Fig.1. TEM image of nanofiber membrane PAN/{Mo_{132}} (left) and structure of Diethyl chlorophosphate (right)

References:

[1] K. Kim, O. G. Tsay, D. A. Atwood, D. G. Churchill, Chemical Reviews, 111 (2011) 5345.
[2] R. Haddad, Current Catalysis, 6 (2017) 97.
[3] R. Haddad, M. Dusti Telgerd, M. Sadeghinia, H. Hadi, Current Applied Polymer Science. DOI : 10.2174/2452271603666190307161415

Synthesis and characterization new macroacyclic complexes containing piperazine moieties with a number of metal ions

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Abstract:

The preparation and characterization of metal complexes with macrocyclic or macro-acyclic ligands was the goal of much research in recent years. Bioinorganic chemistry, material science, catalysis, separation and encapsulation processes, hydrometallurgy, formation of compounds with unusual properties, metal-metal interactions, transport and activation of small molecules have received considerable stimulus from the employment of such ligands [1]. Macro-acyclic ligands have been synthesized to verify the influence of the donor atoms and their relative positions, the number and size of the chelate ring formed, the flexibility and the shape of the coordinating moiety, their planar or tridimensional architecture, etc. on the metal ion binding and selectivity. Piperazine is a cyclic diazine with a rigid cyclohex-ane ring and a suitable structural moiety for macrocyclic and macroacyclic compounds [2].

In this work, we report the synthesis and characterization of new macroacyclic Schiff base complexes have been prepared via the Ni(II) or Co(II) or Zn(II) of 2-((4-(2-aminoethyl)-1,4-diazepan-1-yl)methyl)benzenamine with salicylaldehyde.The complexes have been characterized by elemental analysis, IR and ^{1}HNMR.

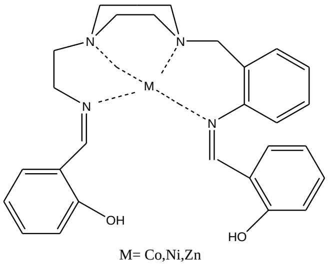

Fig1. macroacyclic Schiff base complexes

References

[1] K. Henrick, P. A. Tasker and L. F. Lindoy, in S. J. Lippard (Ed.), Progress in Inorganic Chemistry, 33 (1985) 1.

[2] H. Keypour, M. Rezaeivala, M. Mirzaei-Monsef, K. Sayin, N. Dilek, H. Unver, Inorg. Chim. Acta 432 (2015) 243-249.

Synthesis and characterization of two new schiff base ligands containing curcumin moiety and corresponding complexes with Fe(III) and Zn^{2+} ions and related anticancer studies

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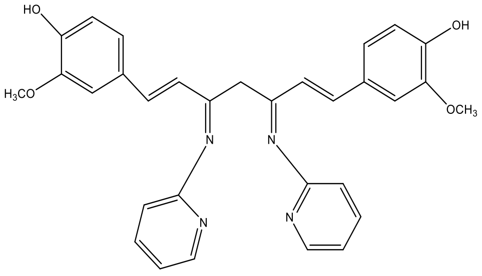
Abstract:

The uses of plants in new drug discovery has been stated in novel reports. Plant have been applied for years in pharmaceuticals, natural therapies and alternative medicine. A plant extract is an active compound that is removed from the tissue of a plant with eligible effects, to be used for a certain purpose [1].

Turmeric is a significant medicinal spice that comes from the root Curcuma longa. The turmeric rhizome contains a variety of pigments among which curcumin is a major pigment that incorporates several functional groups and can be easily dissolved into organic solvent such as methanol, ethanol, and acetone [2].

In this work two new Schiff base ligands, (1 and 2), derived from condensation reaction of 1,7-bis-(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, (curcumin), with 2-amino pyridine and 1,2- diamino ethane, and their complexes of Zn^{2+} and Fe(III) ions were synthesized and characterized. The ligands and complexes were investigated by elemental analysis, IR spectroscopy, ^{1}H and ^{13}C NMR and Mass analysis.



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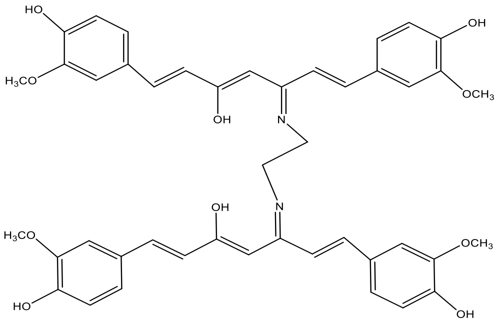

(2)

References:

[1] E.Faramarzi, MM.Zangeneh, A.Zangeneh, R.Moradi,Online Journal of Veterinary Research, 1(2) 6 (2017) 77-80.

[2] P.Yoysungnoen, P.Wirachwong, P.Bhattarakosol et al, Clin-HemorheolMicrocirc 33(2) (2005) 127–135.

Synthesis and characterisation of a new nanobiocomposite based on Dawson-nanocellulose for catalytic synthesis of metal nanoparticles

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Abstract:

Bionanocomposites are bio-based nanocomposites. Actually, they represent an emerging group of nanostructured hybrid materials. Expanding the concept of biocomposites[1] to the nanostructured hybrid materials, “bionanocomposites” can be defined in the following two ways. It could designate nanocomposites as materials made from renewable nanoparticles (e.g., cellulose whiskers and MFC) and petroleum-derived polymers like PP, PE, and epoxies[2].

In this research, the green cellulose-Dawson nanobiocomposites were synthesised using nanocellulose and Dawson heteropolyacid at different loadings including 5, 10, 15 and 20 wt% and used for in-situ synthesis of silver and gold nanoparticles with different sizes and morphologhies. Our findings show that these nanobiocomposites can produce metal nanostructures on their surface and form nanobiocomposites including metal nanostructures . The prepared nano biocomposites characterised by FTIR, XRD, AFM, TEM and SEM analysis. In addition, the metal nanostructure synthesis was investigated by UV-vis spectroscopy step by step. It was shown that the loading amount of heteropolyacid could control the size and shape of metal nanostructures as well as time and pH of their formation.

References:

[1] A.Espert, F.Vilaplana, S.Karlsson, Compos. A-Appl. Sci. Manuf, 35 (2004) 1267-1276.
[2] S.Gilberto, B.Julien, D.Alain, Polymers, 2 (2010) 728-765.

Synthesis, characterization, theoretical calculation and antimicrobial properties of a new zinc chloride complex

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Abstract:

Schiff bases derived from aromatic carbonyl compounds have been widely studied in connection3 with metalloprotein models and asymmetric catalysis, due to the versatility of their steric and electronic properties. Schiff bases and their biologically active complexes have been often used as chelating ligands in the coordination chemistry of transition metals as radiopharmaceuticals for cancer targeting, agrochemicals, as model systems for biological macromolecules, as catalysts and as dioxygen carriers. The phenyl derivatives of schiff bases are used as corrosion inhibitors. Schiff bases derived from aldehyde and diamines constitute one of the most relevant synthetic ligand systems with importance in asymmetric catalysis and they appear to be of importance for a broad range of transition-metal catalyzed reactions including lactide polymerization, epoxidation of olefins, hydroxylation and asymmetric ring opening of epoxides. Schiff bases can be used to obtain optical materials and conducting polymers[1-3]. In this work, we present synthesis and characterization of a new zinc halide complexes with formula of $ZnLCl_2$ in which L= a new ligand formed via condensation of bromobenzaldehyde and bis(2-aminoethyl)amine). The ligand and its complex were characterized by physical and spectral data. After characterization, the ligand and its complex have been subjected to biological standard tests for their antimicrobial activities. Finally, the compound structur was optimized and then some structural parameters and vibrational frequencies were calculated at the B3LYP/LANL2DZ level of theory.

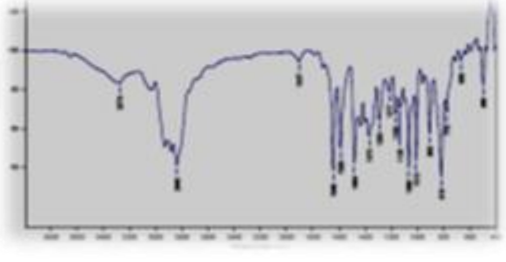

Fig.1. The FTIR of ligand.

References

[1] K. Sztanke, A. Mazark, A. Osinka, M. Sztanke, Bioorg. Med. Chem. 21 (2013) 3648.
[2] J. L. Sessler, E. Tomat, V. M. Lynch, J. Am. Chem. Soc.128 (2006) 4184.
[3] S. Ghanbari Niyaky, M. Montazerozohori R. Naghiha, J. Phys. Org. chem., 30 (2017) 37.

Synthesis and crystal structure determination of a new Nickel(II) macrocyclic complex containing homopiperazine moiety

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macrocyclic ligands have an excellent basis for the study of molecular recognition phenomena due to their cavity size, shape and donor atoms. Macrocyclic structurally reinforced by the inclusion of bridging groups within macrocyclic ring showes much greater rigidity than those its analogues [1]. We have already reported a number of macrocyclic Schiff base complexes containing piperazine and homopiperazine moieties [2]. In this work a new dialdehyde have prepaired by use of Mannich reaction method and related macrocyclic Schiff base ligands synthesised in the presence of 1,4-diamino butane(L_1), and 1,3 diamino propane (L_2). Their related complexes were obtained by using of perchlorate salts of Ni^{2+} and Co^{2+} .The aldehyde and ligands were investigated by elemental analysis ,IR spectroscopy ,^1H and ^{13}C NMR and related complexe were characterizated by elemental analysis , IR spectroscopy and X-ray spectroscopy in the case of NiL_1.

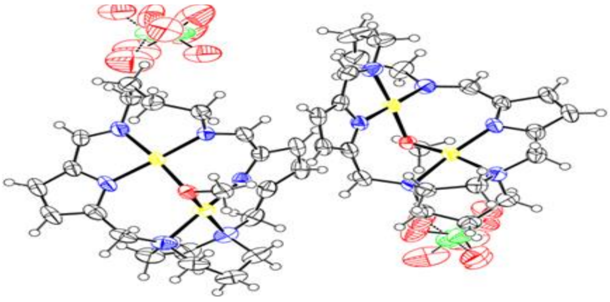

Fig.1. NiL_1 structure

References:

[1] H. Keypour, H. Zeynali, M. Rezaeivala, F. Mohsenzadeh, H. Amiri Rudbari, G. Bruno, A. Sadeghpour, J. Iran Chem. Soc., 12 (2015) 1665-1675.
[2] M. Rezaeivala, H. Keypour, Coord. Chem. Rev., 280 (2014) 203.

Oxidation of Styrene by nano magnetically coordination compound from Fe_3O_4 and Cu(II) complex

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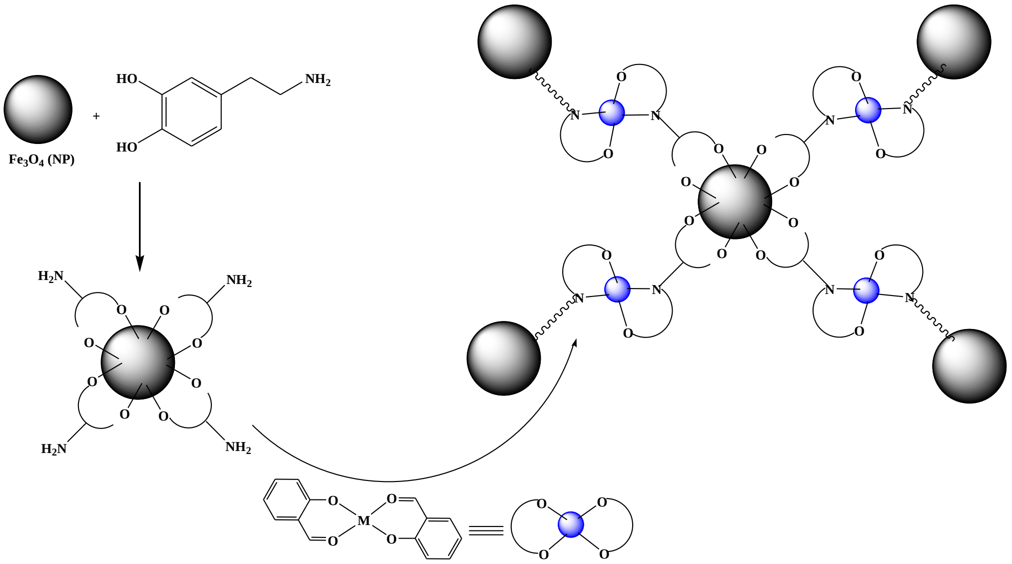
Abstract:
The oxidation of organic compounds using Schiff base complexes has been a field of academic and industrial interest to analyze the catalytic activity of various metal complexes [1–2]. In this project, a new nano-magnetically-compound was synthesized from Cu(II) complex and nano-Fe_3O_4 by covalently bond and characterized by general techniques such as: FTIR, UVD, XRD, SEM and EDX. A Cu complex is covalently anchored to Fe_3O_4 nano-particle by formation of Imine bonds. On the other hand, a Cu-Schiff base complex immobilized on nano-Fe_3O_4 by a Dopamine as a bridge (Scheme.1).



Scheme 1: synthesis root of nano-magnetically Schiff base compound.

As a result, the homogenous complex is easily converted to the heterogeneous-magnetically compound. Then, catalytic property of this compound was studied on oxidation of Styrene by *tert*-butyl hydroperoxide (TBHP) as an oxidizing agent at room temperature. The results showed a solvent free, green, selective, high yield and effective oxidation. The main product is Benzaldehyde. Then, the catalytic properties enhanced by cooperation of Cu complex and Fe_3O_4.

References:
[1]. Z. Xi, H. Wang, Y. Sun, N. Zhou, G. Cao, M. Li, J. Mol. Catal. A Chem. 168 (2001) 299.
[2]. T. Mykaiyama, T. Yamada, Bull. Chem. Soc. Jpn. 68 (1995) 17.

Synthesis and characterizationof macroacyclic Schiff-base ligand containing one mopiperazine moiety and its Zn(II) complex

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Abstract:

The Schiff base ligand (H_2L) by potentially N_6O_2 donor systemhas been prepared from condensation of 2-hydroxybenzaldehyd with polyamin(A). IR spectrum of ligand exhibitsa ν(C=N) vibration in 1634 cm^{-1}.The mass spectrum of ligand (H_2L) shows the peak at 647 m/z that confirms the synthesis ligand. In the ^1H-NMR spectrum of ligand the signal for the imine proton appears at 8.53 ppm. Also the signal for the hydroxyl protons appears at 13.8 ppm. The spectrum of amine proton removed that confirm the synthesize reaction of Schiff base ligand has completed. From direct reaction of this ligand and Zn(II) metal ion,the macroacyclic Schiff-base complex [Zn(H_2L)]was synthesized.IR spectrum of complex exhibit a ν(C=N) vibration in 1611 cm^{-1}.The mass spectrum of ligand (H_2L) shows the peak at 755 m/z that confirms the synthesis ligand. In the ^1H-NMR spectrum of ligand the signal for the imine proton appears at 8.64 ppm, also the signal for the hydroxyl protons appears at 13.7 ppm. The results of elemental analysis confirms the synthesis of ligand and complex [1,2].

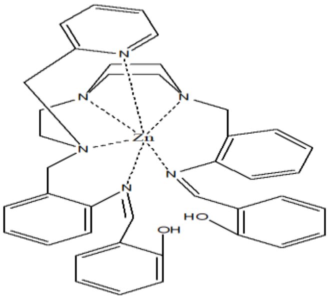

Fig 1. H_2L ligand

References:

[1] M. Rezaeivala, H. Keypour, Coord. Chem. Rev. 280 (2014) 203.

[2] H. Keypour, M. Mahmoudabadi, A. Shooshtari, M. Bayat, R. Karamian, M. Asadbegy, R. W. Gable, InorganicaChimicaActa. 478 (2018) 176.

Synthesis, spectroscopic and crystal structure studies of bidentate Schiff base ligands prepared from 2-(methylamino) and 2-(ethylamino)benzaldehyde

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Abstract:

Nowadays, Schiff base ligands play an essential role in coordination chemistry and their metal complexes exhibit various applications including catalyticactivity in organic reactions,biological activities, solar energy conversion and supramolecular devices [1-3]. In this work, the structures and spectroscopic properties of some new bidentate Schiff base ligands, derived from the reaction of2-(methylamino) or 2-(ethylamino)benzaldehydewithethylenediamine and 4-nitro-1,2-phenylenediaminewere investigated. The prepared bidentate Schiff bases were characterized by FTIR, NMR, UV-Vis spectroscopy, and their crystal structures were determined by single crystal X-ray diffraction analysis.

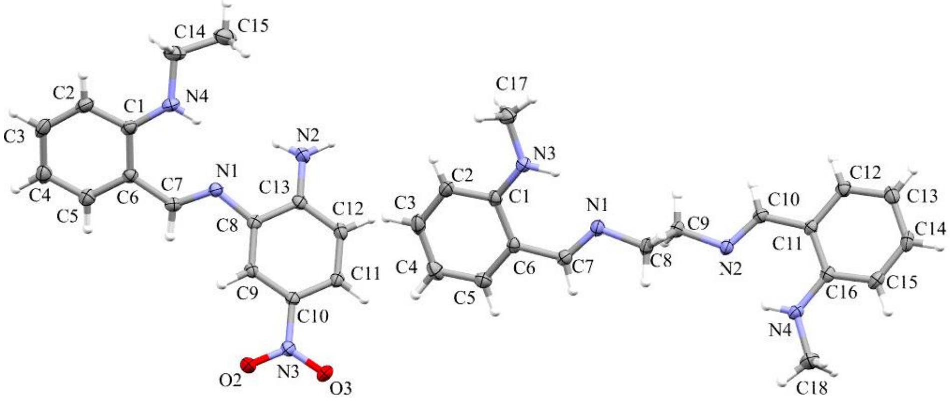

Fig 1. single crystal X-ray of prepared bidentate Schiff base

References:

[1] V. Mirkhani, R. Kia, A. Rostami-Vartooni, D.Milic, Transition Met. Chem., 34 (2009) 225.
[2] N.Armaroli, Chem. Soc. Rev, 30 (2001) 113.
[3] J. Ren, H. Xuan,W. Dai,Y. Zhu,L. Ge, Applied Surface Science, 448 (2018) 609.

Synthesis and characterization of new Schiff baseligands derived from 2′-hydroxyacetophenoneor 5'-chloro-2'-hydroxyacetophenone and their Ni(II) complexes

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Abstract:
The most common method for synthesis of Schiff bases is the reaction of aldehydes or ketones with primary amines in organic solvents [1]. These prepared Schiff base ligands with azomethine linkage (C=N) are able to coordinate with different transition metals in various oxidation states and stabilize them. Some Schiff bases have biological activities such as antibacterial, antifungal, antiviral, antitumor, anti-HIV [2,3]. Also, they have been used as inhibitors for the corrosion of metal alloys in acidic media [4].

In this work, the synthesis and spectroscopic properties of new Schiff base ligands and their Ni(II) complexes were described. These Schiff bases were derived from the reaction of several amines such as ethylenediamineand 4-nitro-1,2-phenylenediaminewith 2′-hydroxyacetophenoneor 5'-chloro-2'-hydroxyacetophenone. The prepared compounds were characterized by FTIR, NMR and UV-Vis spectroscopy.

References:

[1] V. Mirkhani, R. Kia, A. Rostami-Vartooni, H.-K. Fun, Polyhedron, 29 (2010) 1600.
[2]L.J. Li, C. Wang, C. Tian, X.Y. Yang,X.X. Hua, J.L. Du.Res. Chem. Intermed, 39 (2013) 733.
[3]A.M. Abu‐Dief, L.A. E. Nassr, J. Iran. Chem. Soc. 12 (2015) 943.
[4]M.A. Hegazy, Corrosion Science, 51 (2009) 2610.

New Ternary Complexes of Pt(II) with 5-bromo-2-hydroxybenaldehyde N(4)-phenylthiosemicarbazone: Synthesis, Spectroscopic Investigation and Antibacterial Activity

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Abstract:

Thiosemicarbazonesas a class of S-donor Schiff bases are an interesting group of bioligands. On the other hand ternary (heteroleptic) complexes formed between metal ions and two different types of bioligandsmay be considered as models for metal ion mediated biochemical interactions.The effect of one ligand on another through the central metal ion in heteroleptic complexes is very important in coordination and biological chemistry. Complexes of Pt(II) are widely used as chemotherapeutic agents and Pt-S interaction may play a significant role in anti-tumour activity of platinum drugs[1-3].

In this work, we report the synthesis, spectroscopic characterization and antibacterial activity of ternary Pt(II) complexes with 5-bromo-2-hydroxybenaldehyde N(4)-phenylthiosemicarbazone (H_2L). The ligand was prepared by the condensation reaction of the N(4)-phenythiosemicarbazide and corresponding aldehyde. Then the Pt(II) complexes, $[PtL(PPh_3)].C_2H_5OH$ and [PtL(Imd)], have been synthesized by reaction of H_2L with K_2PtCl_4 in presence of PPh_3 or imidazole as auxiliary ligands. New complexes were investigated by elemental analysis, IR and ^{1}HNMR spectroscopy. In all complexes thiosemicarbazoneacts as a tridentate dianionic ligand and coordinates *via* the thiol group, imine nitrogen, and phenolic oxygen. Coordination sphere of complexes are completed by heterocyclic base. The *invitro* antibacterial activity of ligand and complexes has been evaluated against Gram-positive (*Bacillus cereus* and *Staphylococcus aureus*) and Gram-negative (*Escherichia coli* and *Pseudomonas aeruginosa*) bacteria. The results reveal that complexes show good antibacterial activities compared with standard drugs and better activity in comparison to the thiosemoicarbazone (H_2L). The complex containing imidazole, [PtL(Imd)], was more active than the complex with PPh_3.

References:

[1] M. Azarkish, A. Akbari, T. Sedaghat, J. Simpson, J. Mol. Struct., 1156 (2018) 34-42.
[2] A.I. Matesanz, P. Albacete, P. Souza, Polyhedron, 109 (2016) 161-165.
[3] M. Azarkish, A. Akbari, T. Sedaghat, J. Simpson, J. Mol. Struct., 1134 (2017) 126-134.

The inhibition of α-carbonic anhydrase (CA) enzyme by cyanate ion with five-fold ligand: A DFT study

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Abstract:

Density functional theory (DFT) using B3LYP functional and split-valance 6-311G** basis set have been employed tooptimized the geometry ofcyanate ion (OCN^-)inhibitor and complex between this inhibitor with active site of α-carbonic anhydrase (CA) enzyme. The results show that the zinc cation in the active site of the CA enzyme prefers tetrahedral geometry. While the cyanate anion is coordinated to the zinc, the geometry could be change to trigonal bipyramidal or the tetrahedral geometry [1,2],(Figure 1).

It is noteworthy that among the anions studied as inhibitors, including: N_3^-, SCN^-, HS^-, HSO_3^-, CN , cyanateion performs the best inhibitor.

Also the cyanateanion belongs the second group of inhibitors of α-carbonic anhydrase which possess pharmacological applications.

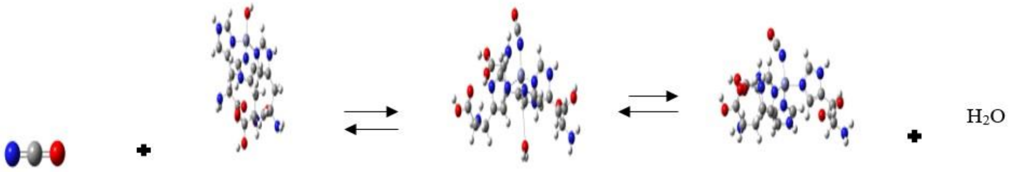

Fig.1. The reaction path between Cyanate Ion and CA

References:

[1] A.Innocenti.C.T. Supuran.et al.. Med. Chem.14 (2004) 3327-3331.

[2] S.DelPrete, C. T. Supuran. et al.. J EnzymInhib Med Ch. 34 (2019) 644–650.

Water soluble ionic $Ni_2L_2(OH)(Cl)$ and $Cu_2L_2(OAC)_2$. $4H_2O$ Schiff base Complexes (L= 5-methyl 1-methylbenzimidazoliumsalicylimine ethylene N, N- dimethyl amine- chloride): Synthesis and Characterization

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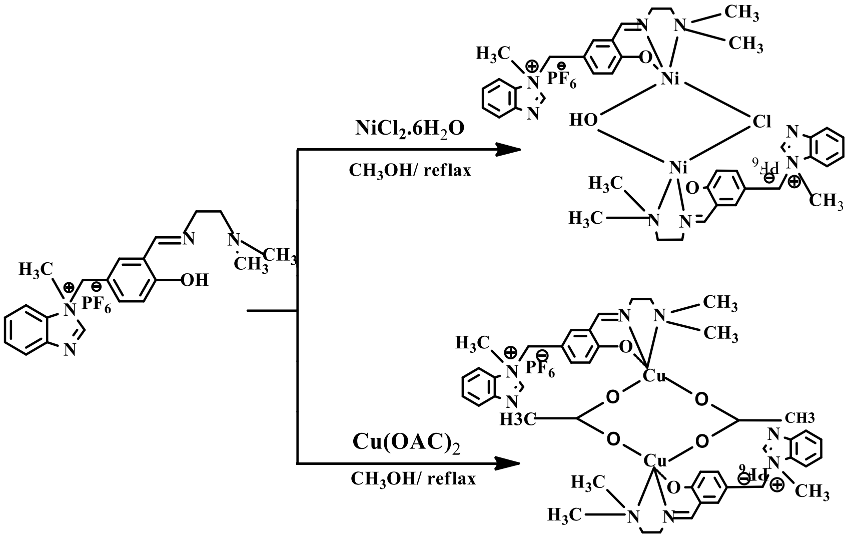
Abstract:

During the last decades the Schiff base chelating ligands or azomethine compounds that are synthesized by reaction of a primary amine and a carbonyl group (aldehyde or ketone) played central role in development of coordination chemistry [1]. They can bind to metal ions and form metal complexes with different properties [2]. Water soluble Schiff base ligands and complexes are rare in literature. Thus in this study we report the synthesis and characterization of two new ionic metal complexes of Ni^{2+} and Cu^{2+} containing the Schiff base ligand of 5-methyl 1-methylbenzimidazoliumsalicylimine ethylene N, N- dimethyl amine- chloride. By reaction of the N-methyl benzimidazole and chloromethylsalicylaldehyde and then by KPF_6, the benzimidazolium methyl salicylaldehydehexafluorophosphate was synthesized. It was reacted by N, N-dimethyl ethylene diamine to synthesis of three dentate Schiff base ligand (L). The reaction of L with $Cu(OAC)_2$ and $NiCl_2.6H_2O$ resulted to synthesis of the $Cu_2L_2(OAC)_2.4H_2O$ and $Ni_2L_2(OH)(Cl)$. The Schiff base ligand and related complexes were characterized via different analytical and spectral methods (CHN, FT-IR, UV-vis).



Scheme 1. Schiff base ligands and complexes

Refrences:

[1] Tahmasebi¸V. Grivani¸ G. Bruno¸ G. J. Mol. Struct. 1123 (2016) 367.
[2] Ji, Y. F. Wang, R. Du. C. F. Liu, Z. L. Inorg. Chem. Commun. 16 (2012) 47.

Intraction of Diorganotin (IV) with Copper Schiff base complexes: Synthesis, Characterization and Adduct Formation Studies

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Abstract:

The equilibrium constant and the thermodynamic parameters were spectrophotometrically measured for the 1:1 adduct formation of the copper (II) Schiff base complexes [CuL] where L= Methyl-2-{N-[2-(2-hydroxy-5-methoxyphenyl)methylidynenitrilo]-ethyl}amino -1-cyclopentenedithiocarboxylate, (H_2cd5OMesalen); Methyl-2-{N-[2-(2-hydroxy-5-bromo-phenyl)methylidynenitrilo]ethyl}amino-1-cyclopentenedithiocarb-oxylate, (H_2cd5Brsalen); Methyl-2-{N-[2-(2-hydroxy-5-nitrophenyl)methylidyn-enitrilo]ethyl} amino-1-cyclopentenedithiocarboxylate, (H_2cd5NO_2salen) [1,2] as donors with R_2SnCl_2 (R= Me, n-Bu) as acceptors in dimethylformamide (DMF) and methanol (MeOH) as solvents at 25°C. Adducts have been characterized by ^{1}H, ^{119}Sn NMR, IR and UV-Vis spectroscopy. Our results revealed the trend of adduct formation constants between Schiff base complexes as donors and tin(IV) as acceptor decreases as follow:
[Cu(cd5OMesalen)] > [Cu(cd5Brsalen)] > [Cu(cd5NO_2salen)];
Me_2SnCl_2> n-Bu_2SnCl_2 and DMF >MeOH.

References:

[1] Sh. Esmaielzadeh, E. Zarenezhad, ActaChim. Slov. 65 (2018) 416–428.
[2] Sh. Esmaielzadeh, L. Azimian, Kh. Shekoohi, Kh. Mohammadi. Spectrochim. Acta Part A: Mole. Biomole. Spectro.133 (2014), 579–590.

Pd [60] fullerene complex immobilized on Graphenenanocomposites: a recoverable and efficient catalyst for the Suzuki–Miyaura reaction

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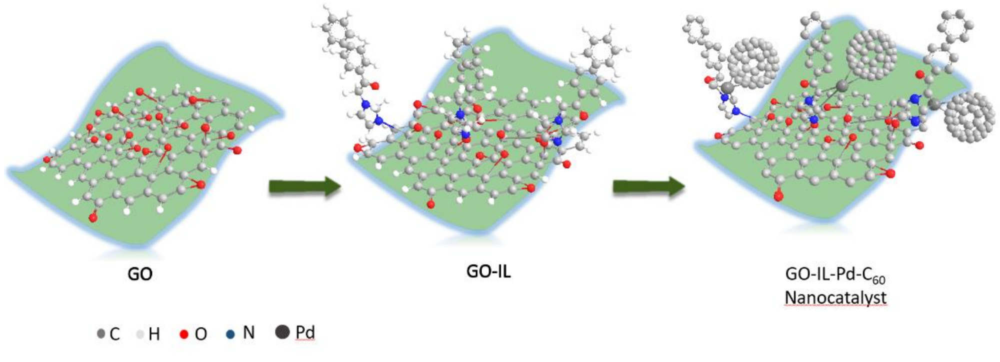
Abstract:

In this study graphene functionalized with a palladium complex (IL-NH) was synthesized. The covalent functionalization reactions of GO include the formation of covalent bonds between the NH functional group of ligand and the epoxy group, followed by the graphene oxide being completely reduced with Pd $(dba)_2$-C_{60}.Recently,Graphene is a novel nanostructured material that can be conveniently used and has gained significant attention in various technological fields including catalytic chemistry, organic synthesis, and electrochemistry [1,2]. The resultant graphene oxide supported C_{60}-Pd-GO composite (GO-supported IL-NH-C_{60}-Pd) was characterized by various spectroscopic and microscopic techniques, including ultraviolet-visible (UV–Vis), Fourier-transform infrared (FT-IR), X-ray powder diffraction (XRD) and Scanning electron microscope (SEM), thermogravimetric analysis (TGA), Energy-dispersive X-ray spectroscopy (EDS). The immobilization of a homogeneous catalyst onto a solid surface was one of the major challenges in catalysis,the results showed that graphenewas a superior substrate to supported metals for applications in the heterogeneous catalysis. The tests of immobilized palladium nanoparticles have shown that they exhibit high activity in the Suzuki–Miyaura carbon-carbon coupling reactions. In addition, this method has several advantages over its homogeneous analogue, such as short reaction time, low catalyst load, high performance and catalytic ability reusability without significant loss of catalytic activity and easy and costly cost of the procedure for Preparation of catalysts [3].



Scheme 1. graphene oxide supported C_{60}-Pd-GO composite (GO-supported IL-NH-C_{60}-Pd)

References:

[1] Li Y, Fan X, Qi J, Ji J, Wang S, Zhang G, Zhang F. Nano Res, 3 (2010) 429–437.
[2] Dreyer DR, Park S, Bielawski CW, Ruoff RS. Chem. Soc. Rev, 39 (2010) 228–240.
[3] Wang GX, Yang J, Park J, Gou XL, Wang B, Liu H, Yao J. Facil. J Phys. Chem. C, 112 (2008) 8192–8195.

