22nd Iranian Inorganic Chemistry Conference

By
Department of Chemistry
University of Kurdistan

With the collaboration of the Iranian Chemical Society

23-25 August, 2023

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About the Conference

The 22nd Iranian Inorganic Chemistry Conference will be held at the University of Kurdistan and will host professors, students, researchers, industrialists and enthusiasts of this scientific event. In the three-day conference, the latest scientific and research achievements in various fields of inorganic chemistry will be discussed. The submitted papers of esteemed colleagues, students, researchers, and industrialists will be reviewed by the scientific committee and presented in two formats of speech and poster. In another part of the conference, in order to benefit more participants with the latest scientific and research findings in the field of topics related to inorganic chemistry and industry, specialized sessions will be held with the cooperation of experts in related fields. Also, during the conference, practical training workshops will be held with the presence of prominent professors. Holding specialized exhibitions on the sidelines of the conference is another program of this scientific event.

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Professor of Inorganic Chemistry

Smohebbi

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Research interests: Nano photocatalyst, Catalyst, and Inorganic Chemistry

Affiliation: University of Kurdistan

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Research interests: Chemistry of polyoxometalates, synthesis and applications

Affiliation: University of Kurdistan

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Research interests: Solar cells, biochemistry, hydrogen storage, nanotechnology, synthesis and identification of porphyrins, and studying their application

Affiliation: University of Kashan

Google Scholar:

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Research interests: Nanotechnology, synthesis and identification of porphyrins, and studying their application

Affiliation: K.N. Toosi University of Technology

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5- Dr. Majid Moghadam

Research interests: Homogeneous and heterogeneous catalysts including metalloporphyrins, Schiff base complexes and polyoxometalates, Photochemistry, and nanochemistry

Affiliation: University of Isfahan

Google Scholar: *https://Google Scholar.google.com/citations?hl=en&user=mIZ_EEkAAAAJ*

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Research interests: Chemistry of polyoxometalates, synthesis and applications Affiliation: University of Isfahan

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Research interests: Designing inorganic and organometallic systems using transition metals and investigating their photophysical and biological properties, Kinetic studies on organometallic complexes, and investigating the catalytic properties of inorganic and organometallic complexes.

Affiliation: Institute for Advanced Studies in Basic Sciences

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8- Dr. Hamid Golchoubian

Research interests: Design, synthesis, and characterization of novel inorganic molecules

Affiliation: University of Mazandaran

Google Scholar: *https://Google Scholar.google.com/citations?hl=en&user=2VAlgxIAAAAJ*

9- Dr. Masoud Mirzaei Shahrabi

Research interests: Metal-Organic Frameworks

Affiliation: Ferdowsi University of Mashhad

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10- Dr. Yasin Gholiee

Research interests: Non-covalent interactions; host/guest chemistry; Protonation and prediction of the protonation constants of polygamous micromolecules; the nature of metal-ligand bonding in complexes; Drug-DNA interactions

Affiliation: Malayer University

Google Scholar: *https://Google Scholar.google.com/citations?hl=en&user=RGL2k_UAAAAJ*

11- Dr. Mehdi Hatefi Ardakani

Research interests: Schiff base complexes, Homogeneous and Heterogeneous nanocatalysts

Affiliation: Vali-e-Asr University of Rafsanjan

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12- Dr. Saeid Farhadi

Research interests: Nanotechnology

Affiliation: Lorestan University

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Research interests: Organometallic

Affiliation: University of Isfahan

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Research interests: Inorganic Chemistry, Nanomaterials and Layered Double Hydroxides(LDHs), and application of nanomaterials in Oxygen Evolution Reaction(OER) Water Oxidation as catalyst, photocatalyst, supercapacitors adsorbents and drug delivery

Affiliation: Azarbaijan Shahid Madani University

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Research interests: Crystallography, nanomaterials, and synthesis and identification of inorganic complexes

Affiliation: Iran University of Science and Technology

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16- Dr. Hadi Kargar

Research interests: Catalyst, Synthesis, Biomimetic, Schiff base, and Porphyrin

Affiliation: Ardakan University

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17- Dr. Akbar Rostami-Vartooni

Research interests: Coordination Chemistry, Nanocomposite, Schiff base, Photodegradation, and Catalysis

Affiliation: University of Qom

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18- Dr. Mohammad Ghadermazi

Research interests: Inorganic Chemistry

Affiliation: University of Kurdistan

Google Scholar: *https://Google Scholar.google.com/citations?user=qQV-JC0AAAAJ&hl=en*

19- Dr. Ezzat Rafiee

Research interests: Nanocatalyst, Heteropoly Acid, and Heterogeneous Catalyst

Affiliation: Razi University

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20- Dr. Seyed Abolfazl Hosseini-Yazdi

Research interests: Inorganic Chemistry, Coordination Chemistry, Macrocyclic Chemistry, and Biological Studies

Affiliation: University of Tabriz

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21- Dr. Khosro Mohammadi

Research interests: Inorganic Chemistry, Coordination Chemistry, Crystallography, polyoxometalates

Affiliation: Persian Gulf University

Google Scholar: *https://Google Scholar.google.com/citations?user=P8n3rusAAAAJ&hl=en*

22- Dr. Hassan Haddadzadeh

Research interests: DNA and BSA Interactions with Metal Complexes and Anticancer Drugs, Organometallics

Affiliation: Isfahan University of Technology

Google Scholar: *https://Google Scholar.google.com/citations?user=yMFH5aEAAAAJ&hl=en*

23- Dr. Ali Hossein Kianfar

Research interests: Metal Schiff base complexes

Affiliation: Isfahan University of Technology

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24- Dr. Mehdi Irani

Research interests: Computational Biochemistry, Kinetics and Mechanism of Reactions

Affiliation: University of Kurdistan

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25- Dr. Mahdieh Ghobadifard

Research interests: Nanophotocatalyst, Heterogeneous Catalyst, Magnetic materials, and Perovskite

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List of Abstracts

Synthesis, characterization, spectroscopic investigation and crystal structure determination of new derivative of *N*-phenylpyrazine-2-carboxamide ligands