A comprehensive study on the synthesisand X-ray characterization of new dimeric palladium(II) complexes of phosphoniumylides

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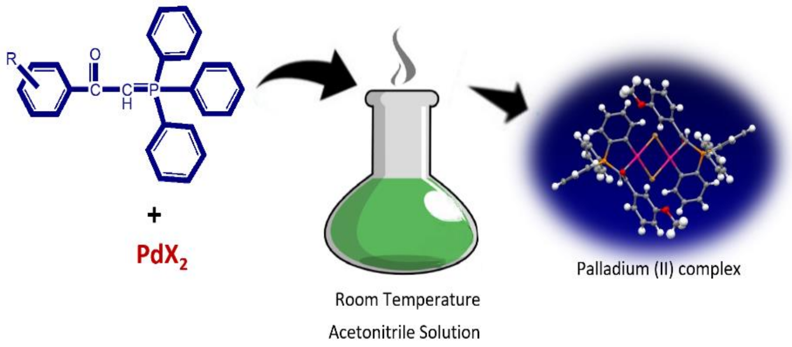
Abstract:

A new series of palladium (II) complexes having α-keto stabilized phosphoniumylides as ligands with general formula $[Pd(\mu\text{-}X)(PPh_3CHC(O)C_6H_4R)]_2$ [X = Cl, R=*m*-OCH_3 (**1**), R=*p*-NO_2 (**2**), X = Br, R=*m*-OCH_3 (**3**), R=*p*-NO_2 (**4**)] was prepared. All complexes were characterized by FT-IR and multinuclear (^1H, ^{13}C, and ^{31}P) NMR spectroscopic techniques. Also, a single crystals X-ray diffraction study was executed for compounds **1** and **3**, which revealed a dimeric square-planar geometry around Pd(II) ions for these complexes. Based on the spectroscopic and crystallographic results, it was found that the phosphoniumylides have coordinated to palladium(II) centers through the coordinatively active ylidic carbon atom and ortho-carbon atom of PPh_3 phenyl ring (ortho-palladation) [1,2].



Scheme 1. Structure of palladium (II) complexe

References:

[1] Wittig, G., and Krauss, D., Liebigs Ann.,34 (1964) 679

[2] S.J. Sabounchei, S. Samiee, D. Nematollahia, A. Naghipour, D.M. Morales, Inorg. Chim. Acta 363 (2010) 3973-3980.

The inhibitory effects of phthalocyaninederivatives as new inhibitors of hCAII enzyme

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Abstract:

In thisstudy, the mechanism of inhibitory performance of silicon(IV)photolocyanineas an inhibitor with carbonic anhydrasII enzyme activesitehas been investigated.The most stable contraormer of this inhibitor ZT-SIQ has been chosen for calculations. All calculations have been done B3LYP level, using 6-31G* basis set.Also thermodynamic functions such as deprotonation enthalpy of inhibitors(ΔH^{0}), standard enthalpies of complexation , standard entropy of complexation (ΔS_{com}^{0}) and standard Gibbs free energy of complexation(ΔG_{com}^{0}) for CA–inhibitor complex are evaluated.In all calculations solvent effects have been considered in water using PCM method. Thus, silicon(IV) photolocyanine derivatives show a new class of carbonic anhydrase inhibitors that might find applications for targeting physiologically relevant isoforms of different forms of CA[1-3].

References:

[1]Arslan, T., Biyiklioglu, Z. and Şentürk, M.,. RSC Advances, 19 (2018) 10172-10178.
[2] Baş, H., Barut, B., Biyiklioglu, Z. and Özel, A., Dyes and Pigments,160 (2019) 136-144.
[3]Ghiasi, M., Kamalinahad, S. and Zahedi, M., 2014. Journal of Structural Chemistry,55 (2014) 1574-1586.

Using linker shapes as a tool to direct MOFs' dimensionality from 2D to 3D and its morphological study

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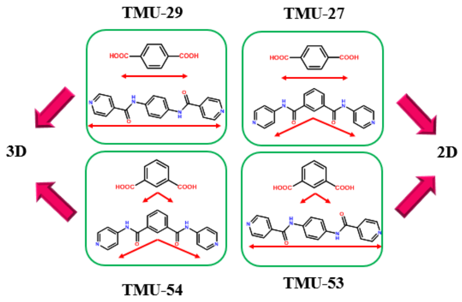
Abstract:

Pillar-layered Metal Organic Frameworks (PMOFs) [1] are a striking branch of MOF materials which investigating their properties as multi donor porous frameworks is of great interest. Rational design and control of the crystal growth, specifically dimensionality is one important goal for inorganic chemists to be achieved. Whether the resulted networks are one, two or three dimensions the related properties and applicability are different. The most important features of 3D networks are their stability and permanent porosity, while 2D frameworks are interesting for their ultrathin thickness and large surface area with highly accessible active sites. Since the crystal growth in pillar-layered MOFs is a spontaneous self-assembly process, predesign of linkers, for conducting the resulted crystals toward 3D or 2D architectures is promising strategy. Hence, linker modification can act as a favorable method for controlling structure assembly.Here in, for the first time, we report a novel strategy to control the dimensionality, topology and further the morphology of four MOFs through adjusting the linker shapes. Our results interestingly indicate that introducing a v-shaped linker along with a linear one lead to formation of 2D network in TMU-27 [Zn(bpipa)(BDC) and TMU-53 [Zn(bpfb)$_{0.5}$(IsoBDC)], whereas applying two v-shaped or two linear linkers into the structures produces 3D frameworks TMU-29 [Zn(bpfb)(BDC). 2DMF] and TMU-54 [Zn(bpipa)$_{0.5}$(IsoBDC)] (BDC: terephthalic acid, Iso-BDC: Isophthalic acid, bpipa: N,N'-di(pyridine-4-yl)isophthalamide and bpfb: N,N'-bis-(4-pyridylformamide)-1,4-benzenediamine). (Scheme 1)For further investigation on the effect of linker shapes on the MOFs properties, the morphological control of the structures through coordination modulation by different capping agents has been done.



Scheme 1. bpfb

References:

[1] F. Zarekarizi, M. Joharian, A. Morsali, J. Mater. Chem. A, 6 (2018) 19288-19329.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Coordination chemistry of new Cu(II) Schiff base complex containing a piperazine head unit

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Abstract:

Schiff base complexes have remained an important and popular area of research due to their simple synthesis, versatility and diverse range of applications [1]. Piperazine is a well-knowbuilding block for novel supramolecular structures due to the presence of two weakly held terminal amino protons. The piperazinemoiety is a structural part of many analgesics, psychotropic and antitumor drugs [2]. A series of complexes containing pipirazine have been reported by us previously [3].

Herein a polyamine containing piperazine moiety and related Schiff base macroacyclic ligand were designed and prepared. Then a new Schiff base complex is synthesized by reaction of prepared ligand with Cu(II) metal ion. In the resulted complex, Cu(II) is coordinated to ligand by four nitrogen (two from piperazine moiety and two nitrogen of imine bonds) and two phenolic oxygen. These Schiff-baseligand and its coppercomplexwere characterized by elemental analysis, IR spectroscopy, EI-Mass and X-ray analysis in the case of ligand (Figure.1).

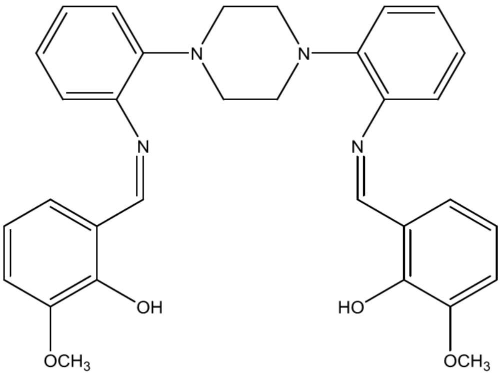

Fig.1. Molecular structure of prepared Schiff base ligand

References:

[1] M. Rezaeivala, H. Keypour, Coord. Chem. Rev. 280 (2014) 203.
[2] Z. H. Chohan, S. H. Sumrra, M. H. Youssoufi, Eur. J. Med. Chem. 45 (2010) 2739.
[3] H.Keypour, M.Mahmoudabadi, A.Shooshtari, M.Bayat, R.Karamian, M.Asadbegy, R.W.Gable, InorganicaChimicaActa, 478 (2018)176.

Intrinsic affinity, size match and solvent hindrance during complexation of cryptands 221 and 222 with Na^+ and K^+ cations; a computational study

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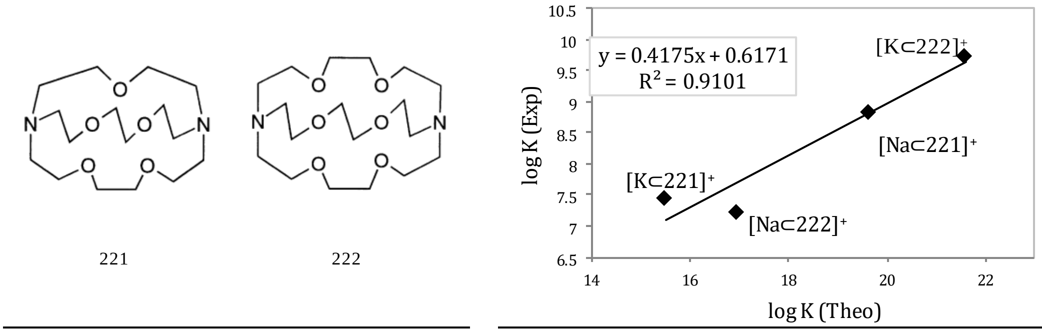
Abstract:

Molecular recognition plays a key role in many biochemical processes, in the design of new materials, and in the development of new procedures for analytical chemistry [1]. Host-guest interactions, which are usually noncovalent, have been modeled in many simple systems using the premises of supramolecular chemistry [2,3]. The 221 and 222 cryptands (see Figure 1a) are synthetic macrocyclic multidentate ligands (hosts) that exhibit high selectivity towards metal ions (guests), and have been used as prototype for molecular recognition by complexation. The experimental observations reveal that 221 is selective for Na^+ over K^+ and 222 is selective for K^+ over Na^+. Herein, we report a theoretical study on complexation of cryptands 221 and 222 with Na^+ and K^+ cations, at BP86/def2-TZVP level of theory. The calculations on the interaction energies in the gas phase show that the interaction of both hosts with sodium ion is larger than that with potassium and this means that 221 and 222 have intrinsically larger affinity for sodium ion. However, the results of calculations on the formation of complexes in solution are in agreement with experimental observations (see Figure 1b). Indeed, in the solution there is a competition between the host and solvent molecules to catch the metal cation.



(a) **(b)**

Fig.1. Chemical structures of hosts studied here (a), correlation between experimental and calculated log *K* values for formation of $[Na\subset 221]^+$, $[K\subset 221]^+$, $[Na\subset 222]^+$ and $[K\subset 222]^+$ complexes in methanol.

References:

[1] J. M. Lehn, Supramolecular chemistry: Concepts and perspectives 1995, VCH, New York.
[2] P. Auffinger, G. Wipff, J Am Chem Soc, 113 (1991) 5976–5988.
[3] S. Salehzadeh and Y. Gholiee, Dalton Transactions 44 (2015) 19708–19716.

A theoretical study on interaction of bispidine analogue of cisplatin $[(C_7H_{14}N_2)PtCl_2]$ with guanine;DFT, EDA-NOCV and NBO analysis

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Abstract:

Since discovery of cisplatin, many efforts have been devoted to understand the mechanisms associated with its antitumor activity, which are nowadays quite well established [1]. The primary target of cisplatin is genomic DNA, and more especially the N7 position of guanine bases. Although there is no doubt that a Pt−N7 bond forms during initial attack, the exact structure of the monofunctional adduct is not well known [2]. A better understanding at the molecular level of the interactions between the Pt and DNA building blocks can be helpful in establishing a new strategy to design cisplatin analogues. In this work we report a theoretical study on the interaction of bispidine analogue of cisplatin $[(C_7H_{14}N_2)PtCl_2]$ (**1**; see Figure 1) with guanine, at BP86/def2-TZVP level of theory. Since the guanine has three possible binding sites with the transition metal, all isomers and conformers of **1**-guanine complexes were optimized. The calculated relative free energies and interaction energies between **1** and guanine showed that the preferred binding site of guanine to complex **1** (similar to cisplatin) is N7. To investigate the nature of interaction between **1** and guanine, the EDA-NOCV and NBO analyses were also performed on **1**-guanine complex. The results of energy decomposition analysis, at BP86-D3/TZ2P level of theory, for all complexes show that the electrostatic nature of interaction between **1** and guanine is more than the covalent (~60% versus ~35%) and contribution of dispersion forces is ~5%.

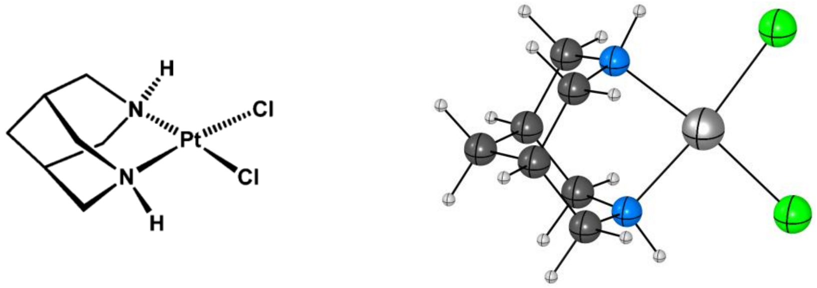

Fig. 1. The molecular (left) and optimized (right) structure ofcomplex **1**, at BP86/def2-TZVP level of theory.

References:

[1] E. R. Jamieson, S. J. Lippard,, Chem. Rev. 99 (1999) 2467–2498.
[2] T. Boulikas, A. Pantos, E. Bellis, P. Christofis, Cancer Therapy, 5 (2007) 537-583.

Docking investigation and binding interaction of gingerol with the liver enzymes, alanine aminotransferase (ALT) and aspartateaminotransferase (AST)

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Abstract:

Gingerols are the major pungent compounds present in the rhizomes of ginger (Zingiber officinale Roscoe) and are renowned for their contribution to human health and nutrition. Medicinal properties of ginger, including the alleviation of nausea, arthritis and pain, have been associated with the gingerols. Gingerol analogues are thermally labile and easily undergo dehydration reactions to form the corresponding shogaols, which impart the characteristic pungent taste to dried ginger. Both gingerols and shogaols exhibit a host of biological activities, ranging from anticancer, anti-oxidant, antimicrobial, anti-inflammatory and anti-allergic to various central nervous system activities. Inclusion of ginger or ginger extracts in nutraceutical formulations could provide valuable protection against diabetes, cardiac and hepatic disorders [1].Alanin aminotransferase (ALT) andaspartate aminotransferase (AST) are the most important enzymes in group of trans-amines.ALT is a specific factor in liver for defining the liver damage. It is only increased in the liver of patients, but AST acts not only as a factor in liver damage but also is increased in heart damages [2].

The purpose of this study was to investigate the effect of ginger on hepatic enzymes including aspartate aminotransferase (AST) and alanine aminotransferase (ALT).The crystal structure of ALT (PDB entry 3IHJ) and AST (PDB entry 1IVR) were obtained from the Protein Data Bank (http://www.rcsb.org./pdb). Molecular docking technique was performed to investigate the probable interactions. B3lyp/6-31g method was used to determine docking data such as binding energy (K_b) and inhibition constant (K_i) values. Molecular docking studies confirms the interaction between gingerol and the enzymes.

References:

[1] semwal, R.B, semwal, D.K, combrinck, S., viljoen, A.M.,Phytochemistry. 117 (2015) 554-568,

[2] Desheesh, M. A., El-Shazly, A. M., El-Deeb, S. T., El-Banna, R. H., Alexandria science exchange journal, 38 (2017) 521-529

Study the antitumor activity of thymoquinone on Plk1 receptor using molecular docking

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Abstract:

Recently, there is growing interest in the natural bioactive components having anticancer activity.Thymoquinone (TQ) is an anticancer phytochemical commonly found in black cumin (nigella sativa). Thymoquinone exhibits anticancer activity via numerous mechanisms of action, specifically by showing selective antioxidant and oxidant activity, interfering with DNA structure, affecting carcinogenic signaling molecules/pathways and immunomodulation [1]. It targets cellular copper, which is presentin the chromatin and is closely associated with DNAbase guanine, and causes oxidative breakage to DNAand consequent cancer cell death [2].A number of carcinogenic signaling pathways or signaling molecules have been reported as thymoquinone'starget.Serine/threonine kinase (Plk1) has been established as one of the most promising targets for molecular anticancer intervention.

In this study, we discuss the potential of thymoquinone as anticancer molecule and its mechanism of action by using molecular docking studies.The crystal structure of serine/threonine kinase Plk1(PDB entry 3FC2) was obtained from the Protein Data Bank (http://www.rcsb.org./pdb). Molecular docking technique was performed to investigate the probable interactions. B3lyp/6-31g method was used to determine docking data such as binding energy (K_b) and inhibition constant (K_i) values. The results show moderate antitumor activity of the thymoquinone.

References:

[1] Asaduzzaman Khan, M., Tania, M., Fu, S., Fu, J., Oncotarget, 8 (2017) 51907-51919

[2] Zubair H, Khan HY, Sohail A, Azim S, Ullah MF, Ahmad A,Sarkar FH, Hadi SM.. Cell Death Dis, 4 (2013) 660.

Sonosynthesis and Characterization of ZrO_2/ TiO_2/ZnO Ternary Nanocomposite for Photodegradation of Congo red

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Abstract:

In this research, the ternary nano-composite ZrO_2/TiO_2/ZnO has been prepared by sol-gel technique under ultrasonic irradiation. For preparation of the nano-composite, Firstly, the sols of ZnO, TiO_2 and ZrO_2 were directly mixed together. After that, the agents were added to form the gel of nanocomposite. The reaction mixture was stirred continuously for 24 hours.And then it placed under ultrasonic irradiation for 30 min. Finally,the filtrated composite gel was washed and calcinated at 500 °C in furnace for 3h. X-ray powder diffraction patterns exhibited well-formed crystal structure, crystalline phases and purity of the produced nanoparticles (NPs).The FT-IR analyses indicated that the positions of peaks related to Zn-O, Ti-O and Zr-O absorption bands does not change in nano-composites. In addition, FESEM images indicated the spherical uniform morphology of the NPs. The mean particles size is 30 nm. The photo-degradation performance of Congo red (as a water pollutant) was obtained. Particle size and band gap of nano-catalyst were considered as important factors on its performance [1-3].

References:

[1] S. M. Saleh, SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy, 211(2019) 141-147.
[2] B. Szczepanik,: A review, Applied Clay Science 141 (2017) 227–239.
[3] J. Wang ,Y. Lv, L. Zhang, B. Liu, R. Jiang, G. Han, R. Xu, X. Zhang, Ultrason. Sonochem.17 (2010) 642–648.

The Influence of synthesized ceramic Incorporation in TiO_2 for Photocatalytic degradation of Organic Dyes

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Abstract:

Pollutants of drinking water, such as dye, are currently being studied due to increased concerns about the dangers ofhumans and the environment [1, 2]. In this study, photocatalytic technology is used for the destruction of contaminationwith new TiO_2/ceramic nanocomposites(TiO_2/C).Because of high surface area, layered or fibrous structure and great adsorption capacities used ceramic as supports in heterogeneous catalysis. Both anatase TiO_2 and ceramic (SiO_2-ZrO_2-Fe_2O_3-Al_2O_3) were successfully prepared usingsimplesolgel method. The new TiO_2/C was deposited on synthesized ceramic by applying co-precipitation techniques.The characterization of theTiO_2/Cwas determined by UV-Vis, XRD, SEM, TEM and FTIR spectroscopy methods. Thephotocatalytic activity of produced materials evaluated by degradation of methylene blue (MB) and methyle orange (MO) dyes under UV light. The results show that the TiO_2/Chave superior photocatalytic activity compared to the pure TiO_2. The project demonstrates that this nanocompositecan be as idealand practical systems for removinghazardous organic materialsin environmentalapplications.

References:

[1]H. Sun, H. Wu, Y.Jin, Y.Lv, G. Ju, L. Chen, Z. Feng, Y. Hu, ,Mater Res Lett, 240 (2019) 100–102

[2]J. Ye, X. Li, J. Hong, J. Chen, Q. Fan, Mater SciSemicond Process, 39 (2015) 17–22.

Mononuclear Ni(II) and Cu(II) Complexes with Schiff base Ligands: Synthesis, Spectroscopic and antibacterial Studies

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Abstract:

Some novel Schiff base ligands of type H_2L was prepared by the condensation of methyl-2-(1-methyl-2'-aminoethane)amino-1-cyclopentenedithiocarboxylate (HcdMeen) [1,2] and 2-hydroxyacetophenon and their derivatives. The metal (II) complexes of Ni^{2+} and Cu^{2+} synthesized and characterized on the basis of physicochemical techniques, namely, elemental analysis, melting point, magnetic moment, molar conductance and spectroscopic (UV-Vis, IR, ^1H, ^{13}C NMR) data. The spectroscopic studies suggested the distorted square planar structures for complexes. To investigate the applications of synthesized compounds, in the next step the compounds were tested for in vitro antibacterial activity against clinically important bacteria.

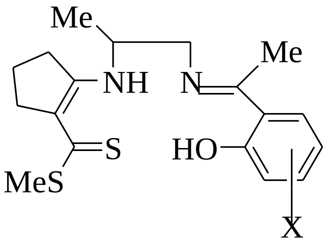

Fig. 1. H_2L

References:

[1] Sh. Esmaielzadeh, E. Zarenezhad, ActaChim. Slov. 65(2018) 416–428.
[2] Sh. Esmaielzadeh, Gh. Mashhadiagha, Bull. Chem. Soc. Ethiop. 31 (2017)159-170.

Evaluation of electronic and structural properties of scandium decorated graphenylene: A DFT-D3 study

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Abstract:

Graphenylene (GPY) is a 2D sp^2-carbon membrane with uniform pores. It has a unique structure which is composed ofperiodic pores with a diameter of 3.2 Å (A ring), cyclohexatriene-like units (B ring) and cyclobutadiene-like units (C ring). GPY is essentially a form of [N] phenylene [1].In this work, DFT-D3 calculations werecarried out using DMol^3 module in Materials Studio software for condensed matter systems to model the surfaces of the electronic structures and the binding properties of the carbon allotropes [2].We used the generalized gradient approximation (GGA) method with the non-empirical local functional, and the Perdew-Burke-Ernzerhof correlation (PBE) and double numerical basis plus polarization (DNP) basis set. In all calculations, a 2×2 supercell of GPY was applied andafter optimization the lattice parameters of GPY obtained a = b = 6.764 Å.

In GPY structure, there are single type of carbon atom, three types of C–C bonds and three different polygons (A, B and C). We examined all of them to find desirable site for Sc adsorption. Results show that after optimization, Sc atom lies only in four sites contain center of ring A, B, C and top of the bond between A and B rings. Corresponding adsorption energies for these sites are –2.478, –3.949, –3.737 and –3.867 eV, respectively. Also, distances of Sc atom and GPY sheet in optimized structures are 0.0, 1.77, 1.97 and 2.0 Å, respectively. Therefore, B ring is the best position for Sc adsorption. Also, band structure diagrams show that pristineGPY is a semiconductor with a direct band gap of 0.862 eV. For Sc decorated GPY, we found that when Sc lies in rings A, B and C, obtained values for band gap are 0.0, 0.491and0.515 eV, respectively.It is seen that Sc decoration causes to decrease the band gap value. Also, PDOS diagrams show strong overlaps between carbon and metal atoms.

References:

[1] Q. Song, B. Wang, K. Deng, X. Feng, M. Wagner, J.D. Gale, K. Müllen, L. Zhi, J. Mater. Chem. C 1 (2013) 38-41.
[2] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, J Chem Phys 132 (2010) 154104.

DFT-D study of hydrogen storageonto Fe decorated monolayergraphenylene

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Abstract: Hydrogen has to be produced, since on the earth it only occurs in the form of water and hydrocarbons.For practical application of hydrogen as energy source, it must be stored, carried and released when it must be consumed. To date,there is no investigated material that exhibits all necessary properties. Moreover, for all methods of hydrogen storage by the structures, there are some key issues. In this work, porousgraphenylene (GPY) functionalized with Fe transition metal was considered for its potential as a high capacity hydrogen storage material.GPY or biphenylene carbon is a 2D sp^2- carbon membrane contains three kinds of polygon [1]. GPY has a unique structure which is composed of dodecagonal, hexagonal and tetragonal rings that we nominated them as A, B and C, respectively.

DFT calculations were done using DMol^{3}package.We used generalized-gradient approximation (GGA) as well as the Perdew–Burke–Ernzerhof (PBE) exchange and correlation functionals with the double numerical polarized(DNP) basis set. A 6×6×1 Monkhorst–Pack k-point mesh with a 13.54 Å × 13.54 Å × 20.00 Å periodic boundary condition for the GPYsheet was applied. To accountVan der Waals forces and dispersion effects, the empirically-correcteddensity functional theory (DFT-D) method in Grimme scheme wasemployed in all computations [2].

In this work, the first attempt was made to consider the best positions for iron atom and then the hydrogen molecule adsorption. Iron metal atomwas placed in five different positions with a different distance from the graphenylene plate, then,the bonding energy was calculated.It was seen that hexagonal ring is the best position with total adsorption energy of –2.66 eV in which distance of Fe from graphenylene sheet is about 1.5 Å.Also, the results show that band gap energy of GPYis 0.894 eV which does not significantly changeafter adsorption of the hydrogen molecule in the hexagonal ring. But, in the presence of Fe and H_2, band gap decreases to 0.666 eV. The results confirm that Fe decoration can extremely improve hydrogenstorage capacity of the GPY and up to 16 H_2 molecules could be adsorbed on Fe decorated GPY that is very higher than that of alkali and alkaline earth metalsdecorated GPY [3].

References

[1] Q. Song, B. Wang, K. Deng, X. Feng, M. Wagner, J.D. Gale, K. Müllen, L. Zhi, J. Mater. Chem. C 1 (2013) 38-41.
[2] S. Grimme, J. Antony, S. Ehrlich, H. Krieg, J. Chem. Phys. 132 (2010) 154104.
[3] T. Hussain, M. Hankel, D.J. Searles, J. Phys. Chem. *C* 121 (2017) 14393-14400.

Intra- and Intermolecular Interactions in Some New Re (I)-tricarbonyl Complexes : Structural and Computational Studies

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Abstract:

Intra- and intermolecular noncovalent interactions are key in many chemical and biological processes[1]. The relatively new discovered noncovalent intra- and intermolecular interactions have attracted growing research interest over the last decade. They are weak in strength but very important in internal geometry and packing arrangement. Although these interactions are widely present in biomolecules and materials, their existence are considered to be counterintuitive [2].

In this study, we report synthesis and structural chemistry of some new complexes of rhenium(I) tricarbonyl, with different NN-diimine ligands in facial geometry. These new complexes were characterized by different spectroscopic methods such as FT-IR, UV-Vis, and ^{1}H-NMRand their solid state structures were determined by single crystal X-ray diffraction. Herein, we are going to investigate the presence of such controversial interaction in synthesized complexes. Further computational calculations for pursuing such interactions with their energy will be done by natural bond orbital (NBO) program.

References:

[1] Emmanuel A. Meyer, Ronald K. Castellano, Francois Diederich. Angew. Chem. Int. Ed. 42 (2003) 1210 – 1250
[2] Egli, MartinSarkhel, Sanjay. Angew. Chem. 128 (2016) 7932 –7936.

Study on cooperativity ofmetal-OH_2 and $H_2O...H_2O$ bonds in $H_2O…H_2O−M$ (M= Li^+, Na^+, K^+, Rb^+, Ca^{2+}, Sr^{2+}, Ba^{2+} and La^{3+}) systems

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Abstract:

The role and importance of non-covalent interactions especially hydrogen bond,have generally been detected in recent decades.Theseinteractions play an important role in chemistry and physics, and furthermore, they have a key importance in the arrangement of biological structures such as DNA [1].In this work,we try to investigate the cooperativity between a $M^{n+}−OH_2$ bond and a $H_2O...H_2O$ hydrogen bond. In fact, the nature and strength of each metal-OH_2 bondand $H_2O...H_2O$ hydrogen bondin a triad system is compared with primary dyad systems.Herein we investigate the $H_2O…H_2O−M$(M= Li^+, Na^+, K^+, Rb^+, Ca^{2+}, Sr^{2+}, Ba^{2+} and La^{3+})compounds, theoretically. The geometries of all compounds in the gas-phase were fully optimized with def2-TZVPD basis set at MP2 and M06 levels of theory using the Gaussian 09 set of programs. The different types of interaction and stabilization energies [2]were calculated and corrected for the basis set superposition error (BSSE) [3].In order to study the cooperativity in these systems, a newly presented method was used[2].The data showed that the total cooperativity of triad correlateswell with the sum of the changes in values of M^{n+}-$OH_2$and$H_2O...H_2O$ interactions,upon the formation of $H_2O...H_2O−M^{n+}$ triad.

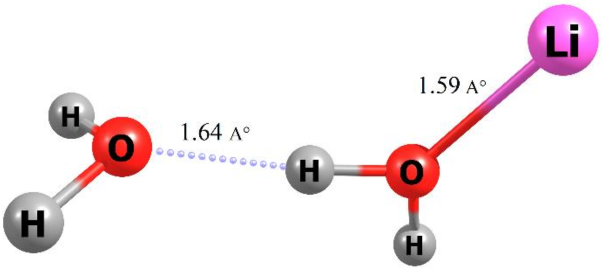

Fig.1. The optimized structure of $H_2O…H_2O−Li$ at MP2/def2-TZVPD level of theory.

References:

[1]Cook, S.A. and A. Borovik,. Accounts of chemical research, 48 (2015) 2407.
[2]Salehzadeh, S. and F. Maleki, Journal of computational chemistry, 37 (2016), 2799.
[3]Maleki, F. and S. Salehzadeh,. The Journal of chemical physics, 149 (2018)064116.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Study on cooperativity of bonds in $NH_3...H_2O{-}M$ ($M= Li^+, Na^+, K^+, Rb^+, Cs^+$ and Sr^{2+}) triads having metal cation and hydrogen bond

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Abstract:

While the structure and properties of small molecules are determined by covalent bonding, in any larger system, noncovalent interactions become equally important[1].Among the non-covalent interactions, hydrogen bonds are the most common type of weak interactions[2]. The hydrogen bond is an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X–H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation[3]. In this work, we try to investigate the cooperativity between a $M^{n+}{-}OH_2$ bond and a $NH_3...H_2O$ hydrogen bond in $NH_3...H_2O{-}M$($M= Li^+, Na^+, K^+, Rb^+, Cs^+$ and Sr^{2+}) triads. The geometries of all dyads and triads in the gas-phase were fully optimized with def2-TZVPD basis set at MP2 and M06 levels of theory using the Gaussian 09 set of programs. The different types of interaction and stabilization energies[4]were calculated and corrected for the basis set superposition error (BSSE)[4].In order to study the cooperativity in these systems, a newly presented method was used[5].The data showed that the total cooperativity of triads correlateswell with the sum of the changes in values of$M^{n+}{-}OH_2$and$NH_3...H_2O$ interactions,upon the formation of $NH_3...H_2O{-}M^{n+}$ triad.

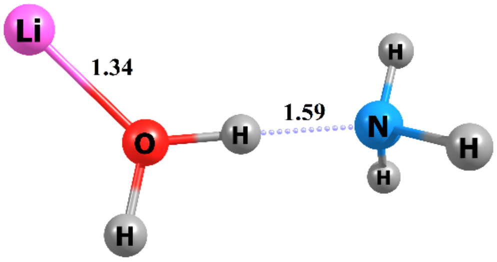

Fig. 1. The optimized structure of $NH_3...H_2O{-}Li$ at MP2/def2-TZVPD level of theory.

References:

[1]Rezac, J. and P. Hobza,. Chemical reviews, 116 (2016) 5038.
[2]Cook, S.A. and A. Borovik, Accounts of chemical research, 48 (2015) 2407.
[3]Arunan, E., et al., Pure and applied chemistry, 83 (2011) 1637.
[4]Salehzadeh, S. and F. Maleki, Journal of computational chemistry, 37 (2016) 2799.
[5]Maleki, F. and S. Salehzadeh, The Journal of chemical physics, 149 (2018) 064116.

Preparation of tetramethylguanidine-functionalized nano size γ-Al_2O_3 as a catalyst for the four-component synthesis of pyrazolopyranopyrimidine derivatives

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Abstract:

Nanocatalysis is a rapidly growing field which involves the use of nanomaterials as catalysts for a variety of chemical reactions. Oxide nanoparticles can exhibit unique physical and chemical properties due to their limited size and a high density of corner or edge surface sites [1]. One of the important methaloxaids is aluminum oxide and among various structures for alumina, γ-alumina is one of the extremely important nano sized materials. It is used as structural composites for spacecraft, and abrasive and thermal wear coatings. γ-Alumina is thermody-namically more stable than the other relatives [2].

At present study a durable nano sized γ-Al_2O_3 functionalized by 1,1,3,3-tetramethylguanidine(TMG) was successfully prepared by the hydrothermal method from aluminum nitrate nonahydrate ($Al_2(NO_3)_3.9H_2O$). The particle size of this catalyst was established by using SEM imaging studyto be in the range of 19 -40 nm. The catalyst was also characterized by various techniques including FT-IR, XRD, TGA and surface area analysis.

The activity of synthesized catalyst was tested in the four-component synthesis of pyrazolopyranopyrimidine derivatives in H_2O, which showed high catalytic activity, producing the desired products in reduced reaction times and excellent yields (90-98%).

References:

[1]. Fang Chen, Xunzhu Jiang, Leilei Zhang, Rui Lang, BotaoQiao; Chinese Journal of Catalysis 39 (2018) 893–898.
[2]. H.H. Kung,: Surface Chemistry and Catalysis; Elsevier: Amsterdam, 1989.
[3]. Seyed Ali Hosseini, AligholiNiaei, Dariush Salari; Open Journal of Physical Chemistry, 1 (2011) 23-27.

Synthesis, Characterization, and X-ray crystal structure of new Cu(II) complex with N-(thiazole-2-yl) picolinamide (L) and CuO nanoparticles as New catalysts in CuAAC reaction and antibacterial studies

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Abstract:

Several attempts proved that Cu^{2+} can catalyze several mechanisms such as cycloaddition reactions between azide and alkyne (a typical click reaction) as well as other types of click reaction. In this case, applying Cu^{2+} nanoparticles to catalyze the specific click reaction in association with carboxamide-based ligands would be a strategic approach to design and implement a highly-efficient catalyst[1].CuO is one of the most important transition metal oxides due to its captivating properties. It is used in various technological applications such as high critical temperature superconductors, gas sensors, in photoconductive applications, and so on. Recently, it has been used as an antimicrobial agent against various bacterial species. Here we synthesized different sized CuO nanoparticles and explored the size-dependent antibacterial activity of each CuO nanoparticles preparation [2].

In this work, five-coordinated copper(II) complex, $[Cu(L)_2(H_2O)].CHCl_3$, was synthesis by N-(thiazole-2-yl) picolinamide (L) with copper(II) acetate. Respectively, Copper oxide (CuO) nanoparticles have been prepared by thermal decomposition using $[Cu(L)_2(H_2O)].CHCl_3$ complexes as a new precursor at 600 °C for 3h under air atmosphere. The complex was characterized using FT-IR spectroscopy, elemental analyses, and their solid state structures were confirmed by single crystal X-ray diffraction. These nanoparticles were identified by fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and thermogravimetry differential thermal analyses (TGA-DTA).The catalytic activity of the complex and nanoparticles were evaluated in one-pot azide–alkyne cycloaddition (AAC) click reaction in water without need of any additional agent.

References:

1.Jennah, O., et al., *P.* Advanced Synthesis & Catalysis, 360 (2018) 4615-4624.
2.Chauhan, M., et al.,. Environmental research, 168 (2019). 85-95.

Preparation and characterization of Mo supported amine functionalized poly-di-phenoxy-phosphazene for epoxidation of alkenes

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Abstract:

Polyphosphazene is an inorganic polymer with wide range of applications. Its backbone comprised from phosphorous and nitrogen atoms with two side groups on phosphorus which controls its physical and chemical properties [1]. In this research polydichloro-phosphazene was prepared from reaction of ammonium sulfate and phosphorous pentachloride in dioxan at 160°C. The produced viscos liquid was then reacted with sodiumphenoxide in dioxane and refluxed for 24 hours to produce polydiphenoxyphosphazene. Then it was treated with concentrated nitric acid to induce nitro group on some phenyl rings. These nitro groups were then reduced to amine with sodium dithionite solution [2]. The produced amine functionalized polyphosphazen was then used to support bis-acetylacetonato-di-oxo molybdenumm complex and used in epoxidation of alkenes. CHN, ICP, XRD, SEM, EDX, FTIR and NMR spectroscopies were used to analyze the product of different steps. The reaction condition was optimized for cis-cyclooctene and then other alkenes were used at these optimum conditions. The optimum conditions were found as 20 mg catalyst in CCl_4 for 0.5 mmolecyclooctene and 1 mmol TBHP as oxidant at reflux temperature. The yield at this reaction conditions was 98% after 3 hours. Recycling experiment was also investigated.

References:

[1] J. E. Mark and H. R. Allcock, Inorganic Polymers , Second Edition.
[2] H. R. Allcock, and S. Kwon,G. phosphate Dehydrogenase, (1986) 1502–1508.

Mn complex immobilized on $CuFe_2O_4$magnetice nanoparticles as an efficient heterogeneous catalyst for the synthesis of 5-substituted 1H-tetrazoles

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Abstract:

Tetrazoles are an important class of heterocycles with wide range of application in coordination chemistry as ligands, in medicinal chemistry as stable surrogates for carboxylic acids, in catalysis technology, in organometallic chemistry as effective stabilizers of metallopeptide structures, in material chemistry as explosives, rocket propellants, etc., and in agriculture. Tetrazoles can be used as isosteric replacements for carboxylic acids in drug design and have found application in various material sciences, including photograph and information recording systems. Also, tetrazoles and their derivatives have been reported as analgesics, antifungal, ant-inflammatory, antibacterial, antiviral and anti-proliferative agents, potential anti-HIV drug candidates and anticancer agents. Valsartan and losartan are two typical examples of the extensive application of these compound in drugs, such as antihypertensive sartan family drugs [1,2].

In this work, tetrazole derivatives were synthesis from reaction between nitrile derivatives with sodium azide in the presence of Mn complex immobilized of $CuFe_2O_4$ magnetic nanoparticles (Fig.1). Then; to determine the best reaction conditions, the effect of various parameters such as solvent, temperature, amount of NaN_3 and amount of catalyst were examined in the cycloaddition reaction of benzonitriles with NaN_3.

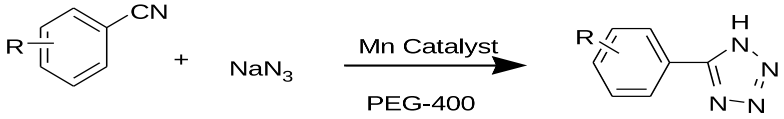

Fig. 1: Synthesis of 5-phenyl-1H-tetrazole derivatives

References:

[1] I.B. Seiple, Z. Zhang, P. Jakubec, A. Langlois-Mercier, P.M. Wright, D.T. Hog, K. Yabu, S. Rao Allu, T. Fukuzaki, P.N. Carlsen, Y. Kitamura, X. Zhou, M.L. Condakes, F.T. Szczypinski, W.D. Green, A.G. Myers, Nature, 533 (2016) 338-345.

[2] F.Abrishami, M. Ebrahimikia, F. Rafiee, Applied OrganometallicChememistry, 29 (2015) 730-735.

Synthesis and identification Ni(II), Cu(II), Mn(II), Zn(II) complexes of anew schiff base ligand

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Abstract:

Schiff bases are generally produced bycondensation reactions of carbonyl moieties (ketone or aldehyde)with primary amines [1].Schiff baseligands are able to coordinate to transition metal ions through imine nitrogenand other atoms such as: oxygen ,sulfur and nitrogen.These compounds, play an importantrole inmedical, industry and biology.They exhibit many biological properties, such as antibacterial, antifungal, and antioxidant activities [2].These compounds are usually prepared by two chemical methods: McCarthy(direct) and template (Morgan and Smith's) procedure. In this projectan asymmetric Schiff base ligand was synthesized.Atthefirst step,1,2 diaminocyclohexane was reacted with 2-acetylpyridine.At the next step,2-hydroxy-1-naphthaldehydewas added to the content of the reaction.TheSchiff base ligand was used to prepare it is Ni(II), Cu(II), Mn(II), Zn(II) complexes.IR, UV-Vis, ^{1}HNMR and^{13} CNMR spectroscopic techniques were utilized to characterize the ligand and the related complexes .More over analytical methods such as :ICP,TGA/DTA, and magnetic susceptibility measurements were used to characterize the schiff base ligand and it's complexes.

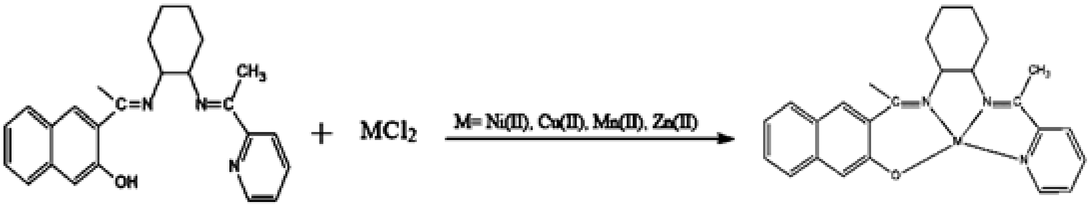

Fig 1. Synthesis of MCl2, [M = Ni(II), Cu(II), Mn(II),Zn(II)] of Schiff base ligand

Reerences
[1] Zoubi, W.A., Kandil, F., Chebani, Kh. " Phys. Sci. Res. Int., 2 (2014) 12-2
[2] Abu-Dief, A. M., Mohamed, I. MBeni-suefuni. J. Basic.. Appl. Sci., 4 . (2015) 119-133

Structural, band-gap and photocatalyticproperties ofAg-Ce codoped ZnO/ reduced graphene oxide nanocomposite

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Abstract:

In this study, Ag-Ce codoped ZnO/ reduced graphene oxide nanocomposite (Ag-Ce-ZnO/ rGO)were synthesized by simple hydrothermal method [1].The structural, morphological, and optical properties of the photocatalysts were done by XRD, FESEM, TEM, UV-Vis, BET and PL.The characterization results suggest thatthe nanocompositeformed arein well-crystalline wurtzite phase, possess reasonably,fine crystallite size and direct band-gap energy transition states.Photocatalytic degradation of aqueous solution of Rhodamine B dye under Vis light illumination was studied by using prepared nanocomposite.The effect of operating parameters such as amount of catalyst, the initial dye concentration, and initial pH on the rate of dye degradation using prepared samples was investigated.The superior photocatalytic activity of these Ag-Ce-ZnO/ rGO could be attributed to the reduce rate of recombination of the photogenerated electrons and holes as well as its lower band gap energy at photocatalyst interfaces. In addition to the enhanced light absorption from UV to visible region, the high specific surface area of prepared nanocomposites also imparts strong adsorption capacity for pollutants over catalyst surface, resulting in high photoactivity [2].

References:

[1] M. Ahmad, E. Ahmed, Z.L. Hong, N.R. Khalid, W. Ahmed, A. Elhissi, , J. Alloys Compd. ,577 (2013) 717–727
[2] Ch. Dong, R.Eldawud, A. Wagner, C.Z.Dinu, ,Appl. Catal. A, 524 (2016) 77–84

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Tin and Copper Dispersed on Metal-organic Framework as a New Fantastic Catalyst for Aerobic Baeyer-Villiger Oxidation of Cyclohexanone

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Abstract:

Baeyer-Villiger (B-V) oxidation reaction is one of the most important reactions in the field of organic chemistry, in which ketones become lactones or esters, which are valuable intermediates in a wide range of chemical industries such as dyestuff, perfume, pharmaceutical, detergent, agriculture, and polymer [1-3].Caprolactone is one of the products produced by this reaction and plays a major role in the pharmaceutical and medical fields as a monomer for the preparation of biodegradable polymers of poly-caprolactone [4,5].Hence, the development of efficient and selective catalysts for oxidative Baeyer-Villiger reaction, economically feasible and with the least amount of environmental damage, is one of the most important challenges in the present era.

In this study, metal-organic frameworks (MOFs) containing two tin and copper metal salts have been used for the first time as efficient catalysts for the Baeyer-Villiger (B-V) oxidation reaction of cyclohexanone.The results showed a synergistic effect on the selectivity and catalyst efficiency, resulting in the simultaneous presence of two copper and tin metal in the MOF.In addition, these catalysts can berecovered during consecutive cycles without notable loss in their catalytic activity.

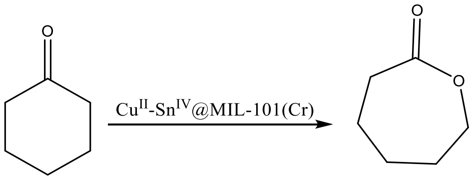

Fig 1. The Baeyer-Villiger (B-V) oxidation reaction of cyclohexanone

References:

[1] A. Berkessel, M.R. Andreae, H. Schmickler, J. Lex, Angew. Chem. Int. Ed. 41 (2002) 4481-4484.
[2] R.A. Michelin, P. Sgarbossa, A. Scarso, G. Strukul, Coord. Chem. Rev. 254 (2010) 646-660.
[3] C. Jiménez-Sanchidrián, J.R. Ruiz, Tetrahedron. 9 (2008) 2011-2026.
[4] G.R. Krow, Org.Reactions. 43 (2004) 251-798.
[5] G.-J. Ten Brink, I. Arends, R. Sheldon, Chem.Rev. 104 (2004) 4105-4124.

Introducing bromoporphyrinato Zinc(II)as a best photosensitizer through the biologicalinvestigation for applying in photodynamic therapy

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Abstract:

Porphine structure include four pyrrole units that connected by four methine bridges(–CH=) [1]. Metalloporphyrins can becoordinated to axial ligands which attached to metal. In this article a table has classified in five categories of metalloporphyrins with high photosensitizer effect. In the class (I) there are tetraphenylporphyrins (*TPP*) metal complexes with and withoutaxial ligands. Classes (II) and (III) are include metalloporphyrins with electron withdrawing and donating groups in para, ortho, and meta situations of phenyl and βsituations of macrocycle in TPP, respectively.classes (IV) and (V) are metalloporphyrins with aromatic functional groups in para situation of phenyl in TPP and meso situations of macrocycle, respectively. In this research, westudiedphotosensitizer effectand toxicity effectof metalloporphyrinsby PASS software. Investigation of photosensitizer effectof metalloporphyrins is important inbiology and medical. As an illustration, in photodynamic therapy (PDT) has been used compounds with high photosensitizer activity. Therefor it'svery essential for cancer treatment that has been evaluated percentage of mentioned activity [2]. The purpose of this article is identification a porphyrin complex with the most photosensitizer activity and the least toxicity. By investigationof the prepared table include 53 porphyrin complexes, was concluded that among 31 compounds with activity probability (P_a) above 90%,compounds number 30 and 31 {2-Bromoporphyrinato Zinc(II):[Zn-1BrP]and Zinc(II)-2,3-di(bromo)-12-formyl-5,10,15,20-tetraphenylporphyrin:[ZnTPP(CHO)Br_2]}has 93.7% and 91.6%respectively without any toxicity.In comparison of compounds 30 and 31,[Zn-1BrP]introduceas the best photosensitizer for utilizing in PDT.

class	No.	Abbrev. Name	% Biological Activities*				% Toxicities*					
			A		T_1		T_2		T_3		T_4	
			P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i
I	1	(Cl)2SnTPP	99.2	0.0	25.4	3.1	--	--	--	--	--	--
	2	PtTPP	98.6	0.0	35.1	1.5	22.2	11.7	--	--	--	--
	3	PdTPP	98.6	0.0	35.1	1.5	22.2	11.7	--	--	--	--
	4	ZnTPP	97.6	0.0	30.1	2.2	18.8	16.7	--	--	--	--
	5	SnTPP	89.4	0.0	53.8	0.7	38.5	3.3	19.0	6.3	27.1	8.5
	6	AlTPP	64.6	0.1	53.8	0.7	38.5	3.3	19.0	6.3	27.1	8.5
	7	PhO-TPP	62.0	0.1	40.3	0.9	35.3	4.2	14.5	9.3	21.6	13.7
	8	Et(AlTPP)	59.9	0.1	46.4	0.7	37.8	3.5	18.6	6.5	28.0	8.0
	9	Ph-COO-AlTPP	56.2	0.1	34.7	1.5	39.8	3.0	--	--	--	--
II	10	ZnTBrPP	96.4	0.0	20.8	5.8	--	--	--	--	--	--
	11	ZnTTP	96.3	0.0	27.2	2.7	--	--	--	--	--	--
	12	T(2,6-ClP)P	96.1	0.0	23.2	3.2	--	--	--	--	--	--
	13	PdAPTTP	95.6	0.0	25.6	3.2	24.9	9.3	--	--	--	--
	14	PtATTP	95.6	0.0	25.6	3.0	24.9	9.3	29.9	3.2	37.4	3.5
	15	Cis-ZnDAPP	95.4	0.0	25.3	3.1	26.0	8.4	24.8	4.4	29.9	0.7
	16	ZnMAPP	95.4	0.0	25.3	3.1	26.0	8.4	24.8	4.4	29.9	0.7
	17	ZnT(2-NO2)PP	94.7	0.0	--	--	--	--	46.3	1.4	47.6	2.2
	18	ZnT(2-N2P)P	94.0	0.0	17.3	11.3	--	--	21.2	5.4	32.0	6.1
	19	ZnCPTPP	93.5	0.0	19.3	7.5	35.3	4.2	--	--	--	--
	20	ZnCPTTP	91.6	0.0	19.7	7.0	31.2	5.7	--	--	--	--
	21	SnTClPP	91.2	0.0	22.9	4.1	--	--	--	--	--	--
	22	Zn(N3P)T(3,5-tBuP)P	89.1	0.0	--	--	--	--	16.7	7.5	21.4	14.0
	23	Zn(BrP)(IP)DMP	88.6	0.0	--	--	--	--				
	24	Zn(p-DNBP)TriPP	86.0	0.0	18.4	0.9	31.3	5.7	29.1	3.3	30.3	6.8
	25	(OH)2SnTTP	72.4	0.1	37.7	1.2	27.8	7.3	18.0	6.0	41.6	3.2
	26	AlTTP	56.0	0.1								
	27	AlTClPP	54.2	0.2	46.6	0.7	42.0	2.6	19.4	6.1	33.8	5.4
	28	Zn(NO2)5TPP	94.3	0.0	--	--	--	--	44.6	1.5	45.8	2.5
	29	Zn(NO2)6TPP	93.6	0.0	--	--	--	--	45.3	1.5	46.3	2.4
	30	Zn-1BrP	93.7	0.0	--	--	--	--	--	--	--	--
	31	ZnTPP(CHO)Br2	91.6	0.0	--	--	--	--	--	--	--	--
	32	ZnDTPTPP	90.2	0.0	18.8	8.4	--	--	--	--	--	--
	33	Zn(2-MeTAC)TPP	79.3	0.1	17.0	12.2	24.1	9.9	--	--	--	--
	34	AcMeZnTPP	76.9	0.1	21.5	5.1	23.5	10.4	--	--	--	--
	35	Zn(4- MeTAC)TPP	75.0	0.1	--	--	--	--	--	--	--	--
	36	Zn(2-Me,4-MeOTAC)TPP	73.0	0.1	--	--	25.5	8.8	--	--	--	--
	37	(2-Me,4-MeOTAC)ZnTPP	72.1	0.1	--	--	--	--	--	--	--	--
	38	(4,2-Me-4-MeTAC)ZnTPP	69.6	0.1	--	--	18.4	17.4	--	--	--	--
	39	(6-Cl,4,2-MeTAC)ZnTPP	66.2	0.1	--	--	--	--	--	--	--	--
	40	(4-ClEt,2-MeTAC)ZnTPP	66.1	0.1	--	--	--	--	18.7	6.2	21.3	14.1
	41	PtTPA	97.7	0.0	23.3	3.9	--	--	--	--	--	--
	42	PdTPA	97.7	0.0	23.3	3.9	--	--	--	--	--	--
	43	ZnDMSPP	92.9	0.0	19.1	7.9	--	--	--	--	--	--
	44	ZnTB9FP	91.4	0.0	22.7	4.2	44.7	2.2	--	--	--	--
	45	(TriAzPyP)TriPP	77.6	0.1	16.6	13.3	--	--	--	--	--	--
	46	ZnBCPF5	73.5	0.1	16.6	13.4	--	--	--	--	--	--
	47	PtTFP	97.3	0.0	29.3	2.3	--	--	19.1	6.2	29.6	7.2
	48	PdTFP	97.3	0.0	29.3	2.3	--	--	19.1	6.2	29.6	7.2
	49	PtOOFP	95.4	0.0	24.4	3.4	--	--	15.9	8.0	25.6	9.6
	50	TFPZn	95.2	0.0	35.9	1.4	--	--	17.0	7.3	22.8	12.4
	51	KP-Zn-CBZ	81.8	0.1	16.1	14.9	24.1	9.9	--	--	--	--
	52	ZnDBuCPF5PP	81.7	0.1	17.8	10.2	--	--	--	--	--	--
	53	ZnBuCEPDMP	78.5	0.1	17.1	11.8	--	--	--	--	--	--

*A= Photosensitizer, T_1= Cytotoxic, T_2= Ulcerogenic, T_3= Mutagenics, T_4= Carcinogeni

References:

[1] R.Zare-Dorabei, R.Rahimi, A.Koohi, S.Zargari.; RSC Advences. 2015.

[2] J. Kou, D. Dou, L. Yang,Porphyrin photosensitizers in photodynamic therapy and its applications, 2018.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Prediction of bio-inorganic activities of metalloporphyrins and phthalocyanines for selecting of the best photocatalysts in 4-chlorophenol degradation: [Zinc(II)5,10,15,20-Tetrakis(2,6-dichloro-3-chlorosulfophenyl) porphyrin]

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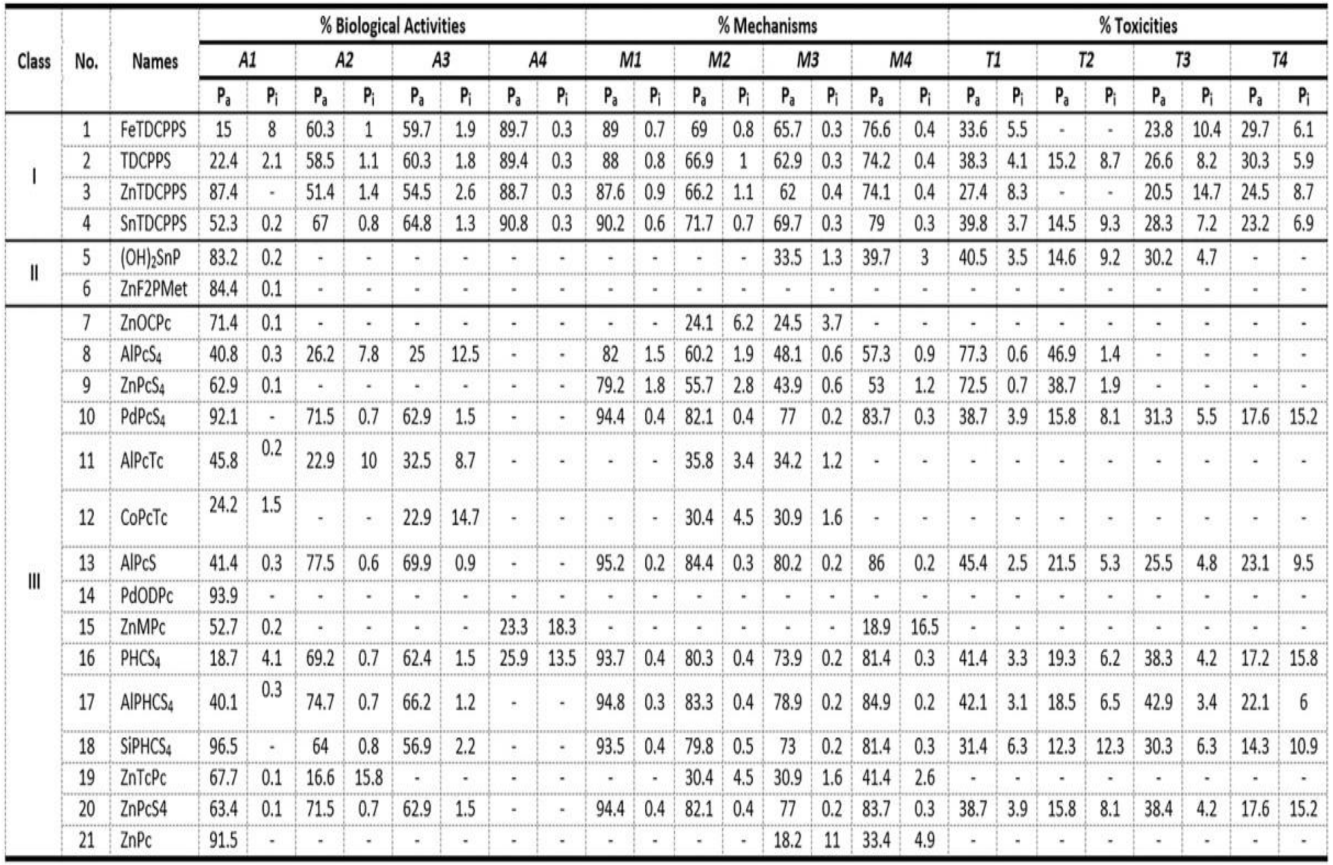
Abstract:

One of the wastewater pollutants is 4-chlorophenol that is extensively used in wood preservation, pesticide and etc. It causesEye and skin irritation [1]. Porphyrins have been utilized as photocatalysts to photodegrade pollutants due toa wide spectrum of light (UV-Vis) absorption,so charge has been transferred easily and this makes good photo physicochemical properties in porphyrin structures [2].In this study porphyrins and phthalocyanines which photodegraded 4-chlorophenol in the same condition are classified into three major groups; tetra sulfonatophenyl porphyrins (I), tetraphenyl porphyrins (II) and phthalocyanines (III). Biological activities, mechanisms, and toxicities of mentioned classes are estimatedthrough PASS software to find out the best compoundin photodegradation of 4-chlorophenol. Each biological activities or mechanism which is higher than 50%, the considered compound is active in that case and the absence oftoxicity is the advantage of photocatalysts. As mentioned points, FeTDCPPS, ZnTDCPPS,and $ZnPcS_4$are better compounds in photodegradation of 4-chlorophenol. The range of activity probability (P_a) of biological activities,mechanisms, and toxicitiesforall of the pointed compoundsare 0.514-0.897, 0.53-0.89 and 0.000-0.725respectively.As a conclusion, for selecting of the best photocatalyst can be shown; ZnTDCPPS>FeTDCPPS>$ZnPcS_4$. Finally,the result of Zinc(II) 5,10,15,20-Tetrakis(2,6-dichloro-3-chlorosulfophenyl) porphyrin:[ZnTDCPPS]with higher average biological activities (0.514-0.887), mechanisms (0.62-0.876) and lower toxicity (0.000-0.274) was satisfying photocatalysts in 4-chlorophenol degradation.



Class	No.	Names	% Biological Activities								% Mechanisms								% Toxicities							
			A1		A2		A3		A4		M1		M2		M3		M4		T1		T2		T3		T4	
			P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i
I	1	FeTDCPPS	15	8	60.3	1	59.7	1.9	89.7	0.3	89	0.7	69	0.8	65.7	0.3	76.6	0.4	33.6	5.5	-	-	23.8	10.4	29.7	6.1
	2	TDCPPS	22.4	2.1	58.5	1.1	60.3	1.8	89.4	0.3	88	0.8	66.9	1	62.9	0.3	74.2	0.4	38.3	4.1	15.2	8.7	26.6	8.2	30.3	5.9
	3	ZnTDCPPS	87.4	-	51.4	1.4	54.5	2.6	88.7	0.3	87.6	0.9	66.2	1.1	62	0.4	74.1	0.4	27.4	8.3	-	-	20.5	14.7	24.5	8.7
	4	SnTDCPPS	52.3	0.2	67	0.8	64.8	1.3	90.8	0.3	90.2	0.6	71.7	0.7	69.7	0.3	79	0.3	39.8	3.7	14.5	9.3	28.3	7.2	23.2	6.9
II	5	$(OH)_2SnP$	83.2	0.2	-	-	-	-	-	-	-	-	-	-	33.5	1.3	39.7	3	40.5	3.5	14.6	9.2	30.2	4.7	-	-
	6	ZnF2PMet	84.4	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
III	7	ZnOCPc	71.4	0.1	-	-	-	-	-	-	-	-	24.1	6.2	24.5	3.7	-	-	-	-	-	-	-	-	-	-
	8	$AlPcS_4$	40.8	0.3	26.2	7.8	25	12.5	-	-	82	1.5	60.2	1.9	48.1	0.6	57.3	0.9	77.3	0.6	46.9	1.4	-	-	-	-
	9	$ZnPcS_4$	62.9	0.1	-	-	-	-	-	-	79.2	1.8	55.7	2.8	43.9	0.6	53	1.2	72.5	0.7	38.7	1.9	-	-	-	-
	10	$PdPcS_4$	92.1	-	71.5	0.7	62.9	1.5	-	-	94.4	0.4	82.1	0.4	77	0.2	83.7	0.3	38.7	3.9	15.8	8.1	31.3	5.5	17.6	15.2
	11	AlPcTc	45.8	0.2	22.9	10	32.5	8.7	-	-	-	-	35.8	3.4	34.2	1.2	-	-	-	-	-	-	-	-	-	-
	12	CoPcTc	24.2	1.5	-	-	22.9	14.7	-	-	-	-	30.4	4.5	30.9	1.6	-	-	-	-	-	-	-	-	-	-
	13	AlPcS	41.4	0.3	77.5	0.6	69.9	0.9	-	-	95.2	0.2	84.4	0.3	80.2	0.2	86	0.2	45.4	2.5	21.5	5.3	25.5	4.8	23.1	9.5
	14	PdODPc	93.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	15	ZnMPc	52.7	0.2	-	-	-	-	23.3	18.3	-	-	-	-	-	-	18.9	16.5	-	-	-	-	-	-	-	-
	16	$PHCS_4$	18.7	4.1	69.2	0.7	62.4	1.5	25.9	13.5	93.7	0.4	80.3	0.4	73.9	0.2	81.4	0.3	41.4	3.3	19.3	6.2	38.3	4.2	17.2	15.8
	17	$AlPHCS_4$	40.1	0.3	74.7	0.7	66.2	1.2	-	-	94.8	0.3	83.3	0.4	78.9	0.2	84.9	0.2	42.1	3.1	18.5	6.5	42.9	3.4	22.1	6
	18	$SiPHCS_4$	96.5	-	64	0.8	56.9	2.2	-	-	93.5	0.4	79.8	0.5	73	0.2	81.4	0.3	31.4	6.3	12.3	12.3	30.3	6.3	14.3	10.9
	19	ZnTcPc	67.7	0.1	16.6	15.8	-	-	-	-	-	-	30.4	4.5	30.9	1.6	41.4	2.6	-	-	-	-	-	-	-	-
	20	ZnPcS4	63.4	0.1	71.5	0.7	62.9	1.5	-	-	94.4	0.4	82.1	0.4	77	0.2	83.7	0.3	38.7	3.9	15.8	8.1	38.4	4.2	17.6	15.2
	21	ZnPc	91.5	-	-	-	-	-	-	-	-	-	-	-	18.2	11	33.4	4.9	-	-	-	-	-	-	-	-

A1: Photosensitizer, A2: Antiseptic, A3: Anti-infective, A4: Cell adhesion inhibitor, M1: Squalene-hopene cyclase inhibitor, M2: Phosphatidylglycerophosphatase inhibitor, M3: Nicotine dehydrogenase inhibitor, M4: (S)-3-hydroxyacid ester dehydrogenase inhibitor, T1: Carcinogenic, T2: Mutagenic, T3: Eye irritation, T4: Skin irritation

References:

[1]. C. J. Monteiro et al., Photochemical & Photobiological Sciences, 4, (2005) 617-624.
[2]. A. D. Schwab et al., "Nano Letters, 4 (2004) 1261-1265 2004.