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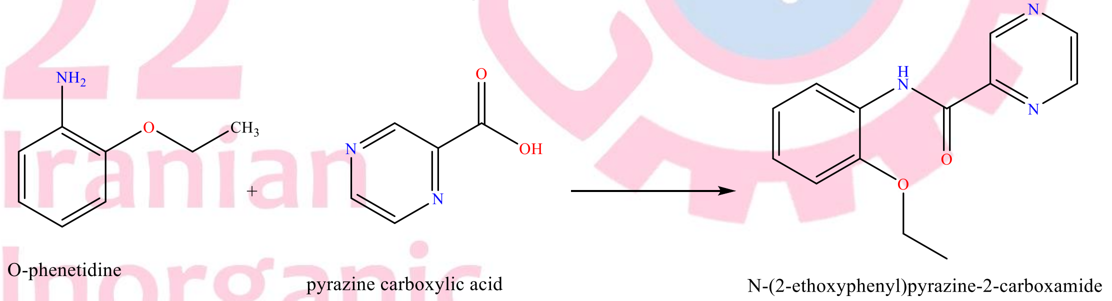
Among organic ligands, carboxamides are of great interest due to the variety of synthetic products and their importance in biological, chemical, and pharmaceutical fields and have many applications such as anti-inflammatory, anti-depressant, anti-tumor, anti-seizure, antibiotic properties, etc. [1,2]. Based on this and considering the variety of biological and medicinal properties of pyrazinamide derivatives and the importance of using these compounds [3], in this research work we synthesized N-(2-ethoxyphenyl)pyrazine-2-carboxamide ligand and after identifying and determining the crystal structure, we investigated the spectral properties of the synthesized compound, in order to investigate their applications.



Keywords: Pyrazine-2-carboxylic acid, Carboxamide Ligand, Crystal Structure.

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Synthesis, characterization, spectroscopic investigation and crystal structure determination of a new copper (II) complex with N-phenylpyrazine-2-carboxamide derivative ligand

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Most of the research that is done in the field of mineral chemistry today is about coordination compounds. Nitrogen-containing heterocycles, especially heterocycles containing pyrazine nuclei, have attracted the attention of organic, pharmaceutical and materials scientists [1]. In addition to coordination chemistry, topics such as crystal engineering have also been raised, which have attracted the attention of scientists in various fields of science. The general goal of crystal engineering is to recognize and use intermolecular interactions in controlling crystal aggregation, designing and synthesizing crystal structures and new solids with desirable and unique properties. The stability and neutrality of carboxamides as well as the simultaneous presence of hydrogen bond donor and acceptor groups in these compounds have caused more attention in recent decades to study and investigate their complexes with intermediate and main metals [2]. For example, the derivative of pyrazine-2-carboxamide compounds can show antimycobacterial and antifungal properties. Therefore, in recent years, the chemistry of intermediate metal ions, including copper (II), with carboxamide groups has found various applications in many fields of chemistry due to their distinct characteristics, including biological activities [3]. In this work, from the reaction of $Cu(NO_3)_2.3H_2O$ with N-(2-ethoxyphenyl)pyrazine-2-Carboxamide Ligand a new complex of Cu(II) was synthesized. Furthermore, this complex was thoroughly characterized by X-ray crystal structure determination, IR, and UV-Vis spectroscopies.

Keywords: Pyrazine-2-carboxylic acid, Carboxamide Ligand, Cu(II) Complexes, Crystal Structure.

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Synthesis and identification of cross-linked chitosan/tripolyphosphat/dacarbazine nano-composite

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Various nanocarrier preparations have been designed to improve therapeutic efficacy and reduce toxic side effects. Nanocarriers prospect a continuous, direct, and controlled drug release to the malignant cells selectively with augmented drug localization and cellular uptake. Nanoparticles can be automated to identify malignant cells and give discriminating and precise drug transfer, evading contact through the normal cells [1].Nanoparticles developed from natural polymers like albumin, heparin and chitosan are used to create nanoparticles for the targeted transport of nucleotide-based drugs, oligonucleotide drugs and proteins [2]. Chitosan (CS) is the most important derivative of chitin which is prepared by the alkaline deacetylation of chitin [3]. The ionic gelation of chitosan by the addition of sodium tripolyphosphate (TPP) is used to prepare chitosan nanoparticles. TPP is a small negative ion that contains three negative charges at physiological pH and its non-toxicity favors its medical application. This compound is able to create five ionic cross-linking points with cationic groups of chitosan. These characteristics make TPP one of the best cross-linking agents for preparation of chitosan nanoparticles [4]. In this study, solution Chitosan and dacarbazine (chemotherapy medication) are mixed together in the dark, then combined with tripolyphosphate solution in a water bath. Using FT-IR, SEM-EDS, NANO DRAP, TGA-DTA and XRD techniques, the structural characteristics of the resulting composite, the percentage of drug use on the Pharmaceutical platform and, also the entrapment efficiency are investigated. As a result, Dacarbazine drug with rod morphology is placed on the chitosan/tripolyphosphate nanocomposite.

Keywords: Chitosan , Tripolyphosphat , Dacarbazine

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Nanomagnetic Cu(II) complex catalyzed synthesis of 2-amino-3-cyano-4H-chromenes

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Heterocyclic systems, in particular oxygen-containing structures, constitute a privileged group of compounds based on their wide range of biological activity. Derivatives of 4H-chromenes have attracted attention because of containing a pharmacophore group that is found in many molecules with pharmacological effects, including anticancer, antifungal, antibacterial, antioxidant, and antiprotozoal agents [1]. 1,10-Phenanthroline-5,6-dione (phendione)-based transition-metal complexes are known for their use in pharmacological and catalysis applications [2,3]. In this work, a novel Fe_3O_4-supported Cu(II)-complex catalyst was synthesized via functionalization of the Fe_3O_4 surface as a support by acetylacetone, followed by treatment with $CuCl_2$ and phen-dione ligands, and identified by Fourier transform infrared spectroscopy (FT-IR), feld emission scanning electron microscopy (FE-SEM), X-ray difraction spectroscopy (EDX), thermogravimetric analysis (TG), and X-ray powder difraction (XRD). The catalytic activity of the Lewis acid catalyst has been successfully examined in a one-pot, three-component condensation reaction of aromatic aldehydes, Lawsone, and malononitrile in ethanol under reflux conditions to furnish 2-amino-3-cyano-4H-chromenes. The proposed approach has some advantages, such as excellent yields, mild reaction conditions, short reaction times, the use of agricultural waste, and an eco-friendly nature.

Keywords: Fe_3O_4; Copper catalyst; 2-amino-3-cyano-4H-chromenes; Levis acid catalyst.

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A novel Cu(II) complex immobilized on $ZrFe_2O_4$ magnetic nanoparticles catalyzed synthesis of pyranopyrazols

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Heterogeneous catalysis plays a crucial role in many chemical processes, including advanced organic preparations and the design and synthesis of new organic moieties [1]. Efficient and sustainable catalysts are vital to ecological and fiscal viability [2]. This is why green multicomponent reaction (MCR) approaches have gained prominence. Owing to a broad range of pharmacological applications, pyranopyrazole syntheses (through the one-pot strategy, employing sustainable heterogeneous catalysts) have received immense attention [3]. Here, the synthesis of efficient heterogenous catalysts for the environmentally friendly and economic synthesis of pyranopyrazoles was reported via multicomponent reactions between hydrazine hydrate, ethyl acetoacetate, malononitrile, and aromatic aldehydes. A nanomagnetic Cu(II) complex was synthesized through the immobilization of tryptophan on the $ZrFe_2O_4$ surface and its complexation with Cu salt. It was characterized by FTIR, XRD, EDX, Map, SEM, TEM, VSM, and BET/BJH methods. The structures of pyranopyrazol compounds were fully confirmed via IR, ^{1}H NMR, and ^{13}C NMR spectroscopic studies. High yields of products, the use of a green solvent, the easy work-up procedure, the short reaction times, and the easily separable catalyst are the main advantages of this protocol.

Keywords: $ZrFe_2O_4$, tryptophan-Cu(II) complex, pyranopyrazoles, Lewis acid catalyst.

References

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Synthesis and electrochemical properties of MIL/Fe_2O_3/PANI/rGO nanocomposite electrode materials for supercacitor applications

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We have successfully synthesized a new nanocomposite made from four component including MIL(100)/Fe_2O_3/PANI/rGO (MFPG) and use them as electrode active materials for supercapacitor fabrication. MIL(101) as a well-known metal-organic frameworks (MOFs), benefits from the valuable properties of MOFs such as high porosity and potential high charge storage abilities [1]. The combination of MIL(100) with nanometal oxide, PANI as a conducting polymer and rGO led to new nanocomposite and it were were characterized by various techniques. The electrochemical properties of the materials were investigated in 1 M KOH as electrolytes. The capacitive properties of MIL-101(Fe) based composite electrodes were found to greatly depend on charge transfer processes, obtained by detailed analyses.

Keywords: Supercapacitor, Electrode material, Metal-Organic Farmeworks, Electrochemistry

References

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Synthesis, spectral and antimicrobial studies of derivative salicylaldehyde schiff base oxidovanadium (IV) complexes

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Vanadium complexes derived from a number of ligands have received great attention in the last few years for their interesting medicinal and biological applications [1]. Schiff bases and their complexes possess wide biological activities, such as antibacterial, antifungal and antitumor aspects [2,3]. Three new vanadium complexes, $[VO(L^{1-3})]$ where L^1 is {[1-methyl-2-(2-hydroxyphenyl)methylidynen-itrilo]ethyl}amino-1-cyclopentenedithiocarboxylate, L^2 is {[1-methyl-2-(2-hydroxy-5-nitrophenyl)methylidynen-itrilo]ethyl}amino-1-cyclopentenedithiocarboxylate and L^3{[1-methyl-2-(2-hydroxy-5-methoxyphenyl)methylidynen-itrilo]ethyl}amino-1-cyclopentenedithiocarboxylate have been synthesized and characterized by elemental analysis, ^{1}HNMR, IR, UV–Vis spectra, Mass spectrometry, powder XRD and EDX. The V atom in complex is in a coordination square pyramidal geometry. Antibacterial activities of the prepared compounds were evaluated in vitro against Staphylococcus Aureus and Escherichia Coli. The ligands and their complexes exhibited significant antibacterial activity. The free ligands showed high activities compared with the VO^{IV} complexes.

Keywords: Oxidovanadium complexes, Antibacterial activities, Schiff base ligands.

References

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Singlet oxygen effect on lipid oxidation in the presence and absence of synthetic/natural antioxidants, using sheep erythrocyte hemoglobin

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Photooxidation of lipids is an undesirable chemical process in which essential fatty acids are converted into peroxides with singlet oxygen ($^1O_2$), which causes oxidative spoilage of meat products [1-3]. Erythrocytes are used as a model for lipid oxidation because residual blood can enhance lipid oxidation upon hemolysis and release of hemoglobin [3]. This study aims at investigation of $^1O_2$ effect on lipid oxidation in erythrocyte model and oleic acid. In this study, hydroalcoholic extracts of Turmeric (Curcuma longa L.) and Cumin (Cuminum cyminum L.) were used as natural antioxidants. Butyl hydroxytoluene (BHT) was used as a synthetic antioxidant and sodium azide (NaN_3) was applied as a well-known singlet oxygen scavenger. The generation or inhibition of $^1O_2$ and peroxide products in the sheep blood erythrocyte and oleic acid in the presence of Rose Bengal photosensitizer, light and various antioxidants were obtained by ^1H NMR spectroscopy, UV-Vis spectroscopy, TBARS assay and iodometric titration. The antioxidant results showed that NaN_3,turmeric, cumin, and BHT were able to prevent the photooxidation of lipids into peroxide products in sheep erythrocyte model, 100%, 70.93%, 62.26%, and 51.92%, respectively. Meanwhile, these inhibition values in the photocatalytic conversion of oleic acid to peroxide products were obtained as 100%, 71.10%, 46.63% and 24.08%, respectively. These results declared that the two methods have a positive correlation for invistigation of lipids and fatty acids phootooxidation.

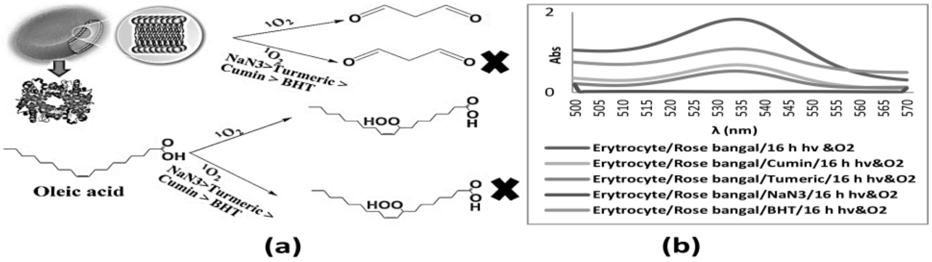

Fig.1 (a) Erythrocyte and oleic acid photooxygenation in the presence and absence of synthetic/natural antioxidants. (b) UV-Vis spectra of (a) based on TBARS method

Keywords: Hemoglobin, lipid oxidation, singlet oxygen, antioxidants

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Synthesis of novel chiral heterogeneous bisoxazoline-based catalyst and its application in the synthesis of chiral allylic esters by synchronous dehydrogenation and allylic oxidation of alkanes