Investigation of photocatalysts property of zinc octacarboxy phthalocyanine $[ZnPc(COOH)_8]$ as a photosensitizer in 4-nitrophenol degradation and its anti-allergic activity

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Abstract:

4-nitrophenol is an organic compound which has been utilized in different industries such as pharmaceutical, textile and etc. human and animal's health are in danger when it's found in water [1]. Photodegradation by porphyrins and phthalocyanines has been studied as a method to degrade this pollutant from water, these are known as good photosensitizers due to π-conjugated, aromatic, rigid and flat structures as well as wide light absorption [2]. In this investigation porphyrins and phthalocyanines degraded 4-nitrophenol in the same pH, temperature and solution. The mentioned compounds are classified into two groups; Tetra phenyl porphyrins (I) and Phthalocyanines (II) which their biological properties, mechanisms, and toxicities are evaluated through PASS software. Biological activities that are higher than 50% and toxicities which are lower than 50% are considered to find out better compound for photodegradation of 4-nitrophenol. By this explanation, structures number 8, 11, 12, and 15 with high activity probability (Pa) are better photocatalysts among all of the structures which are shown in the table. These four compounds can be qualified by the quantity of effects. Each one that has more active from the point of view of biological activities, mechanisms, and inactive toxicities, is the best one. The vantage of these four compound can be shown as follows; ZnPc(COOH)8 > MgPc > ZnPcCl16 > ZnPc(NO2)4. Pa for photosensitivity, anti-allergy, benzoylformate decarboxylase inhibitory and Anthranilate-COA ligase inhibitory of zinc octacarboxy phthalocyanine is 71.4%, 55%, 82.9%, and 70.6% respectively without toxicity. Finally, ZnPc(COOH)8 was selected as a good photosensitizer and anti-allergic.

class	No.	Names	% Biological Activities								% Mechanisms								% Toxicities							
			A1		A2		A3		A4		M1		M2		M3		M4		T1		T2		T3		T4	
			P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i
I	1	$(t\text{-Bu})_4$CuPp	24.2	1.4	51.5	1.7	43.1	5.8	26.5	7.65	32.1	7.1	-	-	-	-	-	-	20.1	15.5	-	-	26.8	8.1	21.2	7.8
	2	$(t\text{-Bu})_2$CuPp	24.2	1.4	51.7	1.7	43.1	5.8	26.5	7.6	32.1	7.1	-	-	-	-	-	-	20.1	15.5	-	-	26.8	8.1	21.2	7.8
	3	(t-Bu)CuPp	24.2	1.4	51.7	1.7	43.1	5.8	26.5	7.6	32.1	7.1	-	-	-	-	-	-	20.1	15.5	-	-	26.8	8.1	21.2	7.8
	4	$(oxyacetat)_4$CuPp	27.3	0.7	34.6	5	36.6	8.9	23.4	9.6	37.3	4.8	-	-	26	11.8	23.2	14.6	22	13.2	12	11.6	28.5	7.1	18.3	9.4
	5	$(py\text{-}4\text{-}COOH)_4$CuPp	24.9	1.2	-	-	23.2	20.1	-	-	25	13.6	23.3	12.4	-	-	-	-	-	-	-	-	-	-	-	-
	6	EthylphenoxyCuPp	27.8	0.7	36	4.5	29.6	14.1	37.8	3.4	31.5	7.4	30.9	8.8	-	-	25.7	10.3	23.5	11.7	12.7	11.7	31.7	5.7	32.5	5
	7	ZnPp	97.6	-	-	-	51.9	3.1	-	-	-	-	-	-	-	-	24.6	12	-	-	-	-	-	-	-	-
II	8	$ZnPc(COOH)_8$	71.4	0.1	-	-	55	2.5	-	-	82.9	0.6	70.6	2.5	24.2	13.9	-	-	-	-	-	-	-	-	-	-
	9	$ZnPcS_4$	63.4	0.1	-	-	27.3	16.1	71.5	0.7	-	-	-	-	-	-	-	-	38.7	3.9	15.8	8.1	38.4	4.2	17.6	15.2
	10	$ZnPcF_{16}$	93.1	-	-	-	47.6	4.2	-	-	-	-	-	-	-	-	-	-	41.2	4.1	-	-	55.8	2.1	28.2	5.2
	11	$ZnPcCl_{16}$	28.6	0.7	99.3	0.2	-	-	-	-	22.2	18.3	-	-	98.5	0.1	-	-	-	-	-	-	-	-	-	-
	12	MgPc	28.6	0.7	99.3	0.2	-	-	-	-	22.2	18.3	-	-	98.5	0.1	87.9	0.1	-	-	-	-	-	-	-	-
	13	ClAlPc	62.7	0.1	-	-	-	-	-	-	24.4	14.4	-	-	23	15.5	22.5	16.2	-	-	-	-	-	-	-	-
	14	ZnPc	91.5	-	-	-	63.4	1.4	-	-	22.2	18.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-
	15	$ZnPc(NO2)_4$	71.3	0.1			34.5	10	-	-	-	-	56.9	4.2	24.8	13.2	-	-	38.2	4.1	41.8	7.1	20.1	15.4	-	-
	16	$ZnPc(NH2)_4$	73.3	0.1	-	-	32.1	12.1	-	-	-	-	-	-	-	-	-	-	31.4	6.3	28	3.6	19.5	15.6	-	-

A1: Photosensitizer, A2: Antioxidant, A3: Antiallergic, A4: Antiseptic, M1: Benzoylformate decarboxylase inhibitor, M2: Anthranilate-COA ligase inhibitor, M3: lipid peroxidase inhibitor, M4: magnesium protoporphyrin IX methyltransferase inhibitor, T1: Carcinogenic, T2: Mutagenic, T3: Eye irritation, T4: Skin irritation

References:

[1] G. Eichenbaum *et al.*, Regulatory Toxicology and Pharmacology, 55(1) (2009) 33-42.

[2] C. M. Drain, A. Varotto, and I. Radivojevic, Chemical Reviews,109(5) (2009) 1630-1658.

Modified UiO-66-NH_2 metal–organic frameworks (MOFs) with Melamine for Knoevenagel condensation

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Abstract:

In recent years, metal-organic frameworks (MOFs) have attracted considerable attention due to their special characteristics such as hybrid compositions, diverse networks, tunable porosity and tailorable surfaces [1, 2]. The application of MOFs as porous heterogeneous catalysts alternative or complementary to microporous zeolites is especially interesting, since the pore size and chemical functionality of MOFs can be modulated within a wider range [3,4].

In this work, Zr-based MOFs,UiO-66-NH_2, was used for post-synthesis by melamine(UiO-66-NH_2-Mlm) (Fig. 1) to provide higher content of primary amine for Knoevenagel reaction. The modified MOFs were characterized with XRD, FT-IR, TEM, SEM, BET, TGA, XPS. The effective parameters in Knoevenagel reaction such as catalyst type, amount, and solvent type were investigated. The modified MOFs exhibited excellent catalyst activities in heterogeneous phase due to their large surface area and porosity.

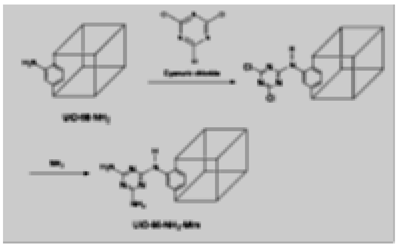

Fig.1. Synthesis of UiO-66-NH_2 (Mlm)

References:

[1] D. Farrusseng, S. Aguado and C. Pinel, Angew. Chem., Int. Ed., 48 (2009) 7502–7513.
[2]A. H. Chughtai, N. Ahmad, H. A. Younus, A. Laypkov andF. Verpoort, Chem. Soc. Rev., 44 (2015) 6804–6849.
[3]Y.-B. Huang, J. Liang, X.-S. Wang and R. Cao, Chem. Soc. Rev., 46 (2017) 126–157.
[4]A. Dhakshinamoorthy and H. Garcia, Chem. Soc. Rev., 41 (2012) 5262–5284.

Investigations UiO-66-NH-EtNH$_2$ ascatalyst for the preparation of enoneα,β-enone

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Abstract:

Metal-organic frameworks (MOFs) are crystalline porous materials [1,2]. MOFs are promising materials for various technological applications, including gas storage, separation, drug delivery, and chemical sensing. In recent years, MOFs have been been used as heterogeneous catalysts [3,4].

In this study, we prepared UiO-66-NH$_2$ (Fig. 1) the using a simpler method and was evaluated as heterogeneou catalyst for reaction between benzaldehyde and malonitrile.The obtained material has been characterized by XRD, FT-IR, TGA, SEM and BET. The effect of various reaction parameters such as type of the solvent and amount of the catalyst were studied. The catalyst shows excellent performance in the reaction ofphenols and aryl halides with good to excellent yield.

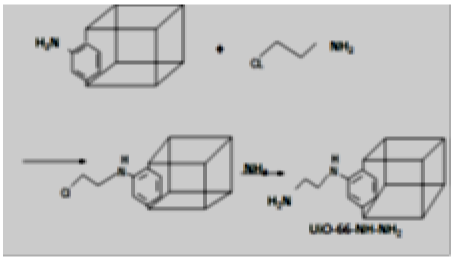

Fig.1. Synthesis of UiO-66-NH-EtNH$_2$.

References:

[1] S. Lee, E. A. Kapustin, O. M. Yaghi. Science 353 (2016) 808−811.

[2] J. A. Mason, J. Oktawiec, M. K.Taylor,M. R. Hudson, J. Rodriguez, J. E. Bachman, M. I. Gonzalez, A. Cervellino, A. Guagliardi, C. M. Brown,P. L. Llewellyn, N. Masciocchi, J.R. Long, 527 (2015) 357−361.

[3] H.A.Hamzah, W. J. Gee, P.R. Raithby, S.J. Teat, M.F. Mahon, A.D. Burrows, Chemistry - A European Journal, 24 (2018) 11094-11102

[4] L. Zhu, X.-Q. Liu, H.-L. Jiang, L.-B. Sun, Chem. Rev. 117 (2017) 8129–8176.

A new selective macroacyclic Schiff base fluorescent chemosensor containinghomopiperazine moiety for Al^{3+} ion

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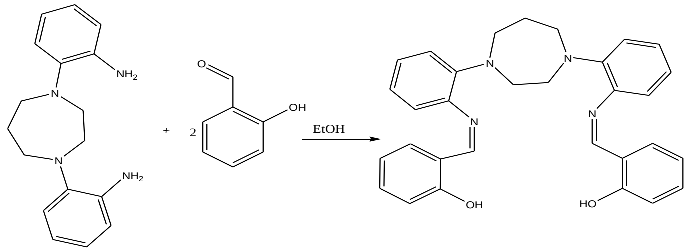
Abstract:

Al^{3+} ions existing in natural waters and most plants can enter the human body through foods and water.Sinceexcess or evendeficiency of aluminum ions can cause many pathological states, developing fluorescent chemosensors for detecting trace amounts of Al^{3+} has attracted increasing attention. a new chemosensor for Al^{3+} based on Schiff base with high sensitivity and selectivity was synthesized by condensation of a polyamine containing homopiperazine moiety with 2-hydroxybenzaldehyde, and characterized by IR, ^{1}HNMR, ^{13}CNMR and mass spectra (Scheme 1). After the addition of different metal ions such as Pb^{2+}, Cr^{3+}, Mn^{2+}, Al^{3+}, Ni^{2+}, Co^{2+}, Zn^{2+}, Hg^{2+}, Fe^{3+}, Zn^{2+},Cd^{2+} only Al^{3+} could increase the fluorescence intensity of the H_2L as a chemosensor(Fig.1 a). Also the fluorescence intensity of the chemosensor in ethanol solution was enhanced after the addition of Al^{3+} over other metal ions (Fig.1 b) [1,2].



Scheme1. The process for the synthesis of macroacyclic Schiff base ligand (H_2L).

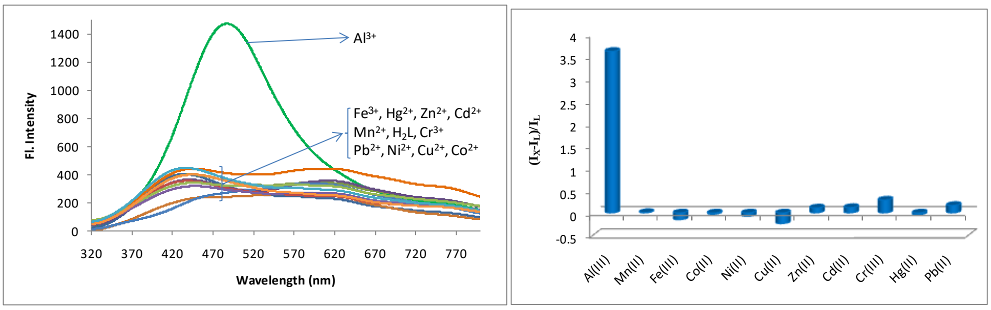


Fig 1.(a) Fluorescence spectra of H_2L in the presence of various metal ions.
(b) changes in fluorescence of H_2L after the addition of Al^{3+} over other metal ions.

References:

[1] R. Azadbakht, T. Almasi, H. Keypour, M. Rezaeivala,Inorg. Chem.Commu.33 (2013) 63-67.
[2] H. Li, J. Wang, Z. Shujiang, C. Gong, F. Wang, RSC Adv.8 (2018) 31889-31894.

Synthesis and Characterization of a Mixed Metal (Fe, Bi) Oxides

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Abstract:

Mixed metal oxide (MMO) plays an appreciable role in many areas of chemistry. In fact, different metals in their various oxidation states can combine in different ratios to produce a variety of materials. The Mixed metal oxides are used in many applications in the electronic industry and various fields of science and technologies, microelectronic circuits, sensors, piezoelectric devices, fuel cells, because of physical, chemical, and morphological properties [1]. These can adopt a vast number of structural geometries with an electronic structure that can exhibit metallic, semiconductor or insulator characters [2].

In this work, we synthesized a mixed metal oxideof Iron(III) and Bismuth (III) and characterized by Infrared(IR) spectroscopy (figure 1) and X-Ray Powder Diffraction (XRD)(figure 2).

The $BiFeO_3$ solution was prepared by dissolving (3mmol, 0.14 g) ratio of $Bi(NO_3)_3.5H_2O$ with (2mmol, 0.8 g) of $Fe(NO_3)_3.9H_2O$ were mixed with deionized water (DI) under continuous magnetic stirring.

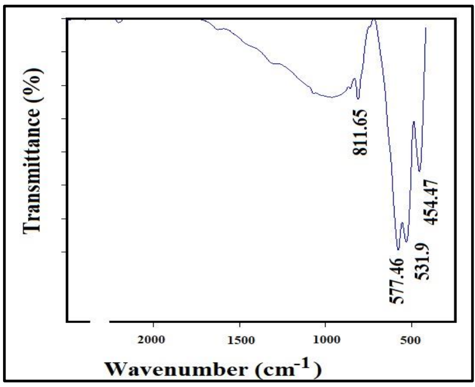

Fig.1.IR spectroscopy of $Bi_xFe_yO_3$

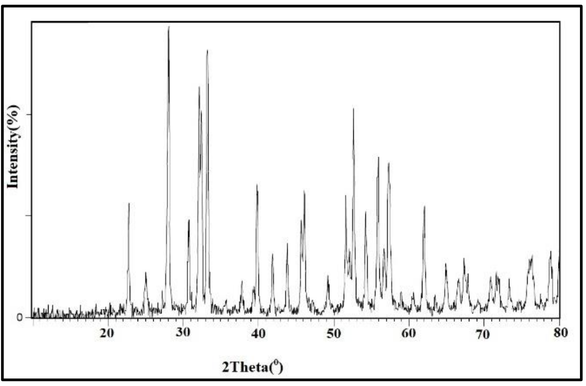

Fig.2.XRD pattern of $Bi_xFe_yO_3$

References:

[1]M. Jabłońska,M.AgoteArán,A. M.Beale,G. Delahay,C. Petitto,M. Nocuń,R. Palkovits, Applied Catalysis B: Environmental, 243 (2019) 66-75.

[2]A.V.Meera, R. Ganesan, T.Gnanasekaran, Journal of Alloys and Compounds, 790 (2019)1108-111.

Synthesis and characterization of naphthalene based Schiff-base receptor for anion detection

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Abstract:

Schiff-base receptors have been of recent interest as colorimetric chemical sensors for detection of anions and cations due to their generally simple method of synthesis [1]. Herein, we report the condensation product of azo-coupled precursor (2-hydroxy-5-(naphthalen-1-yldiazenyl) benzaldehyde) and 4-Chloro-3(trifluoromethyl)benzylamine, 2-((E)-((4-chloro-3-(trifluoromethyl)phenyl)imino)methyl)-4-((E)-naphthalen-1-yldiazenyl) phenol (**L**) acts as a colorimetric chemical sensor. The structure of **(L)** (Fig 1) was studied with the help of UV–Vis, FT-IR and ^{1}H-NMR techniques [2]. The synthesized compound was introduced for the selective detection of anions in organic and semi-organic media. The interaction between the ionophores and anions was investigated by NMR and UV–Vis methods [3].

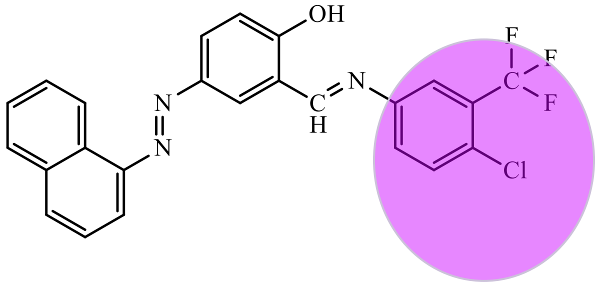

Fig 1.Structure of Schiff-base receptor

References:

[1]. V. Kumar, A. Singh, N. Gupta, Sensors and Actuators B: Chemical- 204 (2014) 125–135.

[2]. J. Kumar, M .Sarma, P. Phukan**,** Dalton Trans**.**44 **(**2015) 4576-4581.

[3]. M. Orojloo, S. Amani, P. Zolgharnein, M. Solimannejad, InorganicaChimicaActa 467 (2017) 227–237.

Synthesis and characterization of a new perovskite of $LaCrO_3$

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Abstract

The name of perovskite was derived from Lev A. Perovski who was a Russian mineralogist [1]. Perovskite structured materials could bethe potential material inthe emerging photovoltaic field due to itsrapid PCE improvement. The common chemical formula for perovskite compounds is ABX_3, where “A” and “B” are two cations.Moreover, ABX_3needs to be a six coordination number element toform octahedron as BX_6. The ratio of ionic radius between A and B isthe major factor in forming perovskite structure. The octahedronsconnect with each other by element X. Every eight octahedronsform a space where a cation is located. The ratio of ionic radiusbetween A and B is calculated by tolerance factor [2]. Tolerance factor between 0.9 and 1.0 leads to form cubic perovskite structure. Tolerance factor between 0.7 and 0.9 leads to form orthorhombic, rhombohedral or tetragonal perovskite structure [3]. In this study, a new perovskite based on chrome(III) metal and lanthanum(III) in a co-precipitation wassynthesized andcharacterized by Infrared (IR) spectroscopy (figure 1) and X-Ray Powder Diffraction (XRD) (figure 2) analysis.5 mL aqueous solution of $La(NO_3)_3$ (0.65 g, 1.5 mmol) was prepared. This solution was slowly added to the aqueous solution (3.5 mL) of $Cr(NO_3)_3$ (0.4 g, 1mmol) under co-precipitation.

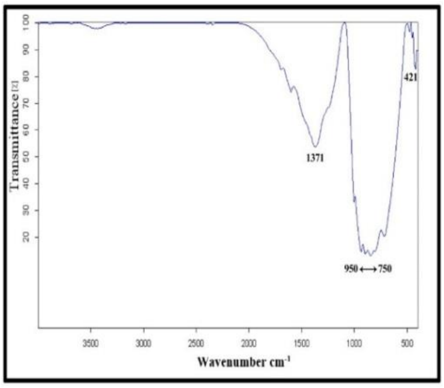

Fig.1.IR spectroscopy of $LaCrO_3$

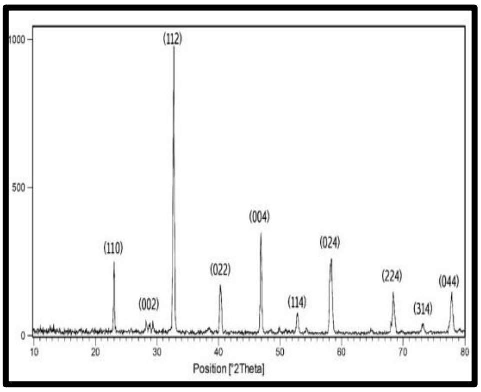

Fig.2. XRD pattern of $LaCrO_3$

References:

[1] M. Kh. A, S. B, R. S, H. H,RENEW. SUST. ENERG. REV.81 (2018) 2812–2822
[2] M. Ch. Wu, W. Ch. Chen, Sh. H. Chan, W. F. Su, Appl. Surf. Sci. 429 (2018) 9–15
[3] T.J. Jacobsson, M. Pazoki, A. Hagfeldt, T. Edvinsson, J. Phys. Chem. C 119 (2015)25673–25683

Some new nano-structure cadmium coordination compounds: Thermal analysis and usage as new precursors for preparation of cadmium oxide nanoparticle

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Abstract:

Nowadays nanostructure compounds are of interest because of notable properties with respect to bulk ones [1]. Schiff bases are the most widely utilized chelating ligands in the development of coordination chemistry. Schiff base compounds containing an imine group are usually formed by the condensation reaction between aprimary amine and an active carbonyl. Because of the possible variety of the initial reactants for the synthesisof Schiff bases ligands, these compounds show a wide variety of chemical structures with differentphysicochemical properties [2].

Synthesis andcharacterization of a new N_2-Schiff base ligand (obtained by condensation reaction between 1,3-propanediamine and methoxycinnammaldehyde) and itsCd(II) complexes are the purpose of this work. All compounds were synthesized in alcohol solutionand after isolation, characterized by FT-IR, NMR, UV–visible spectra and molar conductance. Based on spectral data, the general formula of $CdLX_2$ (X = halide and/or pseudo-halide) was proposed for the cadmium complexes. Thenanostructure cadmium complexes were prepared by sonochemical method. Moreover, CdO nanoparticles were prepared by calcination ofcadmium halide complex at 500 ˚C and characterized by XRD, SEM.Thermal behaviors of allcompounds were studied by TG/DTG analysis data.Furthermore, antibacterial activities of compounds have been screened against various bacteria and fungi by disk diffusion method.

References:

[1] Z. RashidiRanjbar, I. Sheikhshoaie, Z. Bagheri, International Journal of NanoDimension 5 (2014) 409.

[2] S. GhanbariNiyaky, M. Montazerozohori, A. Masoudiasl, J. M. White, J. Mol. Struct. 1131 (2017) 201.

Structural features and Hirshfeld surface analysis of some diorganotin(IV) complexes containingpyridylligands

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Abstract:

Organotin(IV) compounds have been considered as one of the widespread topics in modern coordination chemistry due to their coordinative abilities towards most of the donor ligands especially pyridyl ligands. The penta- and hexa-coordinated organotin(IV) adducts are more common.These compoundsare of particular interest especially in biological fields as anticancer agents andin some cases they show the anticancer activities greater than carboplatinum compound;they may show lower toxicity compared to cisplatin analogues[1-3].Herein, we reportthe preparation, structural characterization of new diorganotin(IV) (R = Ph, Me) complexes containing a related series of pyridyl ligands. The products have been characterized using elemental analysis, IR, multinuclear NMR (^{1}H, ^{13}C, ^{119}Sn), DEPT-135° NMR spectroscopy and X-ray crystal structure determination in most cases.The 3D Hirshfeld surface analysis and 2D fingerprint maps were used for quantitative mapping out of the intermolecular interactions which reveal the presence of several π-π and hydrogen bonding interactions;they are associated between donor and acceptor atoms.

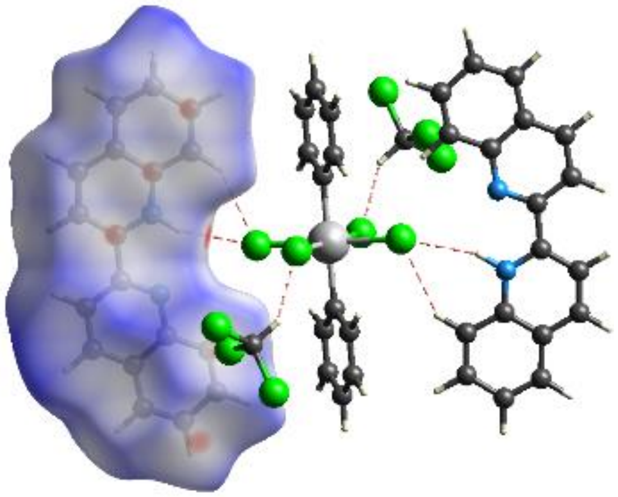

Fig.1

References:

[1] B. Z. Momeni, F. Sefidabi, S. Khademi, N. Fathi, Appl. Organomet. Chem., 32 (2018) 4432.
[2] Y.-X. Tan, Z.-J. Zhang, Y. Liu, J.-X. Yu, X.-M. Zhu, D.-Z. Kuang, W.-J. Jiang, J. Mol. Struct.1149 (2017) 874.
[3] M.K. Amir, S. Khan, Zia-ur-Rehman, A. Shah, I.S. Butler, Inorg. Chim. Acta, 423 (2014) 14.

Enhanced adsorptive removal of anionic and cationic dyes from wastewater using MOF PCN-222(M)

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Abstract:
The toxicity of the dyes and inappropriate discharge of such wastes play major roles in water pollution and spread of diseases [1]. In this work, harmful dyes (anionic dye(MO) and cationic dye(MB)) have been removed from wastewater. The high dye adsorption capacity overPCN-222 (Cu, Fe, Mn)has been estimated and analyzed using Langmuir and Freundlich equations. The adsorption kinetics, thermodynamic parameters, stability and reusability of the adsorbent have also been reported [2]. The results show that PCN-222(M) has maximum loading of MB and MO. The adsorption capacity of metalloporphyrin framework (PCN-222(M) (M= Cu, Fe, Mn)) ranks at top in comparison with metal-free porphyrin framework (PCN-222). Adsorption capacity has been observed up to eight recycles for dye removal with no significant change in crystal structure.The electrostatic interaction between porphyrinic metal center and MO increases dye adsorption capacity.Values of r^2 of a linear plot of the Langmuir model were better than those of the Freundlich model for all three adsorbents (Fig. 1).

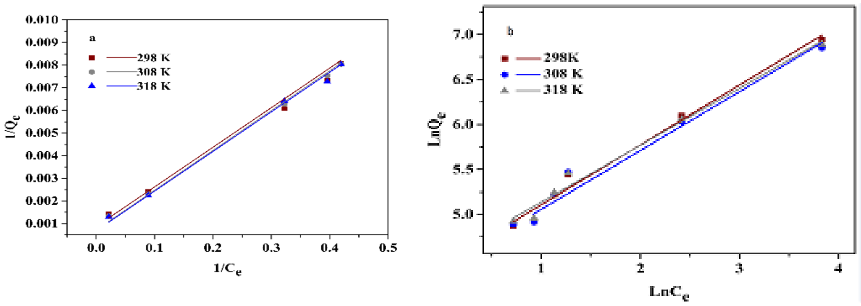

Fig 1. plot of the a)Langmuir andb)Freundlich model

References:
[1]A.A. Mohammadi, A. Alinejad, B. Kamarehie, S. Javan, A. Ghaderpoury, M. Ahmadpour, M. Ghaderpoori, , Int. J. Environ. Sci. Technol. 14 (2017) 1959-1968.
[2]X. Zhao, S. Liu, Z. Tang, H. Niu, Y. Cai, W. Meng, Nat. Publ. Gr. 5 (2015) 1–10.

A facile synthesis of PCN-222(M) (M=Cu, Fe, Mn) and long term stability analysis in aqueous media

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Abstract:

A zirconium based porphyrinic metal-organic framework (PCN-222(M) (M=Cu, Fe, Mn)) has been synthesized by a simple, scalable sonochemical preparation method without high temperature in a short period of time (PCN-222(M)-U). For the first time, stability of PCN-222(M) in the water was investigated for 3 months (PCN-222(M)-3) [1]. In this work, MOFs have been synthesized by heating under reflux and sonochemical irradiation. Sonochemical method has been proven an efficient procedure.MOFs have been characterized by FTIR spectroscopy, Powder X-ray Diffraction (PXRD), Scanning Electron Microscopy (SEM), Thermal Gravimetric Analysis (TGA) and the large specific surface areas have been determined byBrunauer-Emmet-Teller (BET) method.Briefly, 50 mg of PCN-222(M) were dispersed in amount of deionized water for 15 minutes [2]. Then the solution kept at 25^0 C for 3 months.The powder X-ray diffraction (PXRD) patterns of PCN-222(M)-U and PCN-222(M)-3 indicate similar peaks for MOFs suggesting that no extra phase creation or framework collapse happens during ultrasound irradiation method or water aged MOF (Fig. 1).

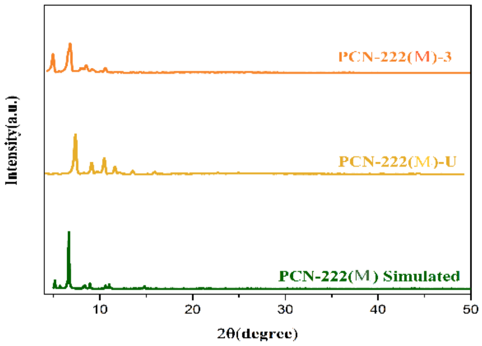

Fig. 1. XRD patterns of PCN-222(M) Simulated, PCN-222(M)-U and PCN-222(M)-3.

References:

[1] D. Feng, Z. Gu, J. Li, H. Jiang, Z. Wei, H. Zhou, Angew. Chemie. 124 (2012) 10453–10456.
[2] H.Molavi, A.Hakimian, A. Shojaei, M.Raeiszadeh, , Appl Surf Sci. 445 (2018) 424-436.

The immobilized azo-azomethine on solid supports: highly selective sensors for naked eye detection of CN^- in water

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Abstract:

A molecular azo-azomethine receptor, **HL**, was synthesized via condensationreaction of 1-(3-formyl-4-hydroxyphenylazo)-4-nitrobenzeneand 3-aminopropyl triethoxysilane in EtOH. The **HL** was characterized using standard spectroscopic techniques.The sensing ability of **HL**was investigated towards the inorganic anions in DMSO and semi-aqueous media. As shownin Fig. 1, upon the addition 10 equiv. of the anions (CN^-, $H_2PO_4^-$,AcO^-, NO_3^- ,HSO_4^-,F^-, Cl^-, Br^-, I^-, and free **HL**) to the DMSO solution of **HL** an instant and noticeable color changes was observed from pale orange to dark blue and gray-blue only in the presence of CN^- and AcO^-, respectively. To further study, UV-Vis experiments were also performed upon the addition 10 equiv. of CN^- and AcO^- to DMSO solution of **HL**.Then, the new solid sensors based **HL** immobilized on amorphous SiO_2, **S-B**, and NaY zeolite, **S-ZY**, was prepared and applied for detection of the mentioned anions, in 100% aqueous media.The fabricated solid sensors were characterized using powder XRD diffraction, TGA-DTA, BET and FT-IR spectroscopy. Surprisingly, **S-B** and **S-ZY** show excellent sensitivity and selectivity against CN^-over the other anions (CN^-, $H_2PO_4^-$,AcO^-, NO_3^-,HSO_4^-, F^-, Cl^-, Br^-, I^- and free **S-ZY**) in water Fig. 2. [1,2]

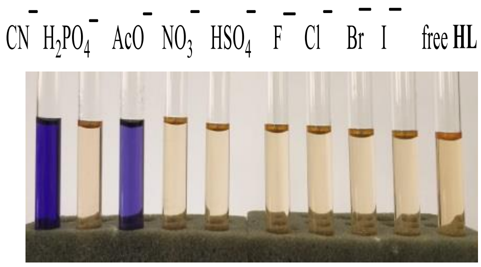

Fig.1. selectivity of molecular azo-azomethine receptor toward CN^- and AcO^-

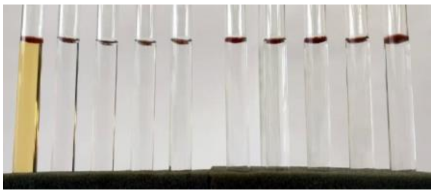

Fig.2. selectivity of molecular azo-azomethine receptor toward CN^-

References:

[1]. S. Mahdavi, H. Khanmohammadi, M. Zendehdel, Spectrochim. Acta A. 199 (2018) 21-31.

[2]. P. Gogoi, A.K. Dutta, S. Saikia, and R. Borah, Appl. Catal. A: Gen., 523 (2016) 321–331.

Functionalized Magnetic Graphene Oxide as a Nanocatalyst for Organic Synthesis

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Abstract:

Recently, graphene and graphene oxide have attracted enormous interest in the development of composite materials and catalysts, due to their remarkable physical, chemical and electrical characteristics, including a very high specific surface area. The synthesis of graphene nanosheets on alarge scale from graphite is a well-established route, where graphene oxide is an intermediate product. The presence of oxygen-carrying functionalities in graphene oxide facilitates their dispersion in water and polar solvents, as well as interrupts the regular p electron distribution. These unique characteristics makes graphene oxide a potent material for the immobilization of various nanoparticles, polymeric composites and catalytic activities [1].

Facile separation and recovery of the catalysts is a significant issue, while imobilization on nanopatricles is a favorable approach. Among different nanoparticles which are used as supports, magnetic graphene oxide (MGO) has attracted interests because of its high surface area, stability, easy separability and unique potential technical applications.

Multi-component reactions (MCRs) are defined as one-pot processes that three or more substrates combine either simultaneously, or through a sequential addition procedure that does not require any change of solvent. Quite recently MCRs have gained importance especially in the total synthesis of natural products, and medicinal heterocyclic compounds, because of their simplicity, higher yield of the products, and lower reaction times[2].

Herein a synergic approach has been presented for performing MCR in the presence of MGO supported catalysts.

References:

[1] Zhu, Y., Murali, S., Cai, W., Li, X., Suk, J. W., Potts, J. R., &Ruoff, R. S.,Adv.mater., 22 (2010) 3906-3924.

[2] Sayahi, M. H., Bahadorikhalili, S., Saghanezhad, S. J., &Mahdavi, M.,Res.Chem. Intermed,44 (2018) 5241-5253.