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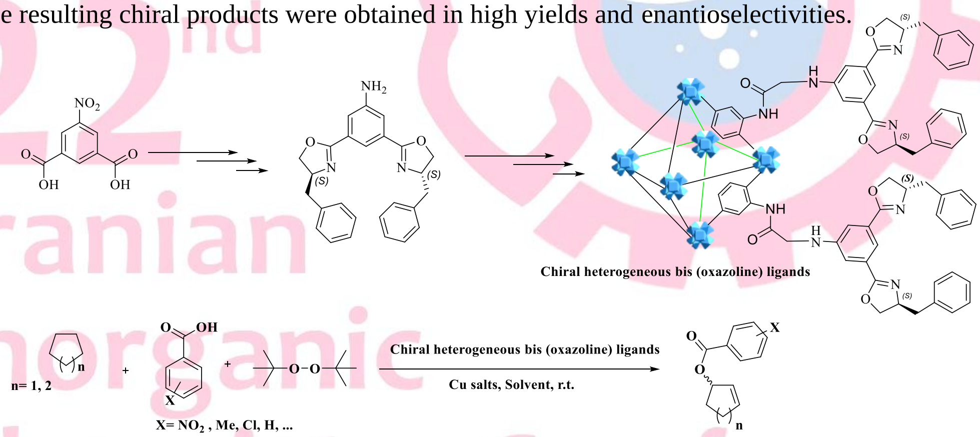
Over the past couple of decades, chiral bisoxazoline (BOX) ligands, mainly prepared from the reaction of various dicarboxylic acids and a range of chiral β-amino alcohols, have gathered increasing attention as promising ligands in numerous catalytic asymmetric transformations [1, 2]. Besides, according to the importance of recyclability of these ligands due to their high value, an excellent selection of a good substrate for immobilization of them could be a suitable idea. Herein, the new chiral amino bisoxazoline ligand was synthesized from the starting material 5-nitro-isophthalic acid in several steps and then immobilized on the functionalized UiO-66-NH$_2$ metal organic framework [3]. The structure of synthesized chiral heterogeneous ligand was characterized by XRD, FE-SEM, BET, FT-IR and TGA techniques. Finally, in order to investigate the catalytic activity of the prepared heterogeneous chiral ligand, it was used in concurrent dehydrogenation of alkanes and allylic oxidation of alkenes as a rare synchronous reaction for the synthesis of chiral allylic esters with various benzoic acid derivatives and oxidants under different conditions (Scheme 1) [4, 5]. The resulting chiral products were obtained in high yields and enantioselectivities.



Scheme 1: Synthesis of chiral allylic esters by using chiral heterogeneous bisoxazoline-based catalysts

Keywords: Chiral bisoxazoline ligands, Dehydrogenation, Allylic oxidation, Chiral allylic esters, Functionalized UiO-66-NH$_2$

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Evaluating anticancer activity and DNA-binding properties of cycloplatinated (II) water-soluble complexes

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According to WHO, cancer is the second leading cause of diseases globally and is responsible for an evaluated 9.6 million deaths in 2018 [1]. Universally, about 1 in 6 deaths is because of cancer [2]. New anticancer chemotherapeutics, that can effectively cure this disease with minimal side effects, maintain initial importance to the world research community [3]. In this study, four Pt-based complexes, [Pt (N^C) (CN) (L)], and [Pt (N^C) $(CN)_2$], in which N^C = deprotonated 2-phenyl pyridine (ppy) or benzo[h]quinoline (bhq), and L = *p*-Tolyl or methyl were synthesized [4,5]. These complexes are characterized by NMR spectroscopy. In addition, the biomolecular interactions of complexes with calf-thymus DNA (CT-DNA) and ethidium bromide (EB) are studied by fluorescence spectroscopy and UV−vis measurements. The potential of Pt complexes (C_1–C_4) to use as an anticancer agent and their cytotoxicity against MCF-7, A549, HT29, and MDA-MB-231 cancer cell lines were measured by using 3-(4, 5-dimethylthiazol-2-yl)-2, 5-diphenyl tetrazolium bromide (MTT) assay. To better understand the nature of the binding, a competitive assay between the complexes and ethidium bromide for DNA binding was studied. According to the results obtained from these analyses, [Pt(ppy)(CN)(*p*-Tolyl)] has more cytotoxicity for MCF-7, A549, and HT29 cancer cell lines, also, [Pt(bzq)(CN)(*p*-Tolyl)] has more cytotoxicity for MDA-MB-231 cancer cell lines. Overall, the present work suggests that a controlled modification could result in new potential antitumor complexes which can survive the repair mechanism and induce facile apoptosis. It can be concluded that the cyclomatalated platinum(II) complexes are highly promising leads for the development of novel effective DNA-targeted anticancer drugs.

Keywords: cyloplatinated (II) complexes, water-soluble, anticancer activity, fluorescence spectroscopy, [Pt(N^C)(CN)(L)] complexes

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Virtual screening of human glyoxalase I inhibitors: A structure-based approach

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Human glyoxalase I (GlxI) is a key metalloenzyme involved in the detoxification of methylglyoxal, a cytotoxic byproduct of glycolysis. GlxI is overexpressed in many cancers and contributes to their proliferation, invasion, and drug resistance. Therefore, this enzyme is a potential target for anticancer drug discovery. In this study, we performed a virtual screening of a large library of compounds to identify novel inhibitors of GlxI. We performed molecular docking using IGEMDOCKv2.1 software to find ligands that bind to the active site of GlxI. We used *S*-P-bromobenzylglutathione, a known inhibitor of GlxI with a very low K_I value of 83 nM [1], as a probe ligand. Docking was performed on the human GlxI structure from the Protein Data Bank entry 1qip [2]. Then we used web servers to generate and search pharmacophore models based on the probe ligand). We selected the top candidates and docked them to GlxI using AutoDock Vina. We ranked the compounds by their binding energies and selected the best ones for further analysis. We evaluated the binding modes and interactions of the selected inhibitors with GlxI and compared them with the known inhibitors. We also performed ADMET prediction and drug-likeness analysis to assess the pharmacological properties of the selected inhibitors. Our results suggest that we have identified some promising candidates that can inhibit GlxI with high affinity and specificity. These compounds may serve as lead compounds for further optimization and development of novel anticancer agents.

Keywords: Glyoxalase I, Drug design, Docking, Virtual screening

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A comparison of organic and inorganic-supports for –SO_3H functionality and their application in known reaction

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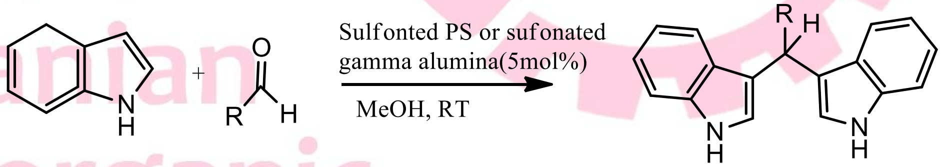
Sulfonation is a major industrial chemical process used to make a diverse range of products, including dyes and color intensifiers, pigments, medicinals,organic intermediates. Sulfonated aromatic rings have been shown to be promising materials for proton exchange membranes (PEM) due to their high thermal and chemical stability as well as lower-cost production compared to commercial available perfluoro sulfonated. for example, Para-toluene sulfonic acid is a typical intermediary for the synthesis of pharmaceuticals, pesticides, and dyes and is a catalyst for organic synthesis[1]. Sulfonation of narrow polydispersity polystyrene, standards remains the method of choice for generating polystyrene sulfonate (SPS), samples with defined composition[2]. In the presenet study, γ-alumina and polystyrene foam were used as support for –SO_3H functional groups. The sulfonated products were charactrized by FT-IR, TGA and ^1H NMR. Eficiently of the above mentioned, solid acid was evaluated in condensation of indoles and aldehydes as a model reaction, under mild conditions. Satisfactory yields of the desired products were obtained.



Keywords: sulfonation, PSF, γ-alumina, indoles, Polystyrene

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Dye decomposition by inorganic−organic hybrid base on Preyssler-type polyoxometalates

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Lately, industrial growth has enhanced intensive environmental difficulty in which pollution of water is the main subject. The existence of dyes along with other pollutants prevent the biological treatment methods also enforce allergic reactions [1]. Rhodamin B (Rh.B) is a carcinogen and dangerous dye for human beings. Several procedures have been presented for the elimination of dyes such as sorption and membrane segregation. But the mentioned methods have disadvantages like high cost, be time-consuming [2]. Polyoxometalates (POMs) are nanoscale anionic metal-oxide clusters of d-block transition metals, which play a very active role in many fields such as homogeneous and heterogeneous catalyses, electrocatalysis, photocatalysis, materials science, molecular magnetism and spintronics, and macromolecular crystallography due to their structural diversity, electronic properties, modifiability, tunability, and redox properties [3]. In the vast family of POMs, the donut-shaped molecule consisting of five PO_4 tetrahedra surrounded by 30 WO_6 octahedra is termed as Preyssler-type POMs ($[M^{n+}P_5W_{30}O_{110}]^{(15-n)-}$, abbreviated as $[M^{n+}@P_5W_{30}]^{(15-n)-}$), Preyssler anions display distinctive properties, among which the most notable are their (1) high negative charges (−12 to −15), (2) large oxidation potential, and (3) reversible transformation. The diameter of the internal cavity of Preyssler clusters approaches 5 Å, large enough to accommodate at least one metal cation (M^{n+}) [4]. In this study, inorganic−organic hybrid consisting of the Preyssler polyoxometalate, $[M^{n+}P_5W_{30}O_{110}]^{(15-n)-}$ with PDA (p-phenylenediamine) were synthesized by a new straight forward method [5]. After calcinated in 500 ˚C, prodact characterized by field emission scanning electron microscopy (FE-SEM), Fourier transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD). At the end, used nanocatalysis for decomposition of organic dye, rhodamine B (RhB), and be reused nanocatalysis for at least 4 cycles.

Keywords: Polyoxometalate, Preyssler, Dyes, Catalysis , Inorganic−organic hybrid

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Synthesis of Fe_3O_4 nanoparticles by co-precipitation method and study of the solvent effect on morphology and crystallinity of particles

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Iron oxides in nano-scale have exhibited great potential for their applications as catalytic materials, wastewater treatment adsorbents, pigments, flocculants, coatings, gas sensors, ion exchangers, magnetic recording devices, magnetic data storage devices, toners and inks for xerography, magnetic resonance imaging, bioseparation and medicine [1-3]. In this research work, Fe_3O_4 nanoparticles were synthesized by co-precipitation method which Iron oxides were normally precipitated from an aqueous solution of Fe(II)and/orFe(III) salts whit addition of an alkali solution along with suitable ageing time.The formation of Fe3O4 can be performed under below the chemical reaction [4]: $Fe^{+2}+2Fe^{+3}+8OH^{-}\rightarrow Fe(OH)_2+2Fe(OH)_3\rightarrow Fe_3O_4+4H_2O$ The effect of solvent on size, morphology and crystallinity of nanoparticles were investigated. The obtained products were characterized by the variety of methods such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and Scanning electron microscopy (SEM).The size of particles was calculated by Sherrer's formula, and then compared with the size of nanoparticles obtained from sem image .The results from the SEM images, show the formation of spherical nanocrystaline iron oxide with average diameter of 37 nm.

Keywords: Magnetite, Co-precipitation, Nanoparticles, Morphology

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Dye decomposition by organo-inorganic catalytic nanocomposite material based on polyaniline (PANI) with Preyssler polyoxometalate

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Organic dyes are important industrial materials and are used in different industries. The extensive use of organic dyes and the indiscriminate disposal of dye-contaminated effluents can cause serious contamination of surface and groundwater[1]. The dyes are toxic and pose a threat to human health, as they can cause mutagenesis, chromosomal fractures, carcinogenesis, and respiratory toxicity[2,3]. Hence, many methods have been proposed to remove dyes from water and wastewater These methods are mainly based on sorption and membrane segregation. But the mentioned methods have disadvantages like high cost and time-consuming [4]. The aim of this study is dye decomposition by organo-inorganic catalytic nanocomposite. For this purpose, an organo-inorganic catalytic nanocomposite material based on conjugated polymer, polyaniline (PANI) with Preyssler polyoxometalate was developed by performing in situ chemical oxidative polymerization of aniline with ammonium persulfate (APS) oxidant synthesized. Then The structural and morphological properties of organo-inorganic PANI nanocomposites were analyzed by X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and Fourier transform infrared spectroscopy (FT-IR), respectively. After that, the catalytic activities of the nanocomposites were evaluated by the catalytic degradation of Methylene Blue (MB) in different conditions.

Keywords: Organo-inorganic hybrid, Nanocomposite, Polyaniline, Polyoxometalates, Preyssler

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Solvothermal synthesis and characterization of nano molybdenum disulfide

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Two–dimensional (2D) materials are widely attractive for applicaiton in next–generation nanoelectronic devices. Transition metal disulfides MS_2 (M = Mo, Ti, W, and V) constitute an important class of inorganic layered compounds. Due to the unique properties, MS_2 nanostructures with sheet–like morphology have been emerging as new potential materials for several applications such as catalysis, transistors, hydrogen storage, solid lubricants, Li–ion batteries, and double–layer capacitors. Bulk MoS_2 is an indirect semiconductor with a bandgap of 1.2 eV, whereas single–layer MoS_2 is semiconducting with a direct bandgap of 1.8 eV. Monolayer MoS_2 could complement graphene in the applications that require thin transparent semiconductors, such as optoelectronics and energy harvesting. Recently, considerable efforts have been paid to the synthesis of these materials on a stable nanometer scale [1-5].In the present study, we describe a solvothermal route to synthesize MoS_2 with a new precusor for source of sulfur. The organic solvents can adhere to the surfaces of MoS_2, leading to the preparation of MoS_2 nanosheets with controllable morphologies. The effect of the solvents on the growth and microstructures of the final products was also investigated. The synthesized molybdenum disulfide was used as photocatalyst for degredation of some organic pollutants.