Molybdenum complex supported on functionalized diatomite and investigation of its catalytic properties

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Abstract:

Diatomite has attracted great interest because of their widely distribution and low cost.Diatomite is a low-density biogenicsediment, and its chemical composition mainly consists amorphous silica (about 70 to 90%) clay, some metallic oxides (e.g. Al_2O_3,Fe_2O_3,MgO and K_2O), etc [1]. In this study diatomite nano-particles were synthesized by sedimentary method. For the preparation of amine functionalized diatomite was refluxed with 3-(tri-methoxysilyl) propylamine (MSPA) for 20 h and then resulting product was functionalized with salicyl aldehyde.MoO_2 $(acac)_2$ was then supported onto the resulting product and heterogeneous catalyst $MoO_2(acac)_2$was prepared.Charactrization of the as-synthesized catalyst were investigated FT-IR, XRD, ICP, SEM, BET and EDX. Epoxides are very important intermediates for the production of fine chemicals and pharmaceuticals.In the past decades, many different kinds of catalysts and reaction systems have been developed for alkenes epoxidation with molecular oxygen, hydrogen peroxide or organic oxidants [2]. Modified diatomite were used to support $MoO_2(acac)_2$ complexes in alkene epoxidation. The various parameters such as type of solvent, time, amount of catalyst, and type of oxidant were optimized for this reaction. The optimum conditions were found as 10 mg catalyst in dichloroethane with t-BuOOH as oxidant which gives 98% yield during 120 minutes.

References:

[1] M. Aivalioti, I. Vamvasakis, E. Gidarakos, Journal of hazardous materials, 178 (2010) 136-143
[2] Y. Nishiyama, Y. Nakagawa and N. Mizuno,Angew. Chem.,Int. Ed., 40 (2001) 3639–3641.

Quantitative Investigation of biological activity, mechanism and Toxicity offluorescence quenchers as a CO_2reductant through the tetrakis (4-sulfonatophenyl) porphyrin (TSPP)

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Abstract:

Tetrakis-(4-sulfonatophenyl) porphyrin is a high Potential molecule because ithas many applications in different fields like photocatalytic and catalytic reactions, photosensitizer and also many studies has done before on application of porphyrins in photoredox system as a catalyst for converting a number of organic compounds like CO_2[1,2] . In this study,23 quenchers have been collected base on the antiseptic and anti-infective activities. The quantitativeactivities have been taken from PASS software. It is asoftware that have good ability to predict biological, toxicity and mechanism of molecules by structure. Each biological activities or mechanism which is higher than 50% is valuable for us. As seen in the table 2, 6-antracenedisulfonate: [ADS],2-naphthalenesulfonate: [2-NS] and 2-anthracenesulfonate: [2-AS]have shown maximum antiseptic and anti-infective ability from 87.8percent for [ADS] to lowest value equal to 50.7 Congo Red[CongoR] .According to the toxicity of all molecules in the table,[ARS] has shown activity probability (P_a) equal to 29.2 for mutagenic (T_1) and 27.8 for skin irritation (T_2).As a conclusion from the point of view of biologicalactivity [ADS] is better than [2-NS] but if we look at toxicity amounts it show lower than that for [ADS] so among these molecules [2-NS] is the best choice.

No	Abbrev name	%Biological activity				%Mechanisms				%Toxicities			
		A_1		A_2		M_1		M_2		T_1		T_2	
		P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i
1	L-phen	---	---	20.3	1.91	21	1.22	---	---	---	---	---	---
2	ADS	87.8	0.4	63.2	1.4	35.9	2.9	---	---	32.5	2.7	31.3	5.4
3	2-AS	86.8	0.4	61.6	1.6	34.1	3.1	---	---	32.3	2.7	22.1	5.9
4	2-NS	87.5	0.4	66.9	1.1	35.9	2.9	---	---	29.2	3.3	27.8	4.3
5	Alizarin	50.3	1.5	39.2	6.3	20.2	1.66	---	---	22.2	5	20.8	11
6	ARS	53.9	1.3	44.4	4.7	21.7	1.31	---	---	47.7	1.3	---	---
7	Congo R	50.7	1.4	33.5	8.3	20.8	1.5	---	---	73.5	6	---	---
8	L-pyrene S	84.2	0.5	63.7	1.4	26.5	6.7	---	---	34.9	2.3	22.3	10
9	NB	---	---	20.8	1.8	---	---	---	---	90.7	3	---	---
10	TNT	38.3	3.3	36.3	7.3	---	---	---	---	90.6	3	32.7	3.1
11	Acid O	18.7	1.35	---	---	20.9	1.49	---	---	51.3	1.2	13.8	11.3
12	EBT	38.5	3.2	29.2	10.1	---	---	---	---	78.1	6	16.7	16.7
13	Methyl O	25.2	8.4	---	---	---	---	---	---	41.7	1.7	---	---
14	Methyl R	34.9	4.2	21.5	16.9	---	---	---	---	43.9	1.5	---	---
15	Tartrazine	---	---	17.4	14.9	---	---	27.5	6	43.5	1.6	---	---
16	FIC	48.6	1.6	35.7	7.5	---	---	36.5	2.9	29.7	3.2	---	---
17	N-1-yl acetate	47.3	1.7	23.8	1.36	34.3	6	---	---	16.9	7.4	31.1	5.5
18	TheoPh	56.3	1.2	46.6	4.2	---	---	84.2	0.4	82.5	5	47	2.1
19	3-phen-1-p	32.9	4.8	---	---	42.6	2.3	36.4	10.1	---	---	42.6	2.6
20	n-butyl p	48.6	1.6	---	---	39.1	3.5	46.4	6.5	---	---	48.5	1.9
21	NB	---	---	20.8	1.8	---	---	---	---	90.7	3	---	---
22	B- uracil	24.7	8.7	22.2	1.56	---	---	87.5	0.2	21.9	5.2	---	---
23	I- uracil	---	---	24.4	1.3	---	---	87.5	0.2	18.6	6.5	---	---

*A1: Antiseptic, A2: Anti-infective, M1: NADH dehydrogenase inhibitor, M2: (NADPH) inhibitor, T1 Mutagenic -T2: Skin irritation, weak

References:

[1] Amao Y, Kataoka R.. Catalysis Today. 307 (2018) 243-247.

[2] Amao Y, Abe R, Shiotani S. Journal of Photochemistry and Photobiology A: Chemistry. 313 (2015) 149-53.

Investigation of biological activity and toxicity of the quenchers that applied for water soluble 5,10,15,20-tetrakis(4-carboxylphenyl)porphyrin (*TCPP*)

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Abstract:

In recent decade porphyrins and metalloporphyrines have been used as chemosensors to sense many materials like metal, toxic and pollutant compounds. Detection of nitro aromatics as explosive compounds is important. One of the suitable method to detect these compounds is fluorescence spectroscopy [1, 2].In this work we investigate some biological activity and toxicity of a number of nitroaromatics by PASS software to choose which one has better antiprotozoal activity as seen in table below. Trinitro-fluoren-9-one [TN-9-one] has 67.2% for antiprotozoal activity which is the greatest value in the range of 41.2% to 67.2%. It has been studied in previous works by Sharma S. and et al. [3]. Also mutagenic and carcinogenic toxicities were compared among molecule sets. If we want to choose the best molecule with respect to T_2 (embryotoxic) amounts there is no choice except [t-p-nitrostilbene]

No.	Compounds	Activity		mechanism		T_1		T_2	
		P_a	P_i	P_a	P_i	P_a	P_i	P_a	P_i
1	TNT	55.8	1.3	94.3	0.2	92.8	0.3	41	8
2	DNT	49.6	2.3	91.8	0.2	91.2	0.3	38.6	9.2
3	2-NBA	41.2	4.3	89.1	0.3	45.6	1.3	32.9	1.3
4	DNBA	46.4	2.9	93	0.2	57.2	0.8	35.7	10.9
5	Nitrostilbene	57.9	1.0	82.5	0.5	62.9	0.7	30.2	15.3
6	DNph	61.6	0.7	87.3	0.3	81.4	0.5	53.5	4.2
7	m-DNB	63.7	0.7	93.9	0.2	87.7	0.4	52.9	4.4
8	NB	62.7	0.7	90.3	0.3	84.3	0.4	48	5.7
9	o_NB	64.6	0.7	90.3	0.3	86.8	0.4	59	2.9
10	o-Nph	58.6	0.9	79.9	0.5	70.2	0.6	51.6	4.8
11	p-DNB	65.2	0.7	92	0.2	86.5	0.4	49.2	5.4
12	p-metNB	53.5	1.6	74.9	0.7	56	0.8	36.2	10.6
13	p-NA	62.9	0.7	82.3	0.5	85.3	0.4	56.3	3.5
14	Picric acid	57.4	1.1	89	0.3	86.1	0.4	41.4	7.9
15	p-NT	57.4	1.1	83.6	0.4	73.9	0.6	39.9	8.5
16	Sodium m-NBS	54.9	1.4	78.7	0.6	59.9	0.7	62.8	2.2
17	t-p-nitrostilbene	56.3	1.3	82.5	0.5	62.9	0.7	30.2	15.3
18	TNB	57.9	1	95.4	0.1	90.9	0.3	53.8	4.1
19	TNF-9-one	67.2	0.6	82.5	0.5	83.6	0.5	44.4	6.7

Activity: Antiprotozoal activity, Mechanism: Chloramphenicol O-acetyltransferase inhibitor T_1: Mutagenic, T_2: Embryotoxic

References:

[1] J.Yang,et al., ACS applied materials & interfaces, **7**(22) (2015) 11956-11964.
[2] Chen, W., et al., Sensors and Actuators B: Chemical, 147(1) (2010) 191-197.
[3] Sharma, S. and N. Anand, Chapter 21 - Miscellaneous Antiprotozoals, in Pharmacochemistry Library, S. Sharma and N. Anand, Editors. Elsevier, (1997) 468-488.

Evaluation of Effective Factors in Antibacterial Performance in Layer-Pillared MOFs

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Abstract:

Today, the problem of bacterial and pathogenic resistance to antibiotics is increasing and has become a major problem in societies, and many efforts are being made to deal with it [1].Metal organic frameworks(MOFs) are porous crystallinematerial that can be synthesis by self-assembly of metal ions and ligands and there are several methods to synthesize them [2,3]. Layer-pillared MOFswith formula [M (bdc) (dabco)$_{0.5}$] are made from two-dimensional paddlewheel cluster layers of M-terephthalatethat convert to three-dimensional structures with dabco [4].Due to the proper properties of MOFs, special attention has been paid to them in the field of antibacterial activity [5].Antibacterial properties of metal ions such as zinc and copper in various MOF have already been proven[6].In this work two layer-pillared MOFs were synthesized by solvothermal and sonochemical methods using copper ions and copper-zinc ions as connectors in their structuresand characterization methods were employed to determine their structures. Antibacterial activities of samples were evaluated by agar well diffusion method against two gram-positive and gram-negative bacteria. The results showed that the antibacterial activity depends on the size of the particles and the type of metal ion used in the MOFs structure.The MOF that had the smallest particle size and made of copper ions only, showed the most antibacterial activity.

References:

[1] P.S. Stewart, J.W. Costerton, , The lancet, 358 (2001) 135-138.
[2] H. Li, M. Eddaoudi, M. O'Keeffe, O.M. Yaghi, nature, 402 (1999) 276.
[3] N. Stock, S. Biswas, Chemical reviews, 112 (2011) 933-969
[4] O. Kozachuk, K. Khaletskaya, M. Halbherr, A. Bétard, M. Meilikhov, R.W. Seidel, B. Jee, A. Pöppl, R.A. Fischer, European Journal of Inorganic Chemistry, 2012 (2012) 1688-1695.
[5] R.K. Alavijeh, S. Beheshti, K. Akhbari, A. Morsali, Polyhedron, 156 (2018) 257-278.
[6] G. Wyszogrodzka, B. Marszałek, B. Gil, P. Dorożyński, Drug Discovery Today, 21 (2016) 1009-1018.

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
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Loading of Chlorhexidine into theHKUST-1 MOF and EvaluatingTheir Antibacterial Performance

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Abstract:

Microbial infection is one of the issues that humans have faced it for many years. Recently special attention has been paid to Metal-organic frameworks (MOFs) in biomedicine [1]. MOFs can be used as controlled delivery platforms for bioactive metal ions and molecules by encapsulating them in their pores or use them as a part of their structures[2]. HKUST-1 is a kind of MOFs that was made from benzene-1,3,5-tricarboxylate (BTC) and copper ion[3]. Chlorhexidine (CHX) is a disinfectant agent and haswidely applications in fighting bacteria [4]. Previouslyseparate use of HKUST-1 and chlorhexidine in the field of antibacterial activity has been carried out [5,6]. In this work,the chlorhexidine was loaded onHKUST-1 and antibacterial activity was studied. Various methods were employed to characterize structures and the successful loading of the chlorhexidine in HKUST-1. Antibacterial activity was evaluated by agar well diffusion test and MIC test.In this way two main bacteria with names Staphylococcus aureus (S. aureus) and Escherichia coli (E. coli) were used.The results showed that antibacterial activity was improved and the synergy effect was also found in CHX@HKUST-1.Another important result was that the release of Antibacterial agents (chlorhexidine and Cu^{2+} ions) became controlled.

References:

[1] P. Horcajada, R. Gref, T. Baati, P.K. Allan, G. Maurin, P. Couvreur, G. Ferey, R.E. Morris, C. Serre, Chemical reviews, 112 (2011) 1232-1268.

[2] R.K. Alavijeh, S. Beheshti, K. Akhbari, A. Morsali, Polyhedron, (2018): 257-278.

[3] S.S.-Y. Chui, S.M.-F. Lo, J.P. Charmant, A.G. Orpen, I.D. Williams, , Science, 283 (1999) 1148-1150.

[4] D. Maki, C. Alvarado, M. Ringer, The Lancet, 338 (1991) 339-343..

[5] A.R. Abbasi, K. Akhbari, A. Morsali, Ultrason. Sonochem, 19 (2012) 846-852.

[6] M.E. Cortés, R.D. Sinisterra, M.J. Avila-Campos, N. Tortamano, R.G. Rocha, J. Inclusion Phenom. Macrocyclic Chem., 40 (2001) 297-302.

Study of spermine as an inhibitor of carbonic anhydrase by anchoring to the zinc-coordinated water molecule.

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Abstract:

Carbonic anhydrases(CAs) have been inhibited by different compounds such as phenols and coumarins. Usually, polyamines, have been used as activators of carbonic anhydrases enzymes, but they have been investigated recently as new inhibitors of human carbonic anhydrase. Spermine is a derivative of polyamines, which is a small aliphatic molecule found in fungi,archaea andplants[1, 2].

In the present research we used the B3lyp method with the standard 6-31+g* basic set to predict the optimized geometries and interaction energies between inhibitors and CA active site.According to our calculated results poly aminescan be used as a suitable inhibitor, which has at least 7 atoms in the chain, with one free NH_2group.Also the results show optimized spermine with threonine (Thr) amino acid have been established by different hydrogen bondings. Thus, an important point of this work is that we observed for the first time the anchoring of a primary amine (as charged ammonium moiety) to the zinc-bound solvent molecule of CA, through a network of hydrogen bonds involving also the conserved amino acidresidue Thr199.Finally, the good agreement between predicted results with X-ray crystallographic data confirm the reliability of selected methods for these kind of molecules.

References:

[1]Casero, R. A., Jr; Marton, L. J. Nature Rev. Drug Discovery, 6 (2007) 373–390.

[2]Woster, P. M. Polyamine structure and synthetic analogs. Wang, J. Y., Casero, R. A., Jr., Eds., Humana Press: Totowa, NJ, (2006) 3-24.

Synthesis, characterization and theoretical studies of two mononuclear Ag(I) and Pd(Π) complexes of apyridiniumylide

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Abstract

Ylides behave as good ligands toward transition metals owing tothe charge density centered on the ylidiccarbon [1]. The majorpart of the reported ylide−metal complexes concerns ylides inwhich the heteroatoms are P, S, or N and the metals belong tothe middle or late transition metals. Pyridiniumylides showinteresting characteristics due to their appreciable stability,quite exceptional for nitrogen ylides, which is attributed to the delocalization of the charge on the heterocycle [2].Following our interest in Ag(I) and Pd(II) complexes of ylides [3],inthe present work,the reaction ofpyridiniumylide$PhC(O)PyCHO_2CCH_2Ph$with $AgNO_3$salt anddichloro(1,5-cyclooctadiene)-palladium(II) complexin methanolandin a 1:1 mole ratioled to the formation of two new mononuclear metal complexes. Characterization of theobtained compounds was performed by elemental analysis and IR, ^1H, and ^{13}C NMR spectroscopic methods.The structures of resulting mononuclear complexes were studied at bp86/def2-TZVP level of theory using Gaussian09 set of programs. The nature of ylide-metal bond in both complexes was also investigated at bp86-D3/TZ2P level of theory using ADF program.

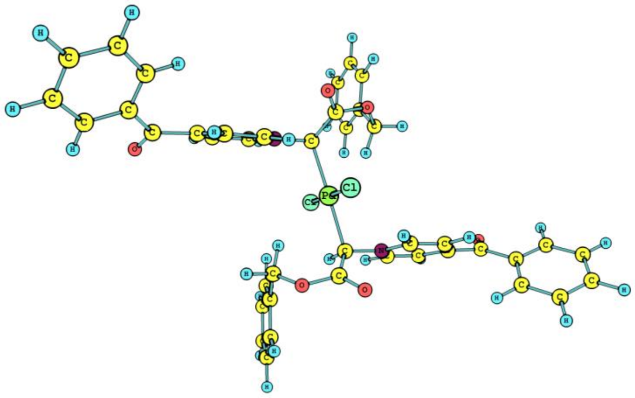

Fig.1. The optimized structure of PdL_2Cl_2 at bp86/def2-TZVP level of theory.

References:

[1] Urriolabeitia, E. P. Top. Organomet. Chem, 30 (2010) 15−48

[2] Jacobs, J.; Van Hende, E.; Claessens, S.; De Kimpe, N.;Curr. Org.Chem. 15 (2011) 1340−1362.

[3]Yousefi, A.; Sabounchei, S.J.; Moazzami Farida, S.H.; Karamian, R.; Rahmani, N.; Gable, R.W.; J.Organomet. Chem., 890 (2019) 21−31.

Synthesis, characterization and theoretical studies of three binuclear Hg(Π) complexes of a new pyridiniumylide

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Abstract:

Phosphonium and sulphoniumylidesstabilization is achieved by the overlap of the formal carbanionic electron pair with the vacant d-orbitals of the adjacent heteroatom. However, in analogous nitrogen compounds such stabilization cannot occur, and consequently most N-ylids are capable of only fleeting existence[1].Following our interest in Hg(II) complexes of various types of ylides [2,3], herein we report the synthesis and characterization of three binuclear Hg(II) complexes. At the first stage, anewpyridinium saltwas synthesized by addition of 4-benzoylpyridine to benzylbromoacetate. Further treatment with NH_3 gave the new pyridiniumylide,PhC(O)PyCHC(O)OCH_2Ph, which is stabilized with a conjugated carbonyl group. The reaction of this ylide with HgX_2 (X=Cl, Br and I) in equimolar ratio using dry methanol as solvent led to the formation of dimeric complexes of the type $[(ylide)HgX_2]_2$ (X= Cl, Br, I).Characterization of the obtained compounds was performed by elemental analysis and IR, ^{1}H, and ^{13}C NMR spectroscopic methods.

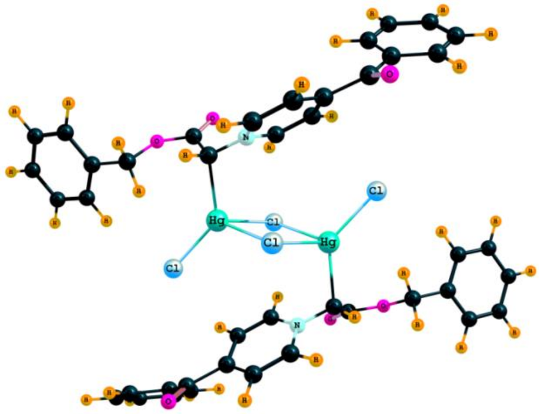

Fig.1. The optimized structure of $Hg_2L_2Cl_4$at bp86/def2-TZVP level of theory. The structure of resulting binuclear complexes was studied at bp86/def2-TZVP level of theory using Gaussian09 set of programs. The nature of ylide-metal bond in all complexes was also investigated at bp86-D3/TZ2P level of theory using ADF program.

References:

[1] Wittig, G.; Krauss, D., Liebigs Ann., 679 (1964) 34.

[2]Sabounchei, S.J.; Sedghi, A.; Bayat, M.; Hosseinzadeh, M.; Hashemi, A.; Yousefi, A.; Gable, R.W.; J. Mol. Struct., 1175 (2019) 346.

[3]Sabounchei, S.J.; Hashemi, M.S.; Karamian, R.; MoazzamiFarid,; S.H.;GohariDerakhshandeh, P.; Gable, R.W.; Van Hecke, K.; J. Coord. Chem., 71 (2018) 3277.

Synthesis and Multinuclear NMR Study of a New Pyridinium Ylide and its Reactions With palladium(II) Chloride

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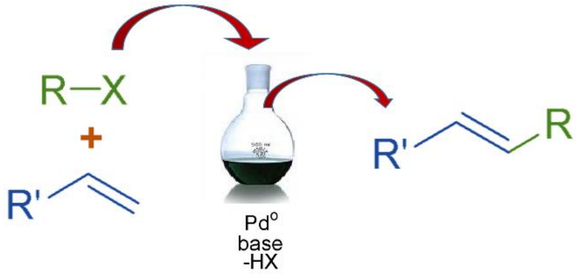
Abstract

Preparation and characterization of α-stabilized Pyridiniumylides and metal complexes in corporating these ylides have attracted much attention. Pyridiniumylides are interesting ligands which have attracted much attention in synthetic, catalytic and theoretical fields of transition metal chemistry [1]. The reaction of Pyridiniumylides of the type NH_5-$C(H)C(O)C_6H_4$-*m*-OCH_3(L) with $PdCl_2$ in equimolar ratios using dichloromethaneas solvent are reported [PdL_2Cl_2]. These complex were fully characterized by elemental analysis and spectroscopic techniques such as IR, ^{1}H, and ^{13}CNMR. This complex has been found to act as efficient catalysts for the Heck reaction. Various aryl halide was coupled with styrene in DMF, under air, in the presence of 0.3mol% of the catalyst to afford corresponding cross-coupled products in good to excellent yields[2,3].



Scheme 1. Catalytic reaction in presence of Pyridiniumylides complex

References:

[1] G. Wittig, Angew. Chem. 92 (1980) 671-675
[2]S.J. Sabounchei, S. Samiee, D. Nematollahia, A. Naghipour, D.M. Morales, Inorg. Chim. Acta 363 (2010) 3973-3980.
[3] Heck, R. F. Org. React. 27 (1982) 345–390.

Structural Chemistry of Nitro-cobaloxime ComplexesSynthesized from their Chloro Precursors in $[Co(DMGH)_2(XPh_3)Cl]$ (X = As & Sb)

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Abstract:

Natural photosynthesis uses sunlight to drive the conversion of energy-poor molecules (H_2O and CO_2) to energy-rich ones (O_2 and $(CH_2O)_n$).Scientists are working hard to develop efficient artificial photosynthetic systems toward the “Holy Grail” of solar-driven water splitting. High on the list of challenges is the discovery of molecules that efficiently catalyze the reduction of protons to H_2. In this case one promising class of molecules are cobalt (III) complexes with equatorial diglyoxime ligands (cobaloximes) [1].Cobaloximes are among the few examples of electrocatalysts based on first-row transition metals complexes that could constitute an effective alternative to the platinum-based catalysts for the economically viable hydrogen production. Alsoover the past four decades cobaloximes have been extensively studied as structural and functional models for the coenzyme vitamin B12. A wealth of information about spectral and structural properties of a great number of cobaloximes has been collected [2]. With regards to the aforementioned properties of cobaloxime complexes, the structural chemistry of such complexes are important for their designated properties.

In this study, the structural chemistry of nitro-substituted cobaloxime complexes, formed by replacing chloro ligand in the precursor complexes, $[Co(DMGH)_2(XPh_3)Cl]$ in which DMGH = dimethylglyoxime monoanion and X = As or Sb., were investigated by X-ray crystallography.These complexes have been also characterized by spectroscopic methods such as FT-IR and^{1}HNMR.

References:

[1] Jillian L. Dempsey, Bruce S. Brunschwig, Jay R. Winkler, and Harry B. Gray.Hydrogen Evolution Catalyzed by Cobaloximes.Accounts of Chemical Research 42 (2009) 1995-2004

[2] Silvia Mirra , Maria Strianese , Claudio Pellecchia , Valerio Bertolasi , Guglielmo Monaco , Stefano.Inorganica Chimica Acta, 444 (2016) 202–208

21st Iranian Inorganic Chemistry Conference
Iranian Chemical Society
28,29 Aug 2019

Synthesis of a new palladacyclopropa[60]fullerene complex containing new unsymmetrical phosphorous ylide and study on its catalytic activity

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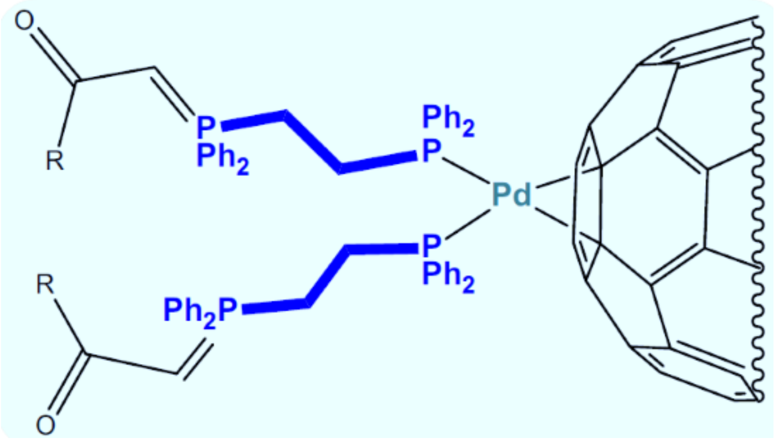
Abstract

Since the discovery of the C_{60} in 1985 by Kroto, Curl, and Smalley [1], coordination chemistry of transition metal-fullerene complexes has attracted the attention of academic researchers more than one decade. Among the myriad of transition metal-fullerene complexes reported today [2], there are only a few metallofullerene complexes synthesized that contain phosphorus ligands.In this work the new Pd[60]fullerene complex incorporating α-keto stabilized phosphorus ylide was synthesized in a three-component reaction of the unsymmetrical phosphorus ylide $[Ph_2P(CH_2)_2PPh_2{=}C(H)C(O)R]$ (Y), C_{60} and $Pd(dba)_2$ (dba= dibenzylideneacetone). The obtained novel P-coordinate complex $[(\eta^2\text{-}C_{60})Pd(\kappa^2\text{-}Y)]$ was characterized successfully by ^1H, ^{13}C and ^{31}P NMR spectroscopic methods and other conventional techniques such as IR, UV-vis and SEM analysis. In addition, a studying between the catalytic activities of the complex was evaluated in the Suzuki and Heck reactions of various aryl halides and olefins in DMF that the coupled products of these reactions were obtained in good to excellentyields and purity, with short reaction times and low catalyst loading.



Scheme 1. Monodentate palldacyclopropa [60] fullerenes containing dppe phosphorous ylide

References:

[1] H. W. Kroto, J. R. Heath, S. C. O’Brien, R. F. Curl, R. E. Smalley, Nature, 318 (1985) 162–163.

[2] D. V. Konarev, S. I. Troyanov, K. A. Ustimenko, Y. Nakano, A. F. Shestakov, A. Otsuka, H. Yamochi, G. Saito, R. N. Lyubovskaya, Inorg. Chem. 54 (2015) 4597–4599.

New composite SBA16 decorated with ZnO for water purification having Azithromycin and optimization of effective parameters by RSM method

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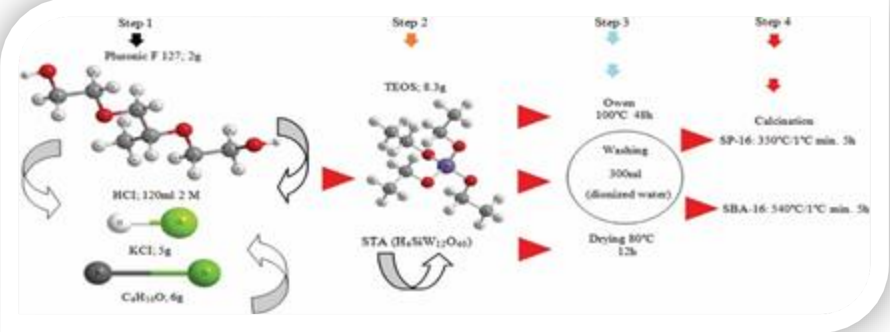
Abstract:

A new mesoporous silica SBA-16/ZnO was prepared by templating method using PluronicF127 as surfactant, TEOS (tetraethyl orthosilicate) as silica source and ZnO nanoparticles as modifier. The physical properties of the materials obtained were investigated by Nitrogen sorptionat 77K (BET), X-ray diffraction (XRD), Fourier transform infrared spectroscopy(FT-IR), Scanning electron microscope(SEM) and MAPPING analysis methods.The characterization results revealed thatthis new composite show highly ordered mesostructure with large surface area and pore diameter,suitable for adsorption applications for eg. antibutics. Today, presence of Azithromycin in environment can be lead to various allergic reactions. According, an effective system needs for removing these compounds. We showed that this materials can be utilizedas purification of water with low pollutant concentrations. Optimization of effective parameters on adsorption percent were performed by Response Surface Method (RSM) [1,2].



Scheme1. New mesoporous silica SBA-16/ZnO composite for water purification

References:

[1] AgnieszkaFelisczak-Guzik , Barbara Jadach , Hanna Piotrowska , Marek Murias , JuninaLulek, Izabela Nowak , Microporous and Mesoporous Materials.220 (2016) 231 – 238.

[2]Gracielle Ferreira Andrade , Daniel cristian Ferreira Soares , Raquel Gouvea dos santos , Edesia Martins Barros Sousa , Microporous and Mesoporous Materials.168 (2013) 102 - 110.

Luminescent Metal–Organic Framework TMU-16as a Sensor for Metal Ions and Small Molecules

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Abstract:

Nowadays, Metal-organic frameworks (MOF) with functional pore structures as a new type of sensing materials have attracted the increasing attention in fluorescence assays [1]. In this research, we explored an interpenetrating microporous mixed-ligand MOF for highly selective and sensitive detection of metal ions. A Zn(II)-based metal-organic framework, $[Zn_2(H_2\text{-}BDC)_2(4\text{-}bpdh)]\cdot 3DMF$ (TMU-16), have been successfully synthesized via a mixed ligand approach using 1,4-benzenedicarboxylate (H_2-BDC) and 2,5-bis(4-pyridyl)-3,4-diaza-2,4-hexadiene (4-bpdh) under solvothermal conditions [2].The TMU-16 displays superb luminescence emission, and it can detect Fe(III) and Cd(II) ions with high selectivity, excellent sensitivity, and short response time (<1 min). The emission intensities of TMU-16 were quenched upon the addition of Fe^{3+} and increased upon the addition of Cd^{2+}. The detection limits of TMU-16 for Fe^{3+}/Cd^{2+} in DMF are estimated to be 0.2 and 0.5 μM, respectively. Furthermore, TMU-16exhibits distinct solvent-dependent luminescent spectra with emission intensity significantly enhanced toward dichloromethane. More importantly, this is the first example of MOF-based luminescent sensor as efficient multifunctional fluorescence material which can use for selective sensing of Fe(III) and Cd(II) ions and small molecules such as CH_2Cl_2 (Fig. 1).

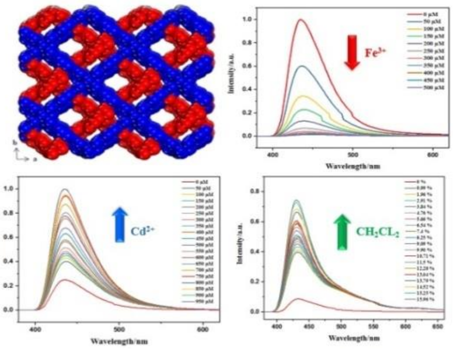

Fig.1. Detection ofFe(III) and Cd(II) ions and CH_2Cl_2 using TMU-16 MOF.

References:

[1] M. Allendorf, C. Bauer, R. Bhakta, R. Houk, Chemical Society Reviews, 38 (2009) 1330-1352.
[2] V. Safarifard, A. Morsali, CrystEngComm, 16 (2014) 8660-8663.

Synthesis and characterization of new binuclear complexes mercury(II) of pyridiniumylide obtained from 2-Bromo-4′-fluoroacetophenone

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Abstract:

Pyridinium ylides are important reagents in organic chemistry, especially in the synthesis of naturally occurring products with biological and pharmacological activities[1]. These compounds have been used as reducing agents in coordination chemistry. They can behave as ambidentate ligands because the carbanion located at the Cα of the ylide or the enolate oxygen is able to donate electron density to a transition metal [2]. Herein, we report the synthesis and characterization of new binuclear complexes of Hg(II) derived from pyridinium ylide $C_5H_5NCHC(O)C_6H_4$-*p*-F (**Y**). Pyridine and 2-Bromo-4-fluoro acetophenone in a 1:1 ratio react in acetone as a solvent to produce the related pyridinium salt. For synthesis ylide, a solution of potassium carbonate in water was added to a solution of pyridinium salt in water. The mixture was stirred for 30 min and then extracted with dichloromethane. The reaction of **Y** with HgX_2(X = Cl, Br and I) in 1:1 ratio leads to binuclear products of the type $[HgX_2(Y)]_2$. Characterization of the complexes by IR, ^{1}H and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom.