Keywords:

Molybdenum disulfide, Synthesis, Characterization, Photocatalyst

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Interrelation of crystal morphology and intermolecular contacts in a new thiophosphoramide structure: an energy framework analysis

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The morphology of the crystal structures is an influencing factor on some physical properties. Particularly, morphology affects the dissolution rate, tabletibility, and stability of pharmaceuticals [1,2]. In a crystal lattice, the morphological feature originates from the intermolecular interactions [3,4]. Understanding the interplay of “intermolecular interactions” and “morphological features” can help to provide insight into changing the properties. Herein, the synthesis, characterization, and crystal structure of a new thiophosphorylated thiourea with the formula $(C_2H_5O)_2P(S)(NHC(S)NHCH_2(C_4H_7O))$ is reported. The N—H···S═C and C—H···S═C hydrogen bonds are the strongest intermolecular interactions, which appear as red spots on the Hirshfeld surface map and propagate the molecular assembly along the *b*-axis. The energy frameworks, calculated using CE-B3LYP/6-31G(d,p) method, show that these interactions take part in the most potent molecular pairs (with the energy values of –57.2 and –48.8 kJ/mol) in the structure. Interaction energies in two other directions are remarkably weaker. The combinations of the interactions in the *b*-direction with some weaker interactions lead to the formation of plates parallel to the *ab*-plane. The plates (with a thickness of about 1 nm) are stacked together with the weakest interactions. This feature reduces the ability of the crystal to grow in the *c*-direction compared to the *a*- and *b*- directions.

Keywords: Thiophosphoramide, Morphology, Interactions, Energy framework, DFT

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Synthesis and characterization of ZIF-67-NiO/graphene sponge for supercapacitor applications

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Nowadays, the use of electrical appliances to supply the daily electrical energy that can replace the use of fossil fuels is very indispensable and important. Not only the harmful phenomena of greenhouse gas production and the increase in earth's heat, but also the dependence of clean energy generation such as solar and wind energy on weather conditions, has pushed researchers towards the challenge of continuous energy supply [1]. Therefore, among electrical devices capable of storing energy, in recent years, supercapacitors (SCs) with high energy density and high charge/discharge speed have attracted the attention of researchers [2]. In this study, to develop supercapacitors, a graphene sponge (GS) has been used as a three-dimensional substrate derived from graphene. Furthermore, to increase the energy density, the GS substrate has been decorated by using nanostructures such as zeolitic imidazolate framework-67 (ZIF-67) and nickel oxide (NiO). In this comparative study, the synthesized GS, ZIF-67, NiO, ZIF-GS, NiO-GS, and ZIF-NiO-GS have been characterized by X-ray powder diffraction, Fourier transform infrared spectroscopy, and field emission scanning electron microscopy coupling with energy dispersive spectroscopy to investigate the structure, functional groups, and morphology with elemental distribution, respectively. The obtained results of XRD show that the target ZIF-67 has been correctly synthesized and has. Furthermore, the images related to the carbon substrate e have shown the favorable sponge shape and it confirms the synthesis of GS successfully. In addition, cyclic voltammetry, electrochemical impedance spectroscopy, and chronoamperometry studies have been used to measure the specific capacitance and the charge transfer resistance of the desired structures.

Keywords: NiO-ZIF-67, Graphene sponge, Supercapacitors, EIS, charge/discharge

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Investigation of electrocatalytic properties of MnO_2-ZnO/rGO aerogel nanocomposite

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In recent decades, environmental concerns and the global energy crisis caused by the reduction of fossil fuels have led to an intensive search for clean and renewable energy sources, especially through electrocatalytic processes. On the other hand, the morphology and structure of the manufactured electrocatalysts can have useful features for better catalytic performance [1][2]. Therefore, the design and synthesis of innovative high-performance nanocomposites in the electrochemical processes, such as the oxygen evolution reaction (OER) and hydrogen evolution reaction (HER), is very important and has attracted a lot of attention in recent years [3][4]. In this study, the novel MnO_2-ZnO/rGO aerogel nanocomposite was synthesised to consider the OER and HER studies. The synthesized rGO aerogel, MnO_2 and ZnO nanoparticles, MnO_2/rGO aerogel and ZnO/rGO aerogel binary nanocomposites, and MnO_2-ZnO/rGO aerogel ternary nanocomposite have been characterized by using X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM) coupling with energy dispersive spectroscopy (EDS), Brunauer-Emmett-Teller (BET) theory to investigate the structure, functional groups, morphology with elemental distribution, and specific surface area of materials, respectively. The obtained results of FE-SEM and XRD revealed that the graphene aerogel has incorporated nanoparticles of MnO_2 and ZnO in the form of a substrate with high porosity and large pore size, without collapsing the surface structure. In addition, cyclic voltammetry, electrochemical impedance spectroscopy, and linear sweep voltammetry have been employed to consider the electrochemical behaviors of synthesized samples. The electrochemical results show that MnO_2-ZnO/rGO only shows lower OER activity than MnO_2/rGO, but in terms of HER, it has good electrocatalytic activity compared to the rest prepared samples.

Keywords: MnO_2-ZnO/rGO, aerogel, HER, OER

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Synergistic effect of graphene oxide on Fe/ZIF-67 for the electrocatalytic reaction of oxygen evolution

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Nowadays, fossil fuels alone will not be enough to meet ever-increasing energy demands to develop sustainable energy. Therefore, a clean pathway to produce sustainable energy carriers has been introduced through electrochemical water splitting containing hydrogen and oxygen evolution reactions (HER and OER) [1]. OER is generally considered to be the rate-limiting step of water splitting, and so the development of inexpensive, low-cost, and efficient OER electrocatalysts is essential [2]. Herein, we propose easily prepared bimetallic zeolitic imidazolate framework-67 (Fe/ZIF-67) on graphene oxide (GO) to investigate the synergistic effect of GO in OER process. The prepared electrocatalyst was characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) coupling Energy-dispersive X-ray spectroscopy (EDS) and Fourier transform infrared spectroscopy (FT-IR). According to the characterization methods the Fe/ZIF-67 nanoparticles were uniformly dispersed on graphene, which provides many more active sites to achieve the better performance of OER. Therefore, Fe/ZIF-67/GO composites compared with ZIF-67 and Fe/ZIF-67 displays low overpotential of 354 and 397 mV at the current density of 5 and 10 mA cm^{-2}, respectively, with a small Tafel slope of 110 mV dec^{-1} in alkaline media. The excellent OER performance is mainly owed to its unique nanoarchitecture and the synergistic effects: not only uniformly dispersed Fe/ZIF-67 nanoparticles on graphene guarantee large specific area and abundant active sites, but also the porous nanostructure benefits electrolyte penetration. This work provides a deep understanding of how to boost catalytic efficiency using GO in the structure of electrocatalysts.

Keywords: Water splitting, Oxygen evolution reaction, Graphene oxide, Zeolite-imidazole framework

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Catalytic effect of CuX (X=F, Cl, Br, I) on nitroso−Diels−Alder reaction, a theoretical study

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In this study, Nitroso−Diels–Alder (NDA) cycloaddition reaction between the $CH_3N=O$ and cis-1,3−butadiene in the presence of the CuX (X=F,Cl, Br, I) as Lewis acid catalyst, using density functional theory calculations at the M06-2X [1] level of theory using the def2-svp basis set, has been studied. The NDA reaction is a chemical reaction for the construction of six-membered rings [2]. The copper(I)-catalyzed such as copper (I) and copper (II) complexes and copper salts have used Lewis acid catalysts in Diels-Alder reactions [3]. The aim of this work was to study various substituents of X (X=F,Cl, Br, I) on the catalytic effect of the Cu catalyst in NDA cycloaddition reaction (Fig. 1). The results showed that the largest effect on activation energies of the reaction belongs to the CuF catalyst.The activation strain model (ASM) [4], the quantum theory of atoms in molecules (QTAIM) and natural bond orbital (NBO) analysis were used to understand the nature of interactions at the TS structures.

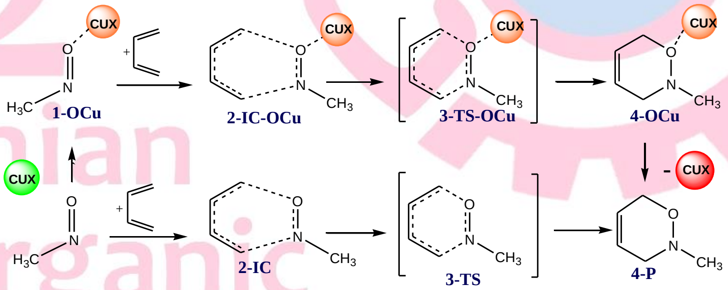

Fig. 1: Uncatalyzed NDA reaction between $CH_3N=O$ and butadiene, versus those catalyzed by a CuX compound (X=F,Cl, Br, I)via Cu···O noncovalent interactions.

Keywords: Nitroso−Diels–Alder, CuX catalyst, DFT

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Tuning the catalytic activity of a Zn-MOF by tandem post-synthetic surface functionalization in the synthesis of benzimidazole derivatives

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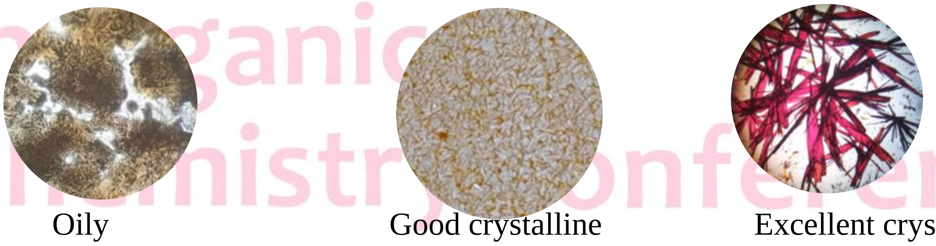
The current work reports the effect of post-synthetic surface modification of a Zn-MOF on the catalytic synthesis of benzimidazole derivatives. For this purpose, the most suitable functional groups for the catalytic formation of benzimidazole derivatives such as Lewis acid, Lewis base, Brønsted acid, and Brønsted base were introduced on the surface of the Zn-MOF. The catalytic reaction was examined in the presence of the resulting functionalized Zn-MOFs as a catalyst. As a result, it was found that the Brønsted acid group has the best performance for the catalytic reaction of benzimidazole derivatives.

Keywords: Post-synthetic modification, Functionalization, Metal-organic framework, Benzimidazole

Table 1 the reaction of benzimidazole derivatives

catalyst	**Efficiency[a] (%)**	**Time[b] (min)**	**Description**
Zn-MOF	<65	>60	good crystalline product
Zn-MOF functionalized by Lewis acid	<80	>60	good crystalline product
Zn-MOF functionalized by Lewis base	<70	>90	oily product
Zn-MOF functionalized by Brønsted acid	>98	<10	excellent crystalline product
Zn-MOF functionalized by Brønsted base	<60	>90	oily product

[a,b] The maximum efficiency/time of reaction for benzimidazole derivatives with each modified Zn-MOF catalyst.



Oily Good crystalline Excellent crystalline

Figure 1 The microscopic images of the synthesis of benzimidazole derivatives

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Post-synthetic modification of a 2D water-stable Zn-MOF; from exfoliated nanosheets to the formation of 3D supramolecular structure functionalized by acid/base groups

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Post-synthesis modification (PSM) is known as a powerful approach that provides the opportunity for the design of new frameworks. The current research reports the PSM of a 2D Zn-MOF in three steps. By removing the coordinated solvent molecules from the 2D structure of Zn-MOF, as pristine structure, Zn-MOF-df with the coordinatively unsaturated site (CUS) as Lewis acid site was prepared in the first step. Then, the 2D packing structure of the Zn-MOF-df was exfoliated to form Zn-MOF-df-ex sheets. At step two, ethylenediamine (en) and 1,3-diamino propane (dap) molecules as amine functional groups were separately added to Zn-MOF-df to obtain Zn-MOF-en and Zn-MOF-dap, respectively. A multi-layer structure was recommended for the Zn-MOF-en, where some of the en molecules act as a cross-linking agent to connect a number of Zn-MOF-df layers to each other, while terminal amine groups acts as Lewis base sites (fig.1). Concerning the Zn-MOF-dap, the dap molecules cross-linked all the layers in the crystal packing and form a 3D supramolecular framework. In the third step of tandem PSM, Zn-MOF-en-ps containing Brønsted acid was synthesized by adding 1,3-Propane sultone (ps) molecules to Zn-MOF-en. Finally, it is believed that through the PSM strategy, it is possible to prepare various MOFs with outstanding properties for designed applications [1-4].