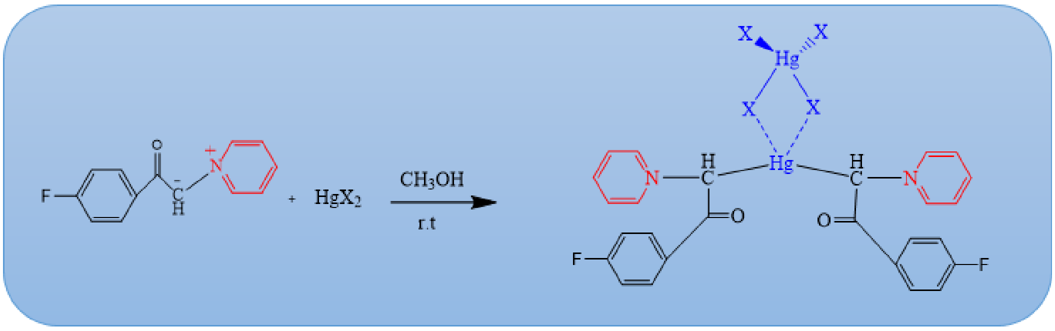

Fig.1. Structure **Y** with HgX_2 (X = Cl, Br and I)

References:

[1] W. Gary. Phillips, Kenneth W. Ratts, J. Organomet. Chem., 35(1970) 3144.
[2] S.J. Sabounchei, F. Akhlaghi, C. Boskovic, R.W. Gable, J. Mol. Struct., 39 (2013) 1046.

Application of modified nanoporous anodic alumina as adsorbent for solid phase extraction of Cr(VI)

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Abstract:

Nanoporous anodic alumina (NAA) is a self-organized material with nanopore arrays. The porous structure can be altered by varying anodization processing parameters and the resulting porous shapes can be tailored with specific pore diameters [1]. NAA has been used in several fields of nanotechnology [2]. In this work, a nanoporous anodic alumina was prepared and used for the solid phase extraction (SPE) of Cr(VI). The metal ion was adsorbed on modified NAA as its complex with 1,5-diphenylcarbazide, then eluted using a mixture of ethanol/HCl and determined by spectrophotometry. The modified NAA was characterized by FT-IR, FE-SEM, EDX analysis and mapping and AFM. The influence of important parameters on the formation of NAA and SPE method such as surface area of aluminum foil, applied voltage, activator acid, pH, type and concentration of eluent as well as adsorption and desorption time was investigated and optimized. Under optimum conditions, the extracted analyte was quantified by UV–Vis spectrophotometry with a detection limit of 1.1 ng mL^{-1} for Cr(IV). This new method was successfully applied to determine Cr(VI) in environmental samples.

References

[1] P. Formentín, Ú. Catalán, L. Pol, S. Fernández-Castillejo, R. Solà and L. F. Marsal, Journal of Biological Engineering ,12(21) (2018) 1-9.

[2] M. F. Shaffei, A. M. Awad, H. S. Hussein and M. S. Mohammed, ARPN Journal of Engineering and Applied Sciences, 10(18) (2015) 7983- 7990.

Study on cell growth and proliferation of nHA/GO/M composite

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Abstract:

Nano Hydroxyapatite (nHA) [$Ca_{10}(PO_4)_6OH_{10}$] is a good selection for different applications because of its similarity of synthesis to mineral phase of the bone, excellent biocompatibility, ability to promote cellular functions andosteoconductivity.

Nano Hydroxyapatite/ graphene Oxide/ doped with metal ions (nHA/GO/M) were prepared using the chemical precipitation method[1].Zinc (Zn) andMagnesium (Mg)were selected as metal ions (M=Mg, Zn).Synthesized samples were identified by the Fourier transform infared (FTIR), Field emission scanning electron microscope (FESEM), X-ray diffraction (XRD), methods. XRD pattern reveals that all reflection peaks of each sample still corresponded to the nHA phase, and that no other phase could be detected. FESEM results showed that nHA andnHA/GO/Zncomposites displayed rod-like and cluster shapes, respectively [2]. An MTT assay was executed to test the in vitro cytotoxicity of doped nHA composites aginst L929 cell lines. The results of the cytotoxicity assay revealed an acceptable limit for the cell growth and proliferation.

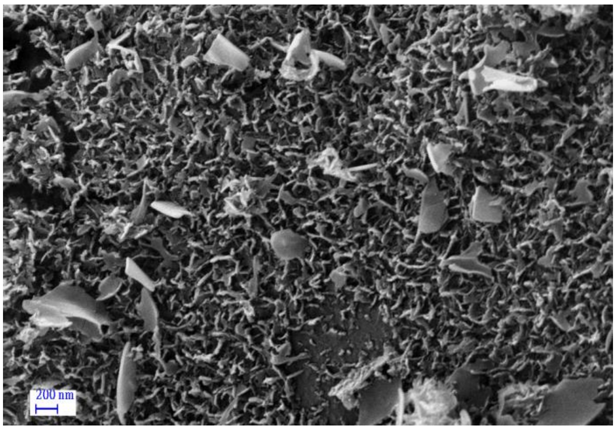

Fig 1. The FESEM patterns of composites nHA/GO/Zn

Refrence:

[1]F. Heshmatpour, S. H. Lashteneshaee, M. Samadipour, J InorgOrganometPolym Mater 28 (2018) 2063-2068.
[2] A. Y. Yilmaz, S. Yilmaz, Ceramics International 44 (2018) 9703-9710.

Synthesis, photochemistry and photosensitizing properties of metallophthalocyanines bearing spiropyrrolizidine oxindoles

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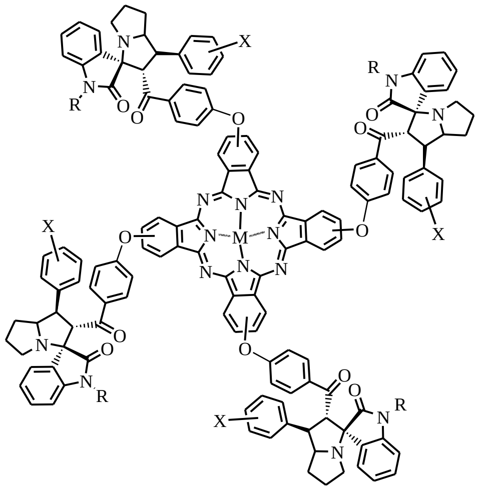
Abstract:

Interestingly, Pc derivatives are promising photosensitizing agents for photodynamic therapy (PDT) due to their intense absorption capabilities in the visible region. An important aim of research into the chemistry of phthalocyanines is to enhance their solubility in various solvents.

A combination of two potentially promising units (i.e. phthalocyanines and spiropyrrolizidine oxindole groups) may improve their organosolubility and biological properties. Herein, we report the synthesis and characterization of several metallophthalocyanines bearing four spiropyrrolizidine oxindole groups which enable the molecules to dissolve in number of organic solvents such as DMF, DMSO and THF. The new metallophthalocyanines (M = Zn and Ni) bearing four spiropyrrolizidine oxindoles at peripheral positions were prepared by tetramerization of corresponding phthalonitriles.

The singlet oxygen generation ability of the ZnPc was quantified as singlet oxygen quantum yields (Φ_{Δ}) and was determined in DMF using 1,3-diphenylisobenzofuran (DPBF) as a chemical quencher. A continuous decrease in DPBF absorbance at 417 nm for phthalocyanine was monitored using a UV-Vis spectrophotometer within 30 min.



References:

[1] Makhseed, S., Machacek, M., Alfadly, W., Tuhl, A., Vinodh, M., Simunek, T., Novakova, V., Kubat, P., Rudolf, E., Zimcik, P.: Chem. Commun. 49 (2013) 11149.

[2] Li, Y., Wang, J., Zhang, X., Guo, W., Li, F., Yu, M., Kong, X., Wu, W., Hong, Z.: Org. Biomol. Chem. 13 (2013) 7681.

Functionalized Magnetic Nanocatalysts Based on Tris-(Hydroxy methyl) amino methane/Triazine as a new inorganic/organic hybrid catalyst for Synthesis of 3,4-dihydropyrano[c]chromene derivatives

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Abstract:

The preparation and the use of inorganic/organic hybrid nanoparticles (HNPs) in organic synthesis has become a subject of intense investigation. In particular, functionalized magnetic nanoparticles (MNPs) which offer advantages in clean and sustainable chemistry as they can be non-toxic, readily available, and recoverable.[1] Dihydropyrano[c]chromenes and their derivatives possess a wide range of biological properties such as anti-cancer, anticoagulant, diuretic, and anti-anaphylactic activities.[2] Therefore, as the importance of these compounds, recently, design of novel nano hybrid catalysts magnetically separable in synthesis of these compounds have been attracted attention.

In this work, mixture of several aromatic aldehydes (1mmol), malononitrile (1mmol) and 4-hydroxycoumain(1mmol) in around bottom flask and catlyst (0.02 g) were stirred at room temperature and solvent free conditions for required time. After completion of reaction, the catalyst easily collected by a magnet to be reused in subsequent reactions [1-3]. The obtained products were recrystallized in ethanol and characterized by ^{1}HNMR, IR and ^{13}CNMR.(Fig. 1)

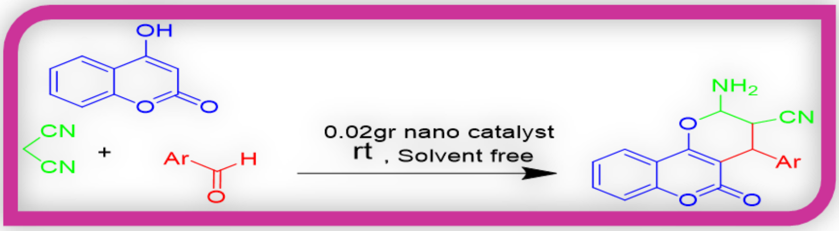

Fig.1. the Synthesis of 3,4-dihydropyrano[c]chromene derivatives by using nano structure catalyst

Referenccces:

[1] N. Azgomi and M. Mokhtary, J. Mol. Catal. A: Chem., 398(2015)58–64.

[2] M. A. Zolfigol, V. Khakyzadeh, A. R. Moosavi-Zare, A. Rostami, A. Zare, N. Iranpoor, M. H. Beyzavie and R. Luque, Green Chem., 15(2013)2132-2140.
[3] K. Niknam, A. Piran Green and Sustainable Chem., 3(2013)1-8.

Esterification of oleic acid with ZrO_2/SO_4^{2-}@MIL-101(Cr) catalyst for biodiesel production

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Abstract:
Biodiesel production is one of the promising ways of saving fossil fuels as it's a renewable and environmentally friendly source of energy which can be produced domestically [1]. In addition to lowering the risk of global warming, biofuel can lead the world to a stable economy while reducing health problems [2]. Esterification and transesterification are two consecutive reactions that can produce FAME or biodiesel from FFA content of edible and non-edible oils such as vegetable oils, animal fats, Karanja, jatropha, and even waste cooking oil. The most common alcohol that is used widely for this process is methanol, which is a short chain and polar and it's relatively cheaper than other alcohols [1]. Esterification is a reversible reaction and it's catalyzed by different kind of homogenous and heterogeneous catalysts. This study aims to present a composite as a solid acid catalyst. MIL-101(Cr) is used as a support for sulfated zirconia in order to improve the %FFA Conversion and also to prevent leaching of sulfate groups. Different factors such as temperature, time, oil to methanol molar ratio, the concentration of catalyst that affect this reaction have been observed and the optimum condition is provided. MIL-101(Cr) and ZrO_2/SO_4^{2-} have shown less catalytic activity compared to synthesized composite under atmospheric pressure. No significant reduction in catalyst activity is seen up to the third cycle.

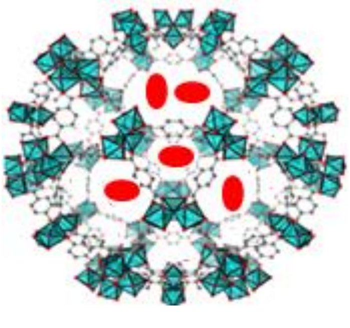

Fig.1. ZrO_2/SO_2^-@MIL-101(Cr)

References:
[1] Kaddour, Mohamed, "Esterification of free fatty acid by selected homogeneous and solid acid catalysts for Biodiesel Production" Thesis, The University of Western Ontario, 2106.
[2] Sani, Yahaya Muhammad, Wan Mohd Ashri Wan Daud, and AR Abdul Aziz. "Activity of solid acid catalysts for biodiesel production: a critical review." Applied Catalysis A: General 470 (2014) 140-161.

Nanoliposome-encapsulated Preyssler Heteropolyacid: Synthesis, Characterization and Invitro Inhibitory Effects on MDA-MB 231 cells

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Abstract:

Breast cancer is the second leading cause of death in Women of the World. And Chemotherapy is one of the most common and most powerful forms during the illness of breast cancer patients. While the chemotheraphy is powerful to kill growing cancer cells, it also can harm healthy cells. In the current study Nanoliposome-encapsulated Preyssler heteropolyacid with diameters of 230-250 nm has been synthesized and characterized by different instrumental techniques. The nanoliposomes were nearly spherical, with entrapment efficiency 53.8%. In vitro antitomur activity of the synthesized nanoliposomes has been investigated using the MTT method on MDA-MB 231 cells Our findings showed enhanced anticancer activity and selectivity for nanoliposome-encapsulated Preyssler (NLEP) compared with Tamoxifen as a commercially drug at 72 h. The present study clearly shows the potential of nanoliposomes as drug carriers for Preyssler. NLEP is a suitable device for an antitumoral drugs application.

References:

[1] Y. Shimizu et al, Jpn. J. Radiol., 36(8) (2018) 511–518.

[2] E. J. Walker et al., Stroke, 43(7) (2012) 1925–1930.

Synthesis, photochemistry and photosensitizing properties of metallophthalocyanines bearing spiropyrrolizidine oxindoles

Application of modified nanoporous anodic alumina as adsorbent for solid phase extraction of Cr(VI)

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Abstract:

Nanoporous anodic alumina (NAA) is a self-organized material with nanopore arrays. The porous structure can be altered by varying anodization processing parameters and the resulting porous shapes can be tailored with specific pore diameters [1]. NAA has been used in several fields of nanotechnology [2]. In this work, a nanoporous anodic alumina was prepared and used for the solid phase extraction (SPE) of Cr(VI). The metal ion was adsorbed on modified NAA as its complex with 1,5-diphenylcarbazide, then eluted using a mixture of ethanol/HCl and determined by spectrophotometry. The modified NAA was characterized by FT-IR, FE-SEM, EDX analysis and mapping and AFM. The influence of important parameters on the formation of NAA and SPE method such as surface area of aluminum foil, applied voltage, activator acid, pH, type and concentration of eluent as well as adsorption and desorption time was investigated and optimized. Under optimum conditions, the extracted analyte was quantified by UV–Vis spectrophotometry with a detection limit of 1.1 ng mL^{-1} for Cr(IV). This new method was successfully applied to determine Cr(VI) in environmental samples.

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[2] M. F. Shaffei, A. M. Awad, H. S. Hussein and M. S. Mohammed, ARPN Journal of Engineering and Applied Sciences, 10(18)(2015) 7983- 7990.

Pseudo Jahn-Teller Effect in Si_4X_4 (X=F, Cl, Br, I) molecules: A theoretical investigation

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Abstract:

The variability of planar rings in Si_4X_4 (X = F, Cl, Br, I) molecules caused by the pseudo-Jahn–Teller impact (PJTE) was evaluated as an original PJTE work. Optimisation and the following frequency calculations in these molecules illustrated that in high-symmetry planar (with D_{4h} symmetry) geometry, all of these compounds were unstable and their structures were puckered to lower C_{2h} symmetry stable geometry. Furthermore, the vibronic coupling interaction between $^1A_{1g}$ ground and the first ^1E_g excited states through $(^1A_{1g} + ^1E_g) \otimes e_g$ PJTE problem was the cause of non-planarity of the four-member ring and the symmetry breaking phenomenon in those series. The calculated gaps (Δ) between the ground state and the E_g excited state, the vibronic coupling (F) and ground state primary force constant values (k_1) were obtained from the numerical fitting of the ground state adiabatic potential energy surface with the analytical expressions of these molecules. Finally, natural bond analysis (NBO) was used for the design of the strongest interaction and natural atomic charges of these structures.

These values are increasing with decreasing of electronegativity of substituent. It can be found a good linear correlation between E_{JT} and Pauling electronegativity (χ_P) of halogens:

$$E_{JT} = -4.6028\ \chi_P + 22.755; \qquad R^2 = 0.9609$$

Therefore, there is stronger Jahn-Teller effect in the less electronegative halogens.

References:

[1] S. Inoue, J. D. Epping, E. Irran, M.Driess, J. Am. Chem. Soc. , 133, 8514 (2011)
[2] I. B. Bersuker, Chem. Rev., 113, 1351 (2013).
[3] I. B. Bersuker, The Jahn-Teller Effect Cambridge University Press: Cambridge, UK 2006.

Post-synthetic modification of IRMOF3 metal-organic framework via Schiff base vanadium complex as catalyst for epoxidtion of allyl alcohols

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Abstract:

Catalytic epoxidation of allyl alcohols is an important synthetic method for both industry and academics [1]. Many transition metal complexes have been used as catalyst for highly selective epoxidation. Among them oxovanadium Schiff base complexes are effective for regioselctive epoxidation of allyl alchols [2]. Due to easier recovery of reaction catalyst in the heterogenous processes, most efforts have been focused on heterogenization of homogenous catalysts. Metal-organic frameworks (MOFs) are crystalline, infinite networks assembled by the bonding of metal ions with polyfunctional organic molecules. MOFs are good candidates for immobilization of catalytically active complexes. in this work IRMOF3 has been synthesized and modified by binding a Schiff base ligand derived from terephetaldehyde and histidine followed by complexation with vanadylsulphate. The success of the postsynthetic modification was assessed by elemental analysis, FT-IR, xrd , BET and SEM techniques. The prepared catalyst successfully catalyzes the epoxidation of geraniol, trans-2-hexen-1-ol and 1-octen-3-ol with 100% conversions and 100% selectivities. The satability and reusability of the catalyst is considerable.

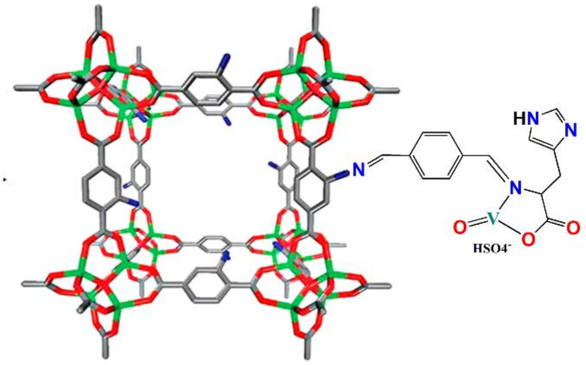

Fig.1. IRMOF3 modified VO Schiff base complex

References:

[1] T. Luts, R. Frank, W. Suprun, S. Fritzsche, E.H. Hawkins, H. Papp, Journal of Molecular Catalyst
273 (2007) 250.
[2] K.A. Jørgensen, Chemical Reviews 89 (1989) 431.
[3] S. Daliran, A. Santiago-Portillo, S. Navalón, A.R. Oveisi, M. Álvaro, R. Ghorbani-Vaghei, D. Azarifar, H. García, Journal of Colloid and Interface Science, 532 (2018) 700.

Antimicrobial activity and thermal analysis of some new zinc halide/pseudohalide complexes

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Abstract:
Schiff bases among the most widely utilized chelating ligands in the development of coordination chemistry. Schiff base compounds containing an imine group (–RC=N–) are usually formed by the condensation reaction between a primary amine and an active carbonyl. Because of the possible variety of the initial reactants for the synthesis of Schiff bases ligands, these compounds show a wide variety of chemical structures with different physicochemical properties[1].

In this research, a new symmetric bidentate Schiff base (L) (bis[3-(4-methoxyphenyl)propenaldehydene)]-1,4-buthanediamine and its zinc complexes with general formula of $ZnLX_2$ (X= chloride, bromide, iodide, nitrate, thiocyanate, azide and nitrate) have been synthesized under ultrasonic conditions. The ligand and its complexes have been characterized by molar conductance measurements, FT-IR, ^{1}H and ^{13}C NMR, UV-Visible spectroscopy and thermal analysis. X-ray powder diffraction and scanning electron microscopy techniques confirmed nanostructure size for these zinc complexes. All the newly prepared compounds were screened for their antimicrobial activities, against four bacterial and two fungal strains using disk diffusion and serial dilution methods. ZnO nanoparticles were prepared by direct calcination process of zinc halide complex at 600°C under air atmosphere.

References:

[1] B. P. Baranwal, K Tripathi, A. K. Singh, S. Tripathi, Spectrochim. Acta A 91 (2012) 36.
[2] M. Montazerozohori, S.A. Musavi, J. Coord. Chem. 61 (2008) 393.

Investigation of the effect of H-ZSM-5 zeolite synthesized by various sources of silicon on the conversion of methanol to propylene (MTP)

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Abstract:

Conversion of methanol, produced from natural gas or coal, to liquid hydrocarbon by zeolite catalysts can be a promising way to save oil reserves(1). According to the literature, H-ZSM-5 zeolite has better performance in the MTP process (2, 3). In this work H-ZSM-5 zeolite catalyst (Si/Al=200) was synthesized by hydrothermal method from various sources of silicon, including Ludox (LHZ), Silicic acid (SHZ), and tetraethyl orthosilicate (THZ). The samples characterization were confirmed using X-ray diffraction (XRD) analysis and fourier-transform infrared (FT-IR) spectroscopy. The relative crystallinity (4) and particle size were compared. Also, LHZ sample characterized by scanning electron microscopy (SEM) and Brunauer–Emmett–Teller (BET) measurements. The catalysts evaluation were performed for all samples in a fixed-bed reactor at 480 °C, 1 bar, methanol weight hourly space velocity (WHSV) of 1 h^{-1} and using feed with methanol to water weight ratio of unity. In order to study the effect of temperature and WHSV on the catalyst performance, LHZ sample studied at four temperatures (420, 450, 480, 510 °C) and three WHSV (1, 2, 3 h^{-1}). According to the results obtained from LHZ, SHZ and THZ samples, LHZ with 99.85% methanol conversion and 55.55% propylene selectivity at optimized conditions T=480°C, WHSV= 1h^{-1}, P= 1atm, MeOH/H_2O= 1Wt had the best performance in the MTP process.

References:

[1] W. Wu et al, Chemical Engineering Science 66 (2011) 4722 –4732.
[2] J. Liu et al, Catalysis Communications 10 (2009) 1506–1509.
[3] C. Sun et al, Chem. Commun., 48 (2012) 5787–5789.
[4] J. Shao et al, Microporous and Mesoporous Materials 273 (2019) 122–132.

Thermal behavior, antimicrobial potential of some new synthesized four coordinated mercury complexes

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Abstract:

Schiff bases are the most widely utilized chelating ligands in the development of coordination chemistry of Schiff base ligands containing an imine group are usually formed by the condensation reaction between a primary amine and an active carbonyl. Because of the possible variety of the initial reactants for the synthesis of Schiff bases ligands, these compounds show a wide variety of antibacterial and anticancer activities, catalysts and luminescent properties [1, 2].

In this study, six new mercury-Schiff base compounds formulated as $HgLX_2$ (L is a new N_2-Schiff base ligand derived from 1,2-diaminopropane and 4-methoxyphenyl propenal and X is (Cl^-, Br^-, I^-, N_3^-, NCS^-, and NO_3^-) were synthesized and characterized by Fourier transform infrared, ^1H and ^{13}C NMR, UV–visible, thermal analyses, and molar conductivity measurements. Mercury complexes have been also prepared in nanostructure sizes under ultrasonic irradiation confirmed by X-ray powder diffraction and scanning electron microscopy. Antibacterial/antifungal activities of the compounds were screened by the disk diffusion method against the Gram-negative bacteria and the Gram-positive bacteria. The results showed remarkable ability of some mercury complexes for DNA cleavage.

References:

[1] M.B. Halli, R.B. Sumathi, Journal of Molecular Structure 1022 (2012) 130.
[2] M. Montazerozohori, S. A. Musavi, A. Masoudiasl, Spectrochim.Acta Part A 137 (2015) 389.

Vanadium complex supported on functionalized diatomite and investigation of its catalytic properties.

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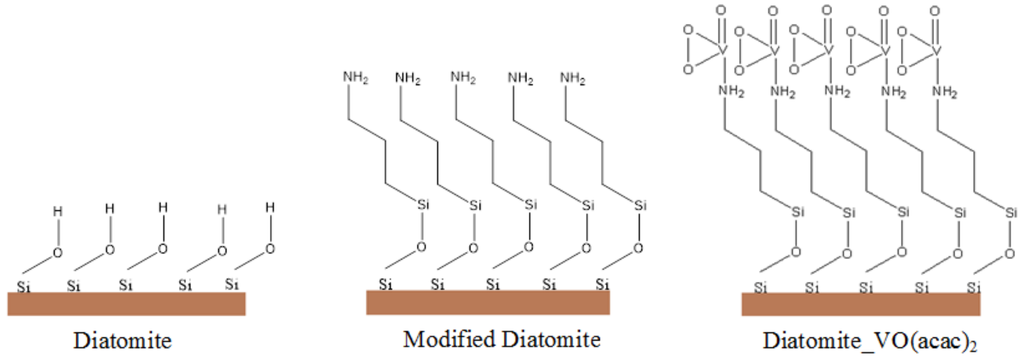
Abstract:

Diatomites are silica based porous material has been attracted attention as support material due to its chemical stability, highly porous structure, high specific surface area and low cost. Due to the porous structure and good surface area, diatomite is considered as a catalyst support[1]. In this study diatomite nano-particles were synthesized by sedimentary method and then For the preparation of amine functionalized Diatomite was refluxed with 3-(tri-methoxysilyl) propylamine (MSPA) for 20 h. VO $(acac)_2$ was then supported onto the resulting product and heterogeneous catalyst Diatomite/VO$(acac)_2$ was prepared. The new catalyst was characterized by FT-IR, XRD, SEM, ICP, BET and EDX. Epoxidation of alkenes is one of the most important chemical processes, the products of this reaction are used as a precursor for the synthesis of many chemicals and pharmaceuticals as well as for the production of many valuable materials including epoxy resins, paints and surfactants [2]. Modified diatomite were used to support bis-acetylacetonato-oxo vanadium complexes in alkene epoxidation. The various parameters such as type of solvent, time, amount of catalyst, and type of oxidant were optimized for this reaction. The optimum conditions were found as 20 mg catalyst in dichloroethane with t-BuOOH as oxidant which gives 98% yield during 180 minutes.[1,2]



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References:

[1] F. Akti, Applied Surface Science, (2018) doi: 10.1016/ j.apsusc.2018.06.019
[2] N. Mizuno, K. Yamaguchi, K. Kamata, Coordination chemistry reviews, 249 (2005) 44-56.

Chemical Activation of Kaolin under Acid and Alkaline Conditions

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Abstract:

In this study chemical activation of kaolin under acid and alkaline conditions was investigated. For this purpose the natural kaolin was heated in a furnace until the metakaolin was formed. Then this reactive kaolin was used for chemical activation. For increasing or decreasing of silica or alumina contents, metakaolin was leached by acids and alkaline [1,2]. The extraction of aluminum and silicon was done by HF and NaOH. After calcination, the percentages of alumina and silica were reached to 41% and 54%, respectively. For reducing silica content and producing higher alumina materials, metakaolin was leached by caustic soda solution at 100 °C. Consequently, the amount of alumina and silica reached to 46% and 48%, respectively. In order to increase the silica content in kaolin, metakaolin has been leached by HF diluted solution at room temperature, in which the amount of alumina and silica reached to 35% and 61%, respectively. In particular, the treated kaolin in this way could be used as raw material to produce zeolite 4A or as a valuable additive in concrete. The XRD patterns of kaolin, metakaolin and leaching process with NaOH were presented in Fig 1: a-c.

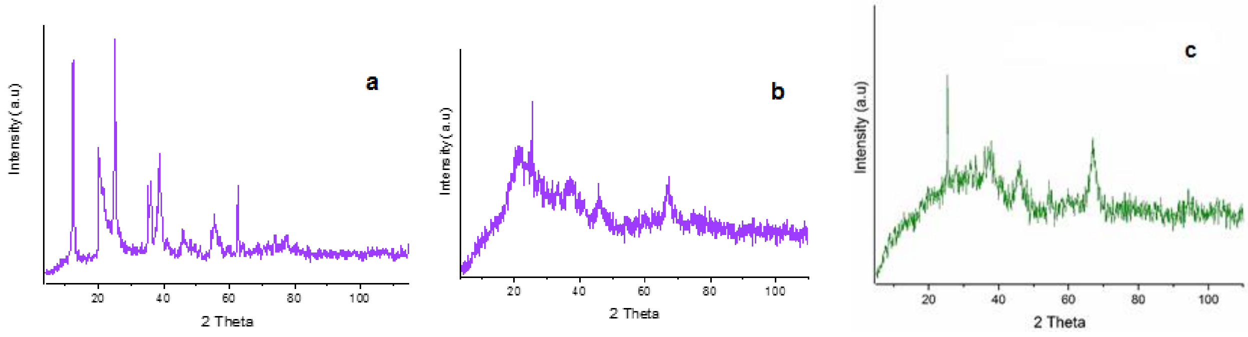

Fig.1

References:

[1] L. Heller-Kallai, "Developments in clay science: handbook of clay science," Thermally Modified Clay Minerals, Elsevier, Oxford, 2006.

[2] F.Hussin, M.K.Aroua, and W. M. A.W. Daud, Chemical Engineering Journal, 170(1) (2011) 90-106.

Synthesis and biologic properties of macroacyclic Schiff-base ligand contaning piperazine and pyridine moieties and corresponding Zn(II) and Cd(II) complexes

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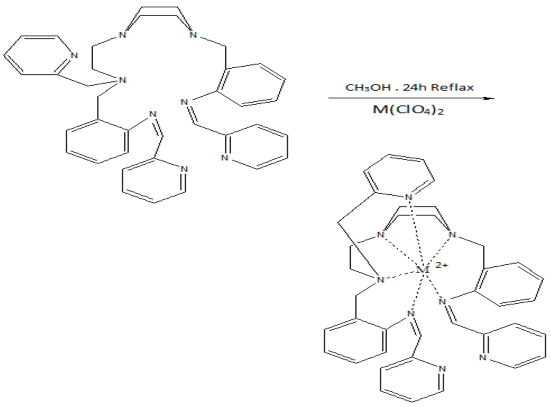
Abstract:
In this paper, the new polyamine 2-((4-(2-((2-aminobenzyl)(pyridin-2-ylmethyl)amino)ethyl)piperazin-1-yl)methyl)aniline (A) was synthesized by the reaction of 2-aminoethylpiperazine with 2-formylpyridine and 2-nitrobenzylchloride. IR spectrum of polyamine exhibit a ν(NH_2) vibration in 3213-3339 cm^{-1}. The mass spectrum of polyamine A shows the peak at 431 m/z that confirm the synthesis of polyamine A. The Schiff base ligand potentially octadentate (L) was prepared from condensation of 2-formylpyridine with polyamine (A). IR spectrum of ligand exhibit a ν(C=N) vibration in 1617 cm^{-1}. The mass spectrum of ligand (L) shows the peak at 609 m/z that confirm the synthesis ligand. From direct reaction of this ligand and Zn(II) and Cd(II) metal ions in methanolic solution four macroacyclic Schiff-base complexes were prepared. The IR spectra of the complexes show the band of ν(C=N) in the 1608 cm^{-1}, which is shifted to lower frequency ongoing from the free ligands. The mass spectra of complexes show the peaks at 675 and 724 m/z that confirm the synthesis of complexes. The elemental analysis and ^1H and ^{13}C NMR confirm the synthesis of products. Furthermore the antioxidant properties of polyamine (A), ligand (L) and its corresponding complexes were investigated [1-2].



References:
[1] M. Rezaeivala, H. Keypour, Coord. Chem. Rev. 280 (2014) 203.
[2] Keypour, M. Mahmoudabadi, A. Shooshtari, M. Bayat, M. R. Karamian, M. Asadbegy, R. William Gable, Inorg. Chim. Acta, 478 (2018)176.

Synthesis and characterization of new palladium(II) complex derived from new phosphonium ylide and investigation of its catalytic activity

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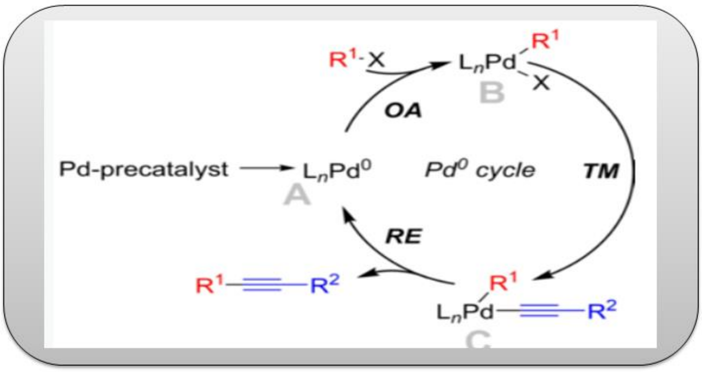
Abstract

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



References:

[1] G,Wittig, and D.Krauss, Liebigs Ann., 697 (1964) 34.
[2] S.J.Sabounchei, A.Sedghi, M.Bayat, M.Hosseinzadeh, A.Hashemi, A.Yousefi, R.W.Gable, J. Mol. Struct., 346 (2019) 1175.
[3] S.J.Sabounchei, M.S.Hashemi, R.Karamian, S.H.Moazzami Farida, P.Gohari Derakhshandeh, R.W.Gable, K.J.Van Hecke. Coord. Chem., 71 (2018) 3277.

[60]Fullerene-based Pt(0) complexes of phosphorus ylide, Efficient Nanodrugs as new anticancer agents

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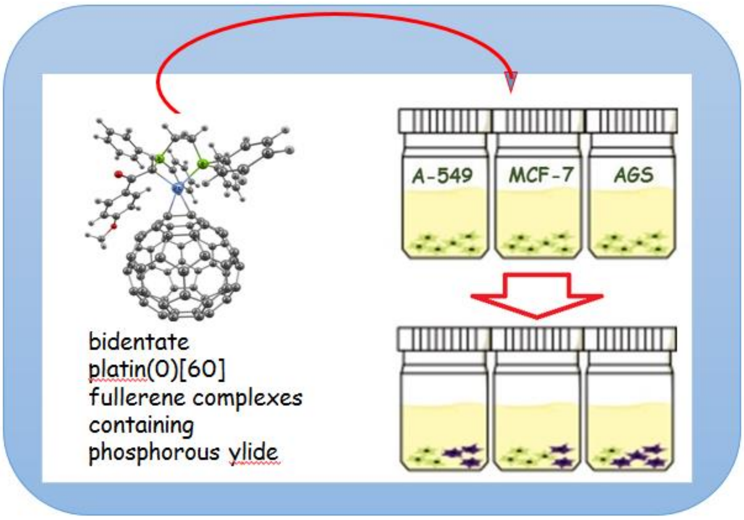
Abstract

In the past two decade, there has been considerable interest in the synthesis, structure, and properties of the transition metals compounds, in which the C_{60} cage is attached to organometallic groups to form corresponding π-complexes [1]. This work reports the synthesis and catalytic properties of new bidentate platin(0)[60] fullerene complexes, prepared by reaction of α-keto stabilized phosphorus ylides $[P_2R_4{=}C(H)C(O)C_6H_4\text{-}p\text{-}R]$ (R = OMe, NO_2 (Y^1, Y^2)), C_{60} and $Pt_2(dba)_3$ (dibenzylideneacetone (dba)). The observed coordination mode is orthometalate P,C-coordinated in the case of $[(\eta^2{-}C_{60})Pt(\kappa^2 -Y^1)]$ (1) and $[(\eta^2{-}C_{60})Pt(\kappa^2{-}Y^2)]$ (2) complexes [2]. All complexes have been fully characterized by ^1H, ^{13}C and ^{31}P NMR spectroscopic methods and other conventional techniques such as IR, thermogravimetry and scanning electron microscopy. Additionally, the current study presents evidence that the investigated compounds induce the anti-proliferative effect in the human gastric (AGS), breast (MCF-7), and lung (A549) cancer cells. Our data indicated that the compounds have excellent anticancer due to Pt nature and ligand properties. It should be noted that although all in vitro experiments hold limitations with respects to possible in vivo efficiency, the results are very promising with regards to possible antineoplastic chemotherapy and form a very sound basis for future research.



References:

[1] M.Robledo, NF.Aguirre, S.Díaz-Tendero, F.Martín, M.Alcamí, RSC Adv., 4(2014)53010–53020.

[2] S.J.Sabounchei, K.Badpa, M.Bayat, R.Karamian F.Ghasemlou, Gable, R. W. & Van Hecke, K., Appl. Organomet. Chem, 33(3) 2019 e4658.

New Tetradentate ligand [N, N´- Bis (Quinoline-2- Carboxamide) - 4- Nitrobenzene] and Cobalt Complexes, Synthesis and Characterization

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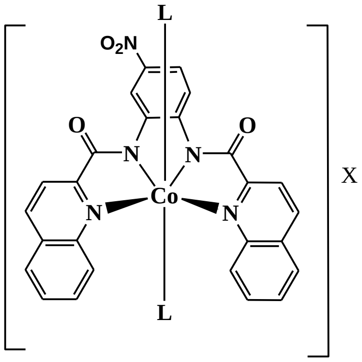
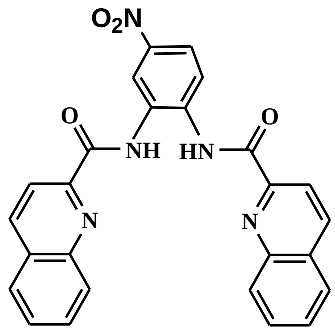
Abstract:

Some cobalt (III) compounds of the type $[Co^{III}(bqbNO_2)(L)_2]X$, L = N_3^-, pipyridine, morpholine, benzylamine, aniline, pyridoxine, pyrrole and X= ClO_4^- , $(n\text{-}Bu)_4N^+$ with New ligand [H_2bqbNO_2 = N, N´- Bis (Quinoline - 2 – Carboxamide) - 4- Nitrobenzene] have been synthesized and characterized by IR and UV–Vis spectroscopy. This ligand is a dianionic tetradentate, furnishing a N_4 set, such that two N atoms of the two pyridine rings and two amido N atoms occupy four equatorial positions, thus deprotonated ligand is a strong σ-donor capable of stabilizing metal ions in high oxidation states. One goal of this project is synthesis of new compounds with using of method ionic liquid as a solvent in which the reaction can be to reduce pollution, high speed and without the use of harmful solvents could be mentioned. Green chemistry searches for environmentally friendly reaction media and strives to increase the reaction rate and efficiency. One of the key is the replacement of hazardous solvents with Ionic liquids [1].

Amide linkages in a biochemical context are called peptide linkages and constitute a defining molecular feature of proteins. Low molecular weight amides, such as dimethylformamide is common solvent and many drugs and dyes, such as penicillin, folic acid, barbiturates and indigo, are amides too. Metal complexes of many amido ligands have been extensively used to mimic the properties of biologically active systems, use in catalysis and for selective binding of the toxic metal ion or as building blocks of new functional metal complexes [2, 3].



trans-$[Co^{III}(bqbNO_2)(L)_2]X$



H_2bqbNO_2

References:

[1] S. Meghdadi, M. Amirnasr, V. Langer, A. Zamanpour, Can. J. Chem. 84 (2006) 971.
[2] S. Meghdadi, K. Mereiter, M. Amirnasr, F. Karimi, A. Amiri, Polyhedron. 68 (2014) 60.
[3] S. Meghdadi, K. Mereiter, N. S. Mohammadi, A. Amiri, Polyhedron. 29 (2010) 2225.

Supported organometallic palladium catalyst into mesoporous channels of magnetic MCM-41 nanoparticles for phosphine-free C-C coupling reactions

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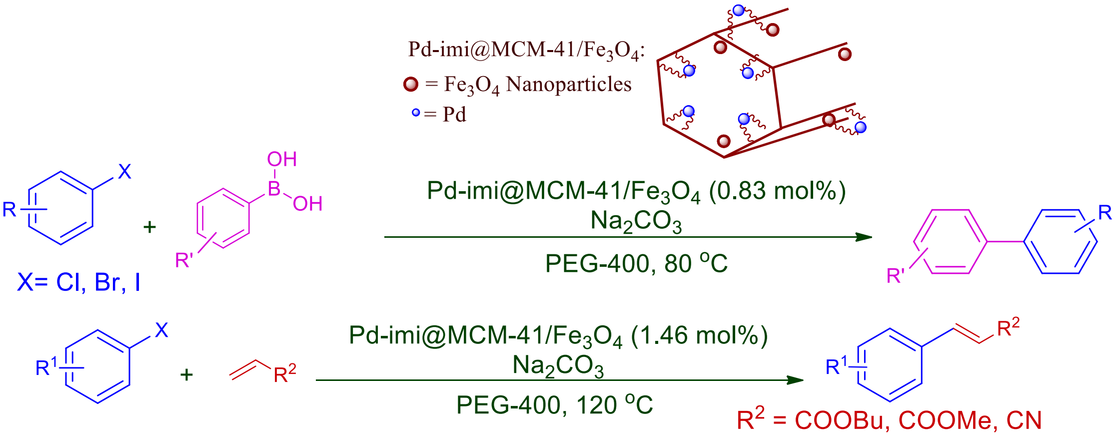
Abstract:

Magnetic MCM-41 nanoparticles were synthesized *via* Fe_3O_4-doped into mesoporous channels of MCM-41 nanoparticles and further, a new organometallic complex of palladium was supported on its inner surface (Pd-imi@MCM-41/Fe_3O_4). This catalyst was applied as highly efficient and magnetically recoverable nanocatalyst in the various C-C coupling reactions under phosphine-free conditions at atmospheric pressure. This catalyst has advantages of both magnetic nanoparticles and mesoporous materials. The structure of this catalyst has been characterized N_2 adsorption–desorption isotherms, TEM, SEM, EDS, WDX, FT-IR, XRD, TGA, ICP, AAS, and VSM techniques. SEM images of this catalyst demonstrate that the particles size are less than 100 nm. VSM curve of the catalyst shows that this catalyst can be recovered using an external magnet; therefore, this catalyst can be reused for several times without significant loss of its catalytic efficiency. Also, all products were obtained in high TON and TOF numbers, which reveals this catalyst has high activity and selectivity in described coupling reactions. Heterogeneity and stability of this nanocatalyst were confirmed by hot filtration test and AAS technique. the selectivity of this catalytic system was confirmed by coupling of 1-bromo-4-chlorobenzene and aryl halides bearing –OH and –NH_2 functional groups with phenylboronic acid.



References:

[1] B. Karimi, D. Enders, Org. Lett. 8 (2006) 1237-1240. DOI: 10.1021/ol060129z

[2] Y.D. Lahneche, A. Lachguar, C. Mouton, J.C. Daran, E. Manoury, R. Poli, M. Benslimane, A. Labande, E Deydier, Inorganica Chim. Acta 492 (2019) 91-97. DOI: 10.1016/j.ica.2019.04.021

Magnetic MCM-41 nanoparticles as support for immobilization of organometallic catalyst of palladium and its application in C-C coupling reactions

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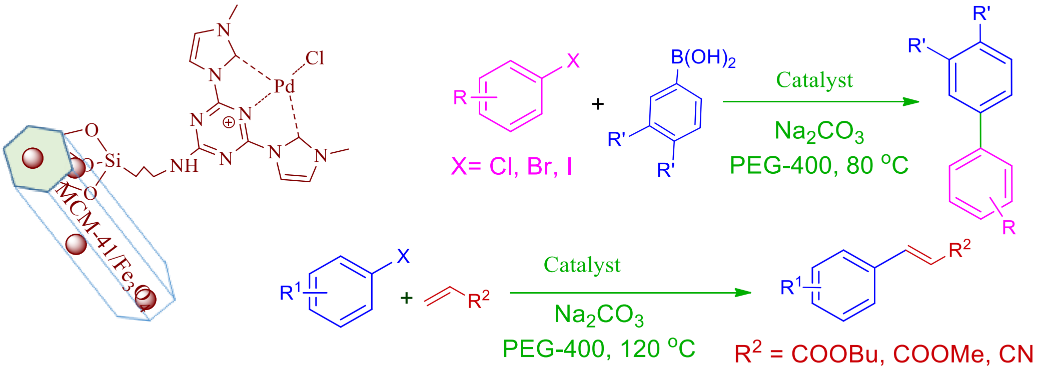
Abstract:

In this work, surface of magnetic MCM-41 nanoparticles were modified by 3-aminopropyltriemtoxysilane and further 1-methyl imidazole anchored on its surface using cyanuric chloride as linker. Then, palladium nanoparticles were immobilized on the its surface (Pd-imi-CC@MCM-41/Fe_3O_4) and further was studied as magnetically recyclable nanocatalyst in carbon-carbon coupling reactions between wide range of aryl halides with butyl acrylate, methyl acrylate, acrylonitrile, phenylboronic acid, and 3,4-diflorophenylboronic acid under phosphine-free ligand and air atmosphere. This catalyst has advantages of both Fe_3O_4 nanoparticles and mesoporous MCM-41. Catalyst structure was characterized using SEM, EDS, WDX, N_2 adsorption–desorption isotherms, XRD, TGA, FT-IR, and AAS techniques. All products from carbon-carbon coupling reaction were obtained with excellent yields and high TON and TOF values, which were indicate the high efficiency and catalytic activity of this catalyst. This catalyst was shows a good selectivity in C-C coupling reactions. Heterogeneity and stability of Pd-imi-CC@MCM-41/Fe_3O_4 was studied by AAS technique, leaching test and poisoning test.



References:

[1] B. Karimi, D. Enders, Org. Lett. 8 (2006) 1237-1240.

[2] Y.D. Lahneche, A. Lachguar, C. Mouton, J.C. Daran, E. Manoury, R. Poli, M. Benslimane, A. Labande, E Deydier, Inorganica Chim. Acta 492 (2019) 91-97.

[3] A. Ghorbani-Choghamarani, B. Tahmasbi, R. H.E. Hudsonb, A. Heidarib. Microporous Mesoporous Mater. 284 (2019) 366–377.

Nickel immobilized on boehmite nanoparticles as a high efficient and recyclable catalyst for organic reactions

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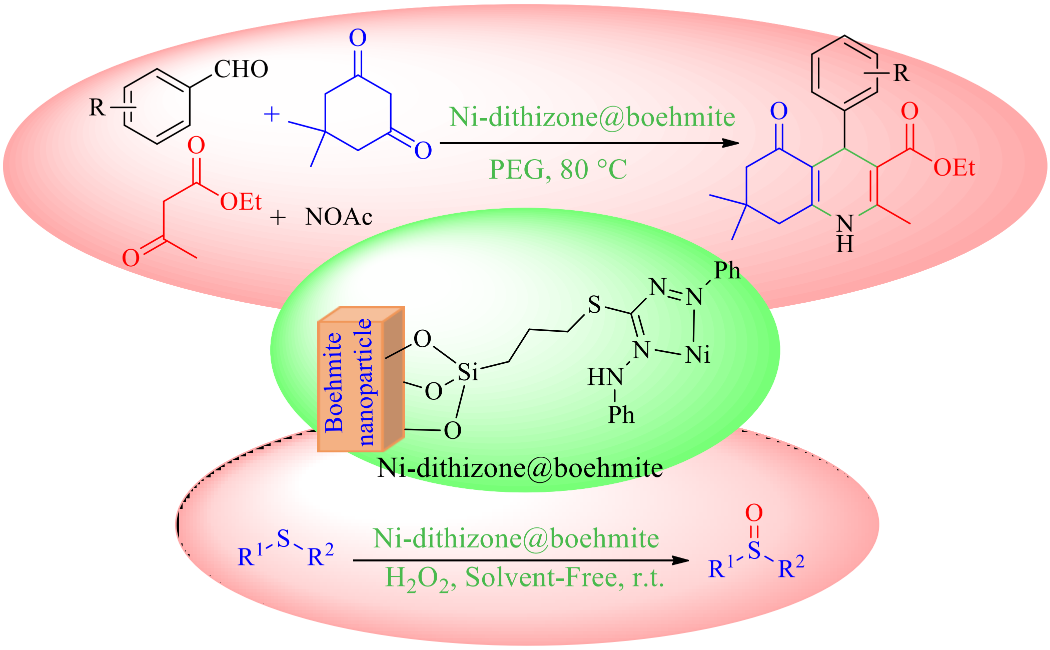
Abstract:

In this work, in the first stage, boehmite nanoparticles were easily fabricated *via* addition of NaOH solution to a solution of $Al(NO_3)_3.9H_2O$ at room temperature in water. Then, Nickel-dithizone catalyst was supported on boehmite nanoparticles (*Ni*-dithizone@boehmite). *Ni*-Dithizone@boehmite is a low-cost, nontoxic, and recoverable catalyst, which provides an environment friendly reaction conditions. In the second stage, catalytic activity of this catalyst was studied in the synthesis of polyhydroquinoline derivatives and selective oxidation of sulfides to sulfoxides. The reactions not require very high temperatures or inert atmosphere. The developed heterogeneous catalyst could be easily separated by centrifugation and recycled for several runs without leaching of Nickel from the surface of the catalyst or significant loss of its catalytic activity.



References:

[1] K. Bahrami, M.M. Khodaei, M. Roostaei, New J. Chem. 38 (2014) 5515-5520.
[2] A. Ghorbani-Choghamarani, B. Tahmasbi, P. Moradi, RSC Adv. 6 (2016) 43205-43216.
[3] X.Y. Chen, H.S. Huh, S.W. Lee, Nanotechnology 18 (2007) 285608-285612.

Synthesis of new octa-nuclear cubic cage of Cu-Mo as a precursor for the synthesis of $CuMoO_4$ nanoparticles

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Abstract:

Within the last two decades, the communicative design and synthesis of inorganic–organic composite materials based on polyoxometalate (POM) building blocks have been attracting great interest, not only in terms of structural versatility but also because of promising applications in the area of adsorption [1], catalysis [2], gas-sorption [3], and magnetism [4,5]. A new coordination polymer of polyoxomolybdate,$\{[Cu_4(phen)_8Mo_4O_{18}]\cdot(H_2O)_4\}$ (**1**) (phen = 1,10-phenanthrolin), has been synthesized under solvothermal reaction, This compound was characterized by elemental analysis, single-crystal X-ray diffraction, IR spectroscopy, UV-vis spectroscopy, cyclic voltammetry and thermal gravimetric analysis (TGA). Single-crystal X-ray analysis reveals that the structure contains a neutral bimetallic $\{Cu_4Mo_4\}$ cluster as the secondary building unit. The thermal stability of compound **1** has been studied by TGA. $CuMoO_4$ nano-structures also were simply synthesized by direct calcination of the single crystals and nano-sized compound **1** at 400 and 600 ^{0}C. The semiconducting properties of these solid-state compounds was revealed from the measurements of the diffuse reflectance UV-vis spectra, in which the band gap values at ca. 2.8 eV are similar to inorganic semiconductor materials, suggesting potential applications in areas of photocatalysis and light-to-electricity conversion.

References:

[1] K. Biradha, M. Fujita, A springlike, Angew. Chem. Int. Ed. 41 (2002) 3392–3395.
[2] Abedi, A. Morsali,, ACS Catal. 4 (2014) 1398–1403.
[3] K. Akhbari, A. Morsali, Dalton Trans. 42 (2013) 4786–4789.
[4] A. Caneschi, D. Gatteschi, N. Lalioti, C. Sangregorio, R. Sessoli, G. Venturi, A. Vindigni, A. Rettori, M.G. Pini, M.A. Novak, Angew. Chem. Int. Ed. 40 (2001) 1760– 1763.
[5] M.A.M. Abu-Youssef, A. Escuer, D. Gatteschi, M.A.S. Goher, F.A. Mautner, R. Vicente, Inorg. Chem. 38 (1999) 5716–5723.

Synthesis and characterization of a novel mixed-ligand diorganotin(IV) complex as a precursor for the fabrication of an organic light emitting diode

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Abstract:

A new mixed-ligand diorganotin(IV) complex, [μ-(4-dpe){$Me_2Sn(cup)_2$}$_2$] (1), was synthesized by reacting dimethyltin(IV) dichloride with 1,2-di(4-pyridyl)ethylene (4-dpe) and ammonium N-Nitroso-N-phenylhydroxylamine (cup). The prepared complex was fully characterized by PXRD, ^{1}H, ^{13}C and ^{119}Sn NMR, IR, and UV spectra and elemental analysis (CHN). The solid-state structure of 1 was also investigated *via* single crystal XRD. By considering the obtained structural parameters, complex 1 consists of centrosymmetric binuclear units that crystallize in the monoclinic system with the space group of $P2_1/c$. Thermal behavior of prepared coordination compound was examined under air atmosphere by thermogravimetric and differential thermal analysis (TGA and DTA). The study of thermal behavior and luminescence properties of prepared diorganotin(IV) complex showed that this compound has the necessary conditions for its use as a precursor in the manufacture of optical devices. The prepared coordination compound was doped into a PVK:PBD blend in two different concentrations as a light emitting material in the fabrication of two organic light-emitting diodes (OLEDs).

References

[1] S.Chang, C.Fan, C.Lai, Y.Chao, S.Hu,. Surf . Coat .Tech. 200 (2006) 3289-3296.
[2] J.Devi, S.Pachwania, Inorg. Chem. Commun. 91 (2018) 44-62.
[3] L.A.Moreno, J. Vis. Exp. 63 (2012) 3066-3070.

Structural optimization of two isoreticular pillared-layer metal-organic frameworks to pore-size-dependent catalytic activity and selective CO_2/N_2 affinity

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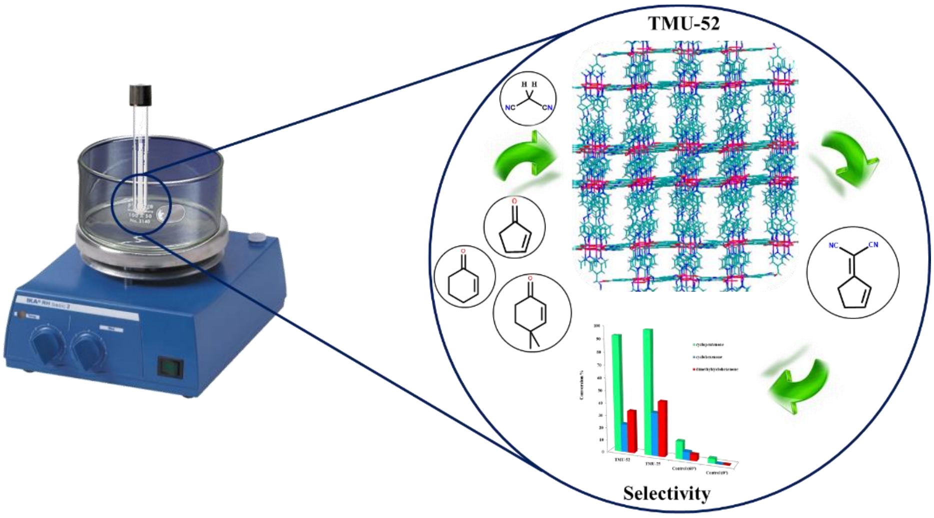
Abstract:

Among different type of MOFs, Pillar-layered Metal Organic Frameworks (PMOFs) [1] are widely studied due to their simple fabrication and structural diversity. Herein, we have synthesized a novel pillared-layer MOF, [Zn(L1)(NH2-bdc)].0.5DMF (TMU-52) by incorporating two different organic linkers, namely 2-aminoterephthalic acid as an oxygen-donor linker and L1 (N4,N4'-bis(pyridin-4-ylmethylene)-phenyl-4,4'-diamine) as a long pillaring linker. The structure of this framework which is isoreticular to our recently reported TMU-25, [Zn(NH2-bdc)(L2)].2DMF, was analyzed using X-ray crystallography, FT-IR spectroscopy, Thermogravimetric and elemental analyses. These two metal-organic frameworks are interesting candidates for comparative size selective catalytic performances. In spite of having the same network topology, the pillaring linkers are different in length and subsequently they provide different frameworks with different pore sizes. The selectively of TMU-52 toward different substrate, as a heterogeneous catalyst in aldol-type condensation reaction was significantly higher than TMU-25.



References:

[1] F. Zarekarizi, M. Joharian, A. Morsali, J. Mater. Chem. A, 6 (2018) 19288-19329.

A microporous functionalized metal-organic framework as a new fluorescent probe for selective sensing of metal cations

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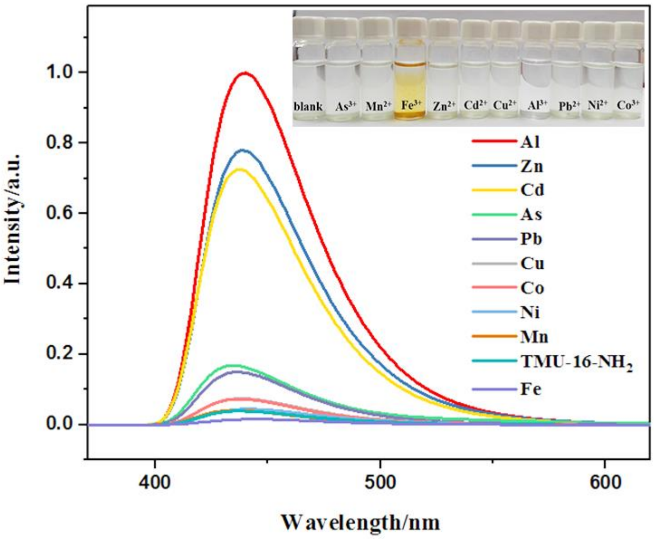
Abstract:

Nowadays metal-organic frameworks with multiple luminescent centers are very fascinating as multifunctional luminescent material because of their luminescence properties, which could be systematically tuned by deliberate use of organic ligands and metal ions [1]. In this research, a two-fold interpenetration pillared-layer amine/imine-functionalized MOF known as TMU-16-NH_2, $[Zn_2(NH_2\text{-}BDC)_2(4\text{-}bpdh)].3DMF$, have been synthesized via a mixed ligand approach using amino-1,4-benzenedicarboxylate (NH_2-BDC) and 2,5-bis(4-pyridyl)-3,4-diaza-2,4-hexadiene (4-bpdh) under solvothermal condition [2]. Sensor TMU-16-NH_2 exhibits Al^{3+}-selective TURN-ON and Fe^{3+}-selective TURN-OFF type fluorescence emission responses, for which the electrostatic interaction between Fe^{3+} and Al^{3+} ions and the inner surface of the micropores may play a critical role. Moreover, the sensor TMU-16-NH_2 shows significantly color change from light yellow to orange and colorless with the addition of Fe^{3+} and Al^{3+} ions, respectively, which is distinguish by naked-eye.



References:

[1] M. Allendorf, C. Bauer, R. Bhakta, R. Houk, Chemical Society Reviews, 38 (2009) 1330-1352.
[2] V. Safarifard, A. Morsali, CrystEngComm, 16 (2014) 8660-8663.

Palladium Supported Mesoporous Silica Nanoparticles as an Efficient Nanocatalyst for the Suzuki Reaction in the Green Reaction Medium

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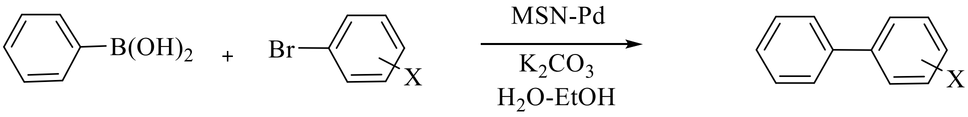
Abstract:

Mesoporous silica materials are important composites because of their wide applications in various fields. Based on the synthesis method and directing agent template, various mesoporous silica compounds have been fabricated and categorized as M41S, SBA, MSU, etc. M41S family is included MCM-41, MCM-50 and MCM-48 and among them, MCM-41 is the most widely studied mesoporous silica. Mesoporous silica nanoparticles (MSNs) are a type of MCM-41 that have particle sizes under 100 nm with interesting properties such as biocompatibility, controllable particle size or shape and have other features of MCM-41 [1-4].

In the present research work, we have prepared MSNs by base catalyzed sol-gel method and MSN-APS synthesized by reaction of MSN with 3-aminopropyl-3-methoxy silane (APTS). Then a Schiff base containing benzimidazole and its Pd(II) complexes have been supported on MSNs. These MSN-Pd nanoparticles were characterized by several techniques such as FT-IR, LA-XRD, FE-SEM, TEM, EDX, BET and TGA. In view of the wide applications of Schiff bases and their complexes and the unique properties of MSNs, this hybrid composite has been successfully used in Suzuki–Miyaura cross-coupling reactions in green reaction medium.



References:

[1] L.Tahmasbi, T.Sedaghat, H.Motamedi, M.Kooti, J. Solid State Chem., 258 (2018) 517-525.
[2] A.M.Trzeciak, A.W.Augustyniak, Coordin. Chem. Rev., 384 (2019) 1-20.
[3] L.B.d.O. Freitas, L.d.M. Corgosinho, J.A.Q.A. Faria, V.M. dos Santos, J.M. Resende, A.S. Leal, D.A. Gomes, E.M.B.d. Sousa, Microporous Mesoporous Mater., 242 (2017) 271-283.
[4] S. Rahmani, J.-O. Durand, C. Charnay, L. Lichon, M. Férid, M. Garcia, M. Gary-Bobo, Solid State Sci., 68 (2017) 25-31.

Synthesis and Characterization of A New Schiff Base Ligand Containing Dinitrogen and Sulfur Atoms and Its Nickel(II) Complex

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Abstract:

Schiff base ligands containing an azomethine group (–CH=N–) are considered as ‘privileged ligands’ because of their capability to stabilize different metals in various oxidation states. Such complexes have been extensively studied due to synthetic flexibility, selectivity and sensitivity towards a variety of metal ions [1]. Schiff base ligands with sulfur and nitrogen donor atoms in their structures, act as good chelating agents for the transition metal ions because of the presence of both hard nitrogen and soft sulfur donor atoms in the backbones of these ligands. These ligands readily coordinate with a wide range of transition metal ions yielding stable and intensely colored metal complexes [2]. In this work, a new tridentate Schiff base ligand was formed by the condensation of cysteamine and 2-pyridinecarboxaldehyde in methanol and 1:1 molar ratio. In order to synthesize of Schiff base complex a solution of $Ni(OAc)_2.4H_2O$ in methanol was added dropwise to a solution of Schiff base ligand in 1:1 stoichiometry. The mixture was heated with stirring on a water bath at 62 °C for 8 hours. The products were characterized by FT-IR, ^{1}H NMR, UV-Vis spectroscopies, elemental analysis, and conductometry.

References:

[1] B. Shafaatian, A. Soleymanpour, N. Kholghioskouei, B. Notash, S.A. Rezvani, Spectrochim. Acta A 128 (2014) 363-369.

[2] Y.P. Tian, C.Y. Duan, C.Y. Zho, X.Z. You, T.C.W. Mak, Z. Zhang, Inorg. Chem. 46 (2007) 4660-4666.

Intraction of [Cp(CO)$_2$ M≡E] with N-Hetrocyclic carben in [Cp(CO)$_2$ M≡E←NHC(R)]$^+$ complexes [E: Si, Ge, Sn, Pb; M: Cr, Mo, W; R:H, F, Cl, Br, CH$_3$, Ph, dipp, Si(CH$_3$)$_3$. A theoretical study

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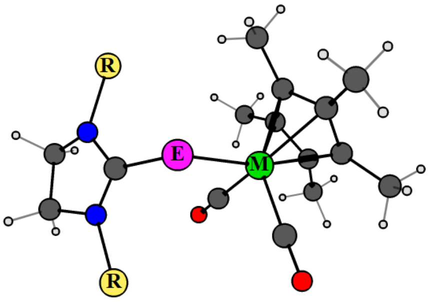
Abstract:

Nowdays, computational chemistry techniques can describe the structure of chemical compounds as well as the nature of chemical bonds with fine accuracy. Theoretical studies including structural, interaction energy, NBO analyze on some N-heterocyclic carbene complexes (NHC) with general formula [Cp(CO)$_2$M≡E←NHC(R)]$^+$ (E: Si, Ge, Sn, Pb; M: Cr, Mo, W; R: H, F, Cl, Br, CH$_3$, Ph, dipp, Si(CH$_3$)$_3$) with M06-2X level using def2-TZVP basis set have been reported. Result showed that the values of interaction energy between NHC(R) and Cp(CO)$_2$ M≡E fragments in the complexes decreased by changing the E atoms from Si to Pb. Also the EDA analyze was used to determine the nature of C→E and M≡E bonds in the complexes with the ADF packages. Results showed that the nature of C→E bond has approximately the same orbital and electrostatic interactions, while the nature of M≡E bond is mainly orbital type.



References:

[1] T.Fukuda, H.Hashimoto, and H. Tobita. J. Organomet. Chem, 848 (2017) 89-94.
[2] K.K.Pandey, M. Lein, and G. Frenking. J. Am. Chem. Soc, 125(6) (2003) 1660-1668
[3] K.K.Pandey and P. Patidar. Polyhedron, 37(1) (2012) 85-93.

Some novel four coordinated nanostructure zinc Schiff base complexes: Thermal behavior and antimicrobial

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Abstract:

Nanometer-size particles of metal coordination complexes enhance their physical and chemical properties that may be due to the large number of surface molecules when are compared with non-nanostructure compounds [1]. Schiff base ligands are considered as very important compounds because of their attractive electronic, chemical, and biological properties [2]. In the last years, most considerable interest has been focused on these compounds, revealing potential applications of them in industrial, medical, biological, and catalysis fields [3].

In this study, a new series of zinc halide/pseudohalide complexes with a novel Schiff base ligand containing 1,3-propanediamine and 3-(4-methoxyphenyl)propenal has been successfully synthesized. The structure of the ligand and its complexes was characterized by analysis tools such as Fourier transform infrared, UV-visible, proton and carbon nuclear magnetic resonance spectra, molar conductance, and thermal analysis. The zinc compounds in nano-structure size were also prepared by sonochemical method. The nano-structure compounds were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Furthermore, the antimicrobial activity of the ligand and its zinc complexes against four gram positive and gram negative bacteria and also two fungi was assessed. Also the zinc complexes were used as precursor for the preparation of zinc oxide nanoparticles.

References:

[1] M. Montazerozohori, H. Mohammadi, A. Masoudiasl, M. Nasr-Esfahani, A. Naghiha, A. Assoud, J. Iran. Chem. Soc. 14(2) (2017) 297

[2] M. Montazerozohori, S. A. Musavi, A. Masoudiasl, A. Naghiha, M. Dusek, M. Kucerakova, Spectrochim.Acta Part A 137 (2015) 389.

[3] Z. Parsaee, K. Mohammadi, M. Ghahramaninezhad, B. Hosseinzadeh, New J. Chem. 40 (2016) 10569.

Catalytic application of transition metal substituted Keggin type polyoxometalates in the oximation of aldehydes and ketones

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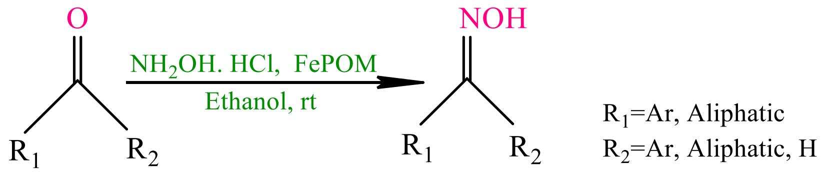
Abstract:

Polyoxometalates (POMs) have received much attention owing to their enormous structural versatility and their present and potential applications. These superior properties allow the POMs-based catalysts to be designed at the atomic and molecular levels. Among a wide variety of heteropolyoxometalates, Keggin structures are the most stable and more easily available [1]. The modification of parent POMs are likely to help in development of new generation catalysts with enhanced properties of acidity, redox potential and stability. This can be basically done by incorporation of transition metal ions into the lacuna in parent POM structures (i.e., transition metal substituted polyoxometalates, TMSPOMs) [2].

Oxime is a chemical compound belonging to the imines, with the general formula $R^1R^2C{=}NOH$, where R^1 is an organic side-chain and R^2 may be hydrogen, forming an aldoxime, or another group, forming a ketoxime. Oximes have been widely used for the prepration of nitro, nitriles, amides and nitrones compounds. Also they present many properties such as antimicrobial, antioxidant, anti-depressive and antiviral agent. The usual method for preparation of oximes involves treatment of carbonyl compounds with hydroxylamine hydrochloride [3].

In this study, transition metal substituted Keggin type POMs (TMPOMs) with some of the first row transition metals, as tetrabutylammonium salt $(TBA)_x[PW_{11}MO_{39}].nH_2O$ (M=Cr, Mn, Fe, Co, Ni, Cu, Zn) have been used in oximation of various aldehydes and ketones in the presence of hydroxylamine hydrochloride at room temperature. The reaction conditions such as kind and amount of TMSPOMs catalyst, amount of hydroxylamine hydrochloride, and type of solvent was initially optimized. Our results showed that among different TMSPOMs, $(TBA)_4[PW_{11}FeO_{39}].nH_2O$ and $(TBA)_5[PW_{11}ZnO_{39}].nH_2O$ have the best activity in oximation of aldehydes and ketones in ethanol. High conversion, short reaction times, room temperature and stability of the catalysts show a new synthetic application for TMPOMs in organic synthesis.



Refrences:

[1] T.Okuhara, N.Mizuno, M.Misono, Adv.Catal. 41 (1996) 113–252.
[2] L.Cronin, A.Müller, Chem. Soc. Rev.
12 (2012) 7325.
[3] E.Abele, E.Lukevics, Org Prep Proced Int. 32 (2000) 235–264

Investigation of 5,10,15,20-tetrakis(4-methyl phenyl)-porphyrinato aluminum(III) as the best restenosis treatment activity through the study of metalloporphyrins

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Abstract:

Restenosis is abnormal narrowing of an artery or a blood vessel that cause disorder in blood flow. One of angioplasty methods is administering green porphyrins have inhibitory properties of the restenosis by removal atherosclerotic plaque in concurrent and following angioplasty [1]. Porphyrins are an aromatic system have cyclic tetrapyrroles with four methine bridges (-CH=) which metal ions can connect to macrocycle. Photodynamic therapy (PDT) is an effective approach to restenosis treatment by porphyrin compounds due to their photosensitizer activity. If the porphyrin complex photosensitizer activity increase, restenosis treatment enhance in vivo [2]. According to the investigation of biological activities of metalloporphyrins which is shown in inserted table, it was identified that some porphyrin complexes has high restenosis treatment activity. In this research for the first time photosensitizer and toxicity activity were studied for a lot of metalloporphyrins. Class (I) is include aluminium porphyrins with different aromatic axial ligands. Classes (II-IV) are involve lanthanide porphyrins with Yb, Er, Tb, Ho, Gd, Dy metal ions and coordinated axial ligand which are similar behavior from the point of view of restenosis treatment activity in spite of metal changing. Research focused on determining one complex with the highest restenosis treatment, photosensitizer activity and lowest toxicity. Through the comparison of activity probability (P_a) above 80%, the maximum restenosis treatment resulted as follows: 1>2>…>6>7 among compounds set involve 50 complexes. Introducing the 5,10,15,20-tetrakis(4-methyl phenyl)-porphyrinato aluminum(III): [AlTTP] as the best compound for restenosis treatment without toxicity and with restenosis treatment and photosensitizer activity; 82.3% and 56.2% respectively.

References:

[1] J. Sh. Lin, C.J. Wang, W, Tyng Li, , 2018.

[2] Granville DJ, Hunt DW, Porphyrin-mediated photosensitization-taking the apoptosis fast lane, 2000.

Evaluate the effect of pore size and functional group of the MOF on the amount of the drug loading

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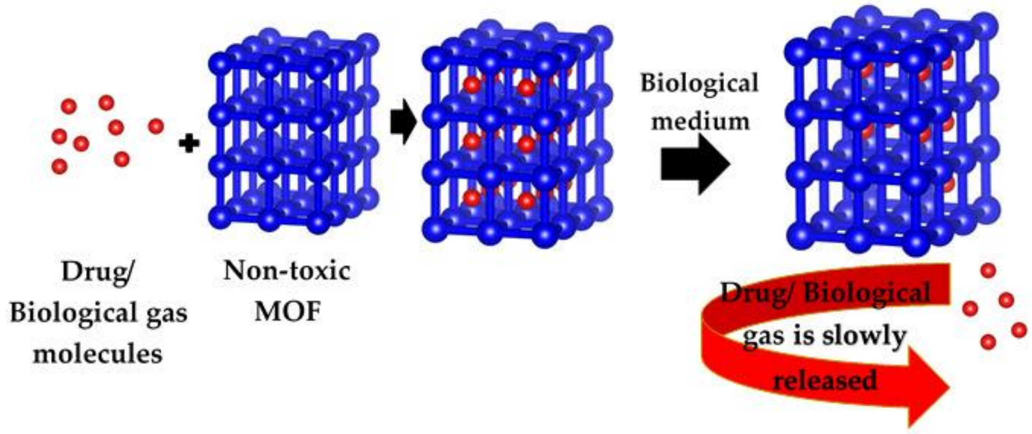
Abstract:

We have witnessed a rapid growth in the field of a new nanoporous material group, metal organic frameworks (MOFs), over the past decade. MOFs possess a wide array of potential applications in chemical engineering, chemistry, and materials science, including gas storage, gas separation, and catalysis[1]. One of the areas MOFs started to appear recently is biomedical applications. The unique physical and chemical characteristics of MOFs make them promising candidates for drug storage and drug delivery, nitric oxide storage and delivery, imaging, and sensing[2]. In this paper, Two 3D, porous Zn(II)-based metal–organic frameworks (MOFs), TMU-5 and TMU-6, containing azine-functionalized pores, were synthesized as potential drug carriers to evaluate the effect of pore size and functional group on the amount of drug loading in a MOF. 5-Fluorouracil (5-FU) is specifically chosen in the study for its small size, which is widely used as an anti-cancer chemotherapy drug for the treatment of colorectal, breast and head and neck cancers was laden into pores of the two structures. These MOFs respectively could adsorb up to 2.1 g and 7.5 g of 5-FU per gram of composites. The drug release for TMU-6 was also monitored and 80% of the loaded drug was released over 12 days.The results showed that pore size has a special effect on the amount of drug loading.



References:

[1] S. Henke, R.A. Fischer, J. Am. Chem. Soc. 133 (2011) 2064–2067.
[2] Q. Hu, J.C. Yu, M. Liu, A.P. Liu, Z.S. Dou, Y. Yang, J. Med. Chem. 57 (2014) 5679–5685.

Modification of boehmite nanoparticles with adenine for the immobilization of Cu(II) as nanocatalyst in organic reactions

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Abstract:

Boehmite nanoparticles are aluminum oxide hydroxide (γ-AlOOH) particles, which has large specific surface area (>120 m^2g^{-1}) and can be prepared using an inexpensive procedure in water. Herein, we present an economical, simple, and environmentally friendly route for the preparation of a copper catalyst on Adenine coated boehmite nanoparticles (Cu-Adenine@boehmite). This catalyst has been characterized by several techniques such as SEM, XRD, AAS, ICP and TGA analysis. Cu-Adenine@boehmite was applied as highly efficient and reusable nanocatalyst in carbon-carbon coupling reactions between various aryl halides and sodium tetraphenyl borate, phenylboronic acid, or 3,4-diflorophenylboronic acid under aerobic conditions, palladium-free and phosphine-free ligand. Also this catalyst was applied for the synthesis of polyhydroquinoline derivatives. In continuation, selective oxidation of sulfides to sulfoxides using hydrogen peroxide (H_2O_2) was studied in the presence of Cu-Adenine@boehmite as catalyst. The synthesis of sulfoxides using H_2O_2 in the presence of Cu-Adenine@boehmite does not generate waste and any byproducts. This catalyst was reused for several times in C-C coupling reaction without loss of its catalytic activity. Reused catalyst was characterized by SEM, XRD and ICP techniques. Heterogeneity and stability of Cu-Adenine@boehmite were studied by hot filtration test, poisoning test and ICP analysis.[1-4]

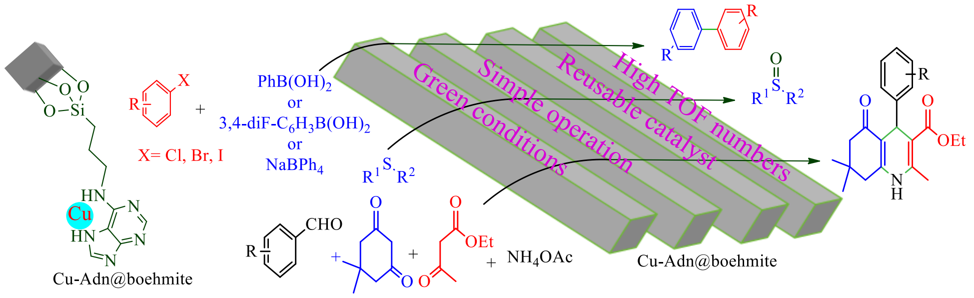

Fig.1

References:

[1] K. Bahrami, M.M. Khodaei, M. Roostaei, New J. Chem. 38 (2014) 5515-5520.
[2] A. Ghorbani-Choghamarani, B. Tahmasbi, P. Moradi, RSC Adv. 6 (2016) 43205-43216.
[3] X.Y. Chen, H.S. Huh, S.W. Lee, Nanotechnology 18 (2007) 285608-285612.
[4] A. Ghorbani-Choghamarani, P. Moradi, B. Tahmasbi, J. Iran. Chem. Soc. 16 (2019) 511–521.

Production of gasoline range hydrocarbons from methanol on hierarchical ZSM-5 catalyst prepared with n-propylamine template

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Abstract:

In methanol to gasoline (MTG) process, due to its unique properties, ZSM-5 zeolite has a high selectivity over gasoline boiling range of hydrocarbons with a research octane number (RON) of 90–96, comparable to that of conventional gasoline[1, 2]. Generally, this zeolite synthesized by TPAOH (TPABr) as template which is expensive. Since it is placed at the intersection of channels after synthesis, it is necessary to burn in calcination step to activate the catalyst and open the cavities. Therefore, the use of cheaper templates will be appropriate[3]. In this study, we tried to use inexpensive Si and Al sources and cheaper template than TPAOH (TPABr) for synthesis of ZSM-5 zeolite and investigate the catalytic performance of this catalyst in MTG process. ZSM-5 zeolite were synthesized via $SiO_2/Al_2O_3=50$ using n-propylamine with a linear carbon chain as the single template, where no secondary template and additives were added. The Si and Al sources were sodium silicate solution and aluminum sulphate-18-hydrate, respectively. The obtained zeolite characterized by FT-IR, XRD and XRF techniques which approved that zeolite was synthesized correctly and with desired SiO_2/Al_2O_3 ratio. The MTG experiment was carried out in a fixed-bed reactor under the operating conditions of T=380 °C, P=10bar and whsv=$2h^{-1}$. Synthesized zeolite exhibited high catalytic activity (100%) during 5h of operating and significant selectivity to the aromatics (44.5%).

References:

[1] C.D.Chang, et al., Process studies on the conversion of methanol to gasoline. 17(3) (1978) 255-260.
[2] C.D.Chang, and A.J.J.J.o.c. Silvestri, The conversion of methanol and other O-compounds to hydrocarbons over zeolite catalysts. 47(2) (1977). 249-259.
[3] L.D.Rollmann, et al., On the role of small amines in zeolite synthesis. 103(34) (1999) 7175-7183.

Curcumin encapsulated MIL-101(Fe) as a sustained release system

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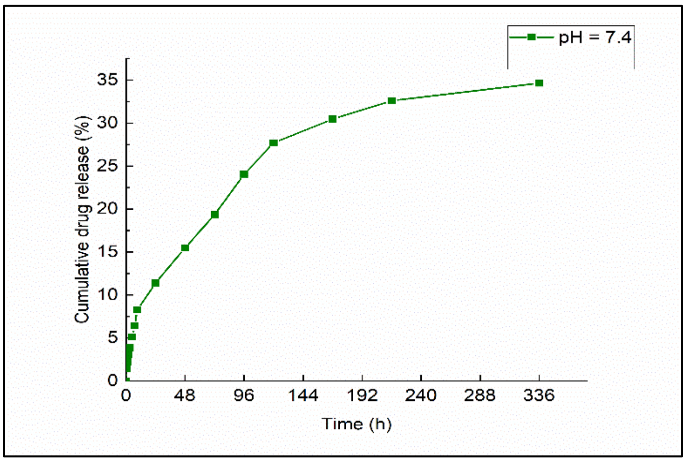
Abstract:

Metal-organic frameworks (MOFs) with unique features of excellent chemical stability, tunable pore size, and high surface area, are appropriate for many applications including gas storage, compound separation, catalysis, and drug delivery [1-3]. In the present study, MIL-101(Fe) was investigated for the load and release of curcumin. This mesoporous MOF is composed of nontoxic components; therefore, it is a suitable candidate for drug delivery field. In the first step, MIL-101(Fe) was synthesized with the reflux method in 110 °C and then activated with the solvent exchange to removing of DMF molecules in the pores. The MOF characterization before and after drug loading was done with some analysis such as X-ray powder diffraction (PXRD), N_2 adsorption/desorption, Fourier-transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), and UV–vis spectroscopy. Obtained results for drug loading was done based on UV-vis analysis. The drug release was monitored in phosphate buffer saline (PBS) at pH = 7.4. Results showed that 34.6% of the loaded drug was released over 14 days. This obtained release profile showed this MOF has the potential for sustained release of curcumin.



References:

[1] B. Lei, M. Wang, Z. Jiang, W. Qi, R. Su, Z. He, ACS applied materials & interfaces, 10 (2018) 16698-16706.
[2] A. Tiwari, A. Singh, N. Garg, J.K. Randhawa, Scientific reports, 7 (2017) 12598.
[3] M. Zheng, S. Liu, X. Guan, Z. Xie, ACS applied materials & interfaces, 7 (2015) 22181-22187.

One-pot Conversion of Starch to Gluconic Acid catalyzed by Multienzymatic Functionalization of Silver dendrites

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Abstract:

The regular cascade processes lead to inspire researchers to bring various biocatalysts together in an artificial way. But, the designed cascade reactions are often restricted due to short lifetime of their enzymes and low activities of micro systems. Therefore, the discovery of convenient and rational strategies for multi-immobilization of enzymes is still of great interest. Multicomponent reactions are an enormous level of interest, which provide rapid and efficient strategies for natural products synthesis and biological screening as well as preparation of biomaterials. In this work, we are going to introduce a brilliant double enzymatic microsystem prepared from co-immobilization of glucose oxidase (GOX) and glucoamylase (GA) on silver dendritic hierarchical nanostructure through Ugi four-component reaction (Ugi- 4CR). A variety of analytical tools were used to study the morphological, structural, and chemical properties of the biocatalysts. The success preparation of the unique biocatalyst system was confirmed by FT-IR, UV-Vis, TGA, XRD and scanning electron microscopy (SEM). The obtained double enzyme microsystem was employed as a biocatalyst for transformation of starch to gluconic acid as an exclusive cascade reaction under mild conditions.

References:

[1] Sheldon RA. Green Chem. 19 (2017) 18-43.
[2] S. Schoffelen, van Hest JCM. Soft Matter. 8 (2012) 1736-46.
[3] Sheldon RA, Pereira PC. Biocatalysis engineering: the big picture. Chem Soc Rev. 46 (2017) 2678-91.
[4] JC.Carlson, S.Li, SS.Gunatilleke, Y.Anzai, DA,Burr, LM.Podust, et al. Nat Chem. 3 (2011) 628-33.
[5] M.Filice, JM.Palomo. ACS Catalysis. 4 (2014) 1588-98.
[6] I.Vilotijevic, TF.Jamison.Angew Chem Int Ed. 48 (2009) 5250-81.
[7] ET.Hwang, B-k.Seo, Mb.Gu, A-P.Zeng. Catal Sci Tech. 6 (2016) 7267-72.
[8] SM.McKenna, S.Leimkühler, S.Herter, NJ.Turner. Green Chem. 17 (2015) 3271-5.

Geometrical aspects in coordination of a N_4-donor macrocyclic ligand toward Cu^{2+} ion along with docking studies

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Abstract:

Macrocycles are Large loop molecules that contain 12 or more atoms. From the point of view of drug chemistry, macrocycles are commonly known as a therapeutic agent. With regard to medicinal applications, they are used in the modelling of metallobiosites and metalloenzyme active sites [1] and also have also shown anti-fertility, anti-bacterial and anti-fungal [2]. A new macrocyclic compound of copper containing 1,3,6,10,12,15-hexaazatricyclo[13.3.1.1^{6,10}]eicosane ligand (L), [Cu(L)NCS]NCS, was prepared by template synthesis and ion exchange reaction. Then characterized by CHN analysis, FT-IR spectroscopy single crystal X-ray diffraction. In the coordinated macrocycle (figure 1), the copper center bonds to two secondary and two tertiary amines on the macrocycle and one nitrogen atom on the thiocyanato ligand, with a coordination number of five and square pyramidal geometry ($\tau = 0.46$).

The ability of complex to interact with ten selected biomacromolecules (BRAF kinase, CatB, DNA gyrase, HDAC7, rHA, RNR, TrxR, TS, Top II, B-DNA) was investigated by docking calculations. Based on this study, this complex can be considered as biologically active compound.

m.p. 148 °C, decomposed. Anal. Calcd for $C_{64}H_{118}Cu_4N_{32}O_3S_8$ (%): C, 50.23; H, 7.77; N, 5.49. Found: C, 50.38; H, 7.79; N, 5.63. IR (KBr, cm^{-1}): 3439 m (ν O−H), 3130 m (ν N−H), 2951 m (ν_{as} CH_2), 2855 m (ν_s CH_2), 2061 s (ν CN^{NCS}), 1647 w (δ H_2O), 1455 m (δ_{as} CH_2), 1379 m (δ_s CH_2), 1064 m (ν C−N), 818 m (ν C–S), 624 w (ρ_r H_2O), 537 (ρ_w H_2O).

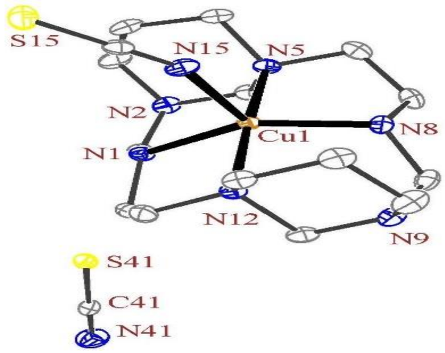

Fig. 1. An ORTEP plot of the complex, showing thermal ellipsoids at 50% probability.

References:

[1] S. R. Collinson, D. E. Fenton, Coord. Chem. Rev., 148(19) (1996).
[2] A. Chaudhary, N. Bansal, A. Gajraj, R. V. Singh, J. Inorg. Biochem., 96 (2003) 393

Cytosine complex of copper on MCM-41 nanoparticles as a highly efficient and reusable nanocatalyst for organic reactions

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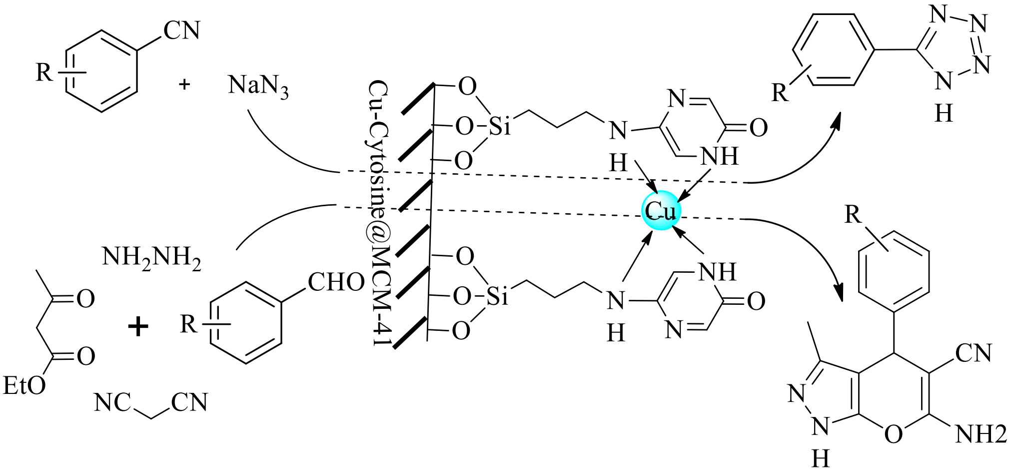
Abstract:
MCM-41 nanoparticles have a large specific surface area (>1200 m^{2}g^{-1}) and can be prepared using an inexpensive procedure in water. In this work, we present an economical, simple, and environmentally friendly route for the preparation of a complex of copper on MCM-41 nanoparticles (Cu-Cytosine@MCM-41) as heterogeneous catalyst. This catalyst has been characterized by several techniques such as N$_2$ adsorption–desorption isotherms, SEM, EDS, XRD, TGA, Ft-IR, and AAS techniques. Based on SEM images of Cu-Cytosine@MCM-41, the particles size of this catalyst were obtained in 80-120 nm of diameters. Cu-Cytosine@MCM-41 was applied as highly efficient and reusable nanocatalyst in multicomponent reactions such as synthesis of 5-substituted tetrazoles and pyranopyrazole derivatives. Tetrazoles and pyranopyrazoles have a wide range of biological activities such as antibacterial, antifungal, anticancer agents, anti-infammatory and insecticidal properties. This catalyst was reused for several times without loss of its catalytic activity. Heterogeneity and stability of Cu-Cytosine@MCM-41 were studied by hot filtration test and AAS analysis.



References:
[1] A. Ghorbani-Choghamarani, P. Moradi, B. Tahmasbi, J. Iran. Chem. Soc., 16 (2019) 511.
[2] A. Ghorbani-Choghamarani, P. Moradi, B. Tahmasbi, RSC Adv., 6 (2016) 56638.
[3] X. Xiong, C. Yi, X. Liao, S. Lai, Tetrahedron Lett.60 (2019) 402.
[4] B.J. Khairnar, D.V. Mane,B.R. Chaudhari, J. Applicable Chem. 8 (2019) 425.

MoO$_2$(acac)$_2$ supported on graphene oxide as a highly efficient and reusable catalyst for epoxidation of styrene

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Abstract

Epoxidation of alkenes catalyzed by metal complexes is an important reaction in organic synthesis because these compounds serve as useful intermediates that can be used for synthesis of a wide variety of other compounds [1]. Transition metals such as manganese and molybdenum have been used for alkene epoxidation [2]. Recently, metal acetylacetone complexes have been grafted onto supports as heterogeneous catalysts for the oxidation of olefinns or other substance [3]. Graphene oxide (GO), due to the presence of plenty of oxygen functionalities, such as hydroxyl and epoxide groups on both sides of its surface, has been acknowledged as one of the most promising supports to immobilize various homogeneous materials, including transition metal complexes [4]. Different approaches have been used to immobilize molybdenum on various supports to obtain heterogeneous catalysts [5]. This paper describes a catalytic system bases on graphene oxide modified with imidazole which was used as supports for MoO$_2$ (acac)$_2$. The heterogeneous catalyst, was characterized by FT-IR, UV-Vis and SEM. Characterization results showed that dioxomolybdenum (VI) complex was successfully grafted onto graphene oxide and the structure of the graphene oxide was well preserved after several stepwise synthesis procedures. The catalytic activity and reusability of catalyst in the styrene epoxidation was investigated. In addition, the heterogeneous catalyst could be reused five times without significant loss of activity.

References:

[1] M. Yan, F. Jin, Y. Ding, G, Wu, R. Chen, L. Wang, Y. Yan, Ind. Eng. Chem. Res. 58 (2019) 4764-4773.

[2] F. Esnaashari, M. Moghadam, V. Mirkhani, S. Tangestaninejad, I. Mohammadpoor-Baltork, A. R. Khosoropour, S.Hushmandrad, Polyhedron 48 (2012) 212-220.

[3] Z. Li, S. Wu, D. Zheng, J. Liu, H. Liu, Q. Kan, Appl. Organometal. Chem. 28 (2014) 317-323.

[4] R. Yadav, A. Subhash, N. Chemmenchery, B. Kandasubramanian, Ind. Eng. Chem. Res. 57 (2018) 9333−9350.

[5] A. Saroja, B. R. Bhat, Ind. Eng. Chem. Res. 58 (2019), 590–601.

Adsorptive removal of Pb(II) from water using metal-organic frameworks Cu-BTC and Zn-BTC

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Abstract:

Metal-organic frameworks are a kind of porous nanoscale materials, which features attractive adsorption of small molecules, large pores, high surface areas, etc., making them attractive for analytical applications [1]. In this study, two MOFs, which named by Cu-BTC and Zn-BTC, with the benzene-1,3,5-tricarboxylic acid linker, were successfully synthesized. Various variables including contact time, pH solution, initial concentration of metal ions and the effect of absorbent dose using ultrasonic device were studied. The use of an ultrasonic device plays an important role in shortening the absorption time of lead ions by increasing the absorbent dispersion in the solution [2]. For Pb(II) metal ions the sorption capacities of 333 mg g^{-1} and 312 mg g^{-1} were obtained effectively by Cu-BTC and Zn-BTC structures, respectively. The experimental adsorption data for the Cu-BTC and Zn-BTC MOFs, are well suited with the pseudo-second-order kinetic model ($R^2 = 0.99$), and adsorption isotherms of Pb^{2+} metal ions with the Langmuir model are in good agreement. This work exhibits two BTC-based MOFs to remove Pb^{2+} from pollutant water in less than 30 min effectively.

References:

[1] A. Hakimifar, A. Morsali, Inorganic chemistry, 58 (2018) 180-187.
[2] M. Roosta, M. Ghaedi, A. Daneshfar, R. Sahraei, Journal of Chromatography B, 975 (2015) 34-39.

Design, synthesis and luminescence properties of a new Zn(II)-tetracarboxylate metal–organic framework

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Abstract:

Metal–organic frameworks (MOFs) are an interesting category of crystalline porous materials, composed of metal nodes/clusters and organic linkers. MOFs have attracted much attention in separation science, gas storage, catalysis, drug delivery systems, and as synthetic precursors of porous materials [1]. More recently, metal-organic frameworks are introduced as luminescent sensors due to their unique crystallinity, tunable porosity and structural diversity [2,3]. Among a number of ligands have been used in the structure of MOFs, multi-carboxylate linkers are an important family of O-donor ligands for the construction of MOFs with fascination architectures and properties.

The present work demonstrates the design and synthesis of a new zinc(II)-tetracarboxylate metal–organic framework and its potential sensing applications. The Zn-MOF, namely, $[Zn_4(H_4L)(DMSO)_2]_n$ was prepared via the reaction of zinc(II) nitrate and a tetracarboxylate ligand under solvothermal condition. The title compound was characterized by FT-IR, CHNS, TGA, PXRD, and single crystal X-ray diffraction. In addition, (bio)sensing behavior of the Zn-MOF in detection of some drugs has been studied.

References:

[1]] D.J.T.Ryan, J.Kuppler, Q.R.Fang, J.R.Li, T.A.Makal, D.YMark, D.Young, D.Zhao, W.Zhuang, H.C.Zhou, Coord. Chem. Rev. 253 (2009) 3042-3066.

[2] Y.Zhang, S.Yuan, G.Day, X.W.Xinyu, H.Zhou. Coord. Chem. Rev. 354 (2018) 28-45.

[3] S.Carrasco,. Biosensors, 8(4) (2018) 92.

Synthesis of layered perovskite Ag, F-Bi_2MoO_6/rGO: A surface plasmon resonance and oxygen vacancy promoted nanocomposite as a visible-light photocatalyst

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Abstract:

Heterojunction z-scheme based Ag,F co-doped Bi_2MoO_6/reduced graphene oxide (Ag,F@BMO/rGO) photocatalysts were synthesized via a facile solvothermal method. The present work describes the improved photocatalytic activity of BMO/rGO nanocomposite by co-doping of F^- and Ag^+ ions, to remove RhB from aqueous solution. The XRD, N_2 adsorption, SEM, TEM, EDS, UV–Vis DRS, FT-IR, Raman, and PL measurements were employed to characterize the crystallographic, morphological, and optical properties. X-ray diffraction analysis suggests that crystal growth of all the as-prepared nanoparticles with different F^- and Ag^+ contents has occurred in Aurivillius phase and the crystal structure did not affected by doping. The insertion of Ag^+ and F^- into Bi_2MoO_6 led to a red-shift in the absorption edge of nanocomposite and decrease the band gap energy from 2.78 eV to 2.6 eV, due to the synergetic effects of Surface Plasmon Resonance and surface oxygen vacancy induced by Ag^+ and F^-, respectively. These beneficial properties are explored toward the photodegradation of RhB under visible-light source, resulting in better yields at lesser exposure time. The photocatalytic activity was significantly influenced by rGO in the nanocomposite, which was 2 times higher than that of pure Bi_2MoO_6, by effective separation of the charge carriers. The separation behaviors of photogenerated electron-hole were also systematically investigated by the PL. Based on the radical trapping experiments, photogenerated holes and $O_2\bullet^-$ were the main active species in RhB photodegradation and the detailed decolorization pathway has been suggested, using liquid chromatography/mass spectrometry (LC/MS) technique. In addition, the Ag,F@BMO/rGO nanocomposite does not display dramatic reduction of catalytic performance after four recycles, reveals its great prospect and promising application for water purification.

A Density Functional Theory (DFT) and Experimental study on F-doped Bismuth Molybdate Nanoplates; The effects of pH on Photocatalysis and Adsorption

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Abstract:

The present work describes two-dimensional plate architecture of F/Bi_2MoO_6 toward photodegradation of RhB in aqueous solution. The effects of F-doping on the physicochemical properties of Bi_2MoO_6 are confirmed by XRD, XPS, SEM, FTIR, Raman, PL, EDX, EDX mapping, and UV−Vis diffuse reflectance spectra. Under the influence of CTAB surfactant, Bismuth, Molybdenum, and Fluorine source self-assemble into nanoplate architectures, whereas FE-SEM images confirm two-dimensional plate morphology. The photocatalytic activity of the nanoplates is studied under visible-light (λ>420 nm) irradiation toward the photodegradation of RhB. It is interesting to find that the F-doped sample showed enhanced photocatalytic activity. In addition, density functional theory (DFT) calculations performed to study the Frontier orbital character.

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