Keywords: Post-synthetic modification, Functionalization, Metal-organic framework

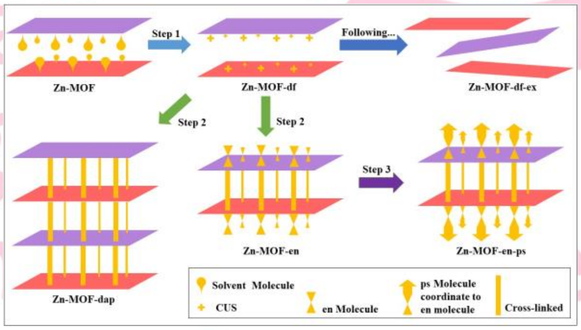

Fig. 1. Tandem post-synthetic modification on 2D Zn-MOF

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Post-synthetic metal exchange on an amine-functionalized zinc coordination polymer for hydrogen sulfide capture

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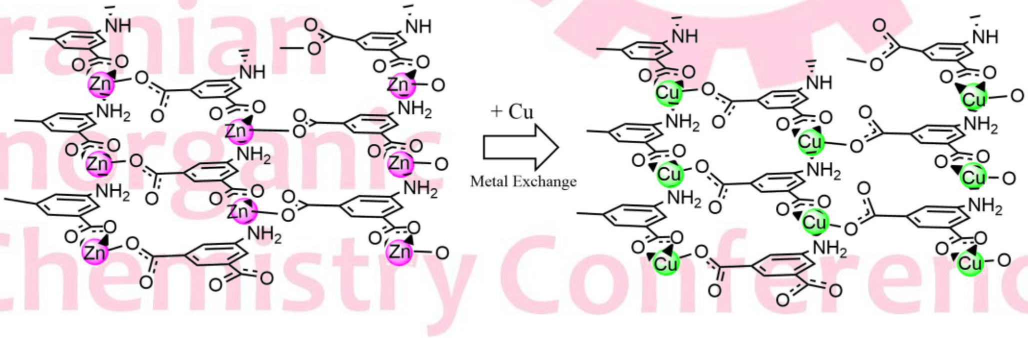
Tandem post-synthetic modification is an interesting approach for improving the properties of coordination polymers. In this work, we report surface functionalization by amine group under ultrasonic condition and tandem post-synthetic metal-exchange (PSE) on zinc coordination polymer (Zn-CP). During the metal exchange process Cu^{2+} ions were replaced by Zn^{2+} ions in methanol . Due to the existence of two suitable sites in the obtained product, i.e. copper metal nodes and amine surface functional groups, it acquires the ability to enhance the hydrogen sulfide (H_2S) capture [1-3].

Keywords: Post-synthetic modification, Metal exchange, Functionalization, Metal-organic framework, H_2S capture.



Scheme 1. Post-synthetic metal exchange approach

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Investigation of structural and optical properties of $Ba_{0.6}Mg_{0.2}Ca_{0.2}Al_2O_4$ ceramic

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Barium aluminate ($BaAl_2O_4$) is an insulator with hexagonal crystal structure, and it crystallized in space group P63 (No. 173) symmetries with cell parameters a = b= 10.449, c = 8.793 Å. It belongs to the family of stuffed tridymite tetrahedral structures. This structure consists of twisted AlO_4 tetrahedral linked to each other by their corners [1]. Metal ion-doped $BaAl_2O_4$ ceramics possess wide applications in the fabrication of efficient phosphor materials. In researches [2 and 3], a broad emission band at about 405 nm in the spectrum of undoped, non-reduced $BaAl_2O_4$ were reprted. Pandey and Chithambo [2] measured PL with UV-excitation at 248 nm and thermoluminescence, while the Benourdja et al. [3] evaluated CL spectra. Both author groups ascribed the broad emission band to native defect state transitions in $BaAl_2O_4$. Suriyamurthi and Panigrahi [4] reported the PL at room temperature of undoped $BaAl_2O_4$ by excitation with near UV light at 346 nm. They measured a main emission band at 500 nm and a shoulder at 430 nm and relatively assign these emission bands to V_k^{3+} defect centres. These contradictory results indicate that apart from the processes mentioned above, viz. annealing and excitation, there could be non-registered parameters such as synthesis conditions, purity, storage condition, etc. that affect the nature and concentration of defects in $BaAl_2O_4$. In this research, $Ba_{0.6}Mg_{0.2}Ca_{0.2}Al_2O_4$ ceramic was fabricated by sol-gel route and its optical and structural properties was evaluated compared to $BaAl_2O_4$ by techniques such as X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), *energy*-disspersive X-ray spectroscopy (EDS), ultraviolet-visible (UV–Vis), and *photoluminescence* (PL).

***Keywords**: ceramic, optical properties, structural properties, sol-gel approuch*

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Structural, electrical, and dielectric properties of $Mg_{0.8}Ba_{0.2}Al_2O_4$ ceramic fabricated by gel-combustion route

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In this research, the structural, electrical, and dielectric properties of $Mg_{0.8}Ba_{0.2}Al_2O_4$ nanocrystalline ceramic were investigated. The ceramic was synthesized by gel-combustion method. Different techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy–energy dispersive X-ray spectroscopy (SEM–EDX), surface area analyzer (BET), and impedance spectroscopy were used to study the structural, microstructural, morphological, electrical, and dielectric properties of the prepared $Mg_{0.8}Ba_{0.2}Al_2O_4$ ceramic. In particular, the magnesium aluminate ($MgAl_2O_4$) has well known for its normal spinel structure. The physical properties of the magnesium aluminate system are more suitable for microwave device fabrications. The insulating properties of spinel aluminate materials favor various applications by way of catalyst, catalyst support and intrinsic dielectric materials, chemical attacks towards the high resistive integrate electronic circuits and also act as a good refractory material. The distinct dielectric properties possessed by the magnesium aluminate system make it more suitable for microwave and microelectronic devices [1]. Padmaraj et al. reported a specific surface area of 162.704 m^2/g for the prepared $MgAl_2O_4$ nanocrystalline powder in their research.While using a new and affordable sol-gel method, Habibi et al. were able to report a spinel with a high specific surface area of 264 m^2/g at low temperature [2]. Additionally, the nanocrystalline $MgAl_2O_4$ pellet was found to have a calculated conductivity value of 4.9213×10^{-13} S cm^{-1}[3].

Keywords: Gel-combustion, Electrical properties, Structural properties, Ceramic

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Degradation of an anti-inflammatory drug using magnesium ferrite in the Fenton oxidation process

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Abstract:The growth of the global economy is exponentially increasing. The rapid growth of urbanization and industrialization releases a huge volume of wastewater that imposes adverse effects on human health[1]. The presence of organic compounds such as painkillers in water is a threat to public health; because many of them are poisonous; endocrine disruptor and mutagenic for humans and animals[2]. Fenton advanced oxidation process is one of the most cost-effective methods for wastewater treatment[3]. In this research, the Fenton oxidation process using a ferrite-based catalyst, i.e. magnesium ferrite ($MgFe_2O_4$), has been used to remove diclofenac sodium (DS) from an aqueous solution. DS is a nonsteroidal anti-inflammatory drug (NSAID) used to block substances that cause inflammation and pain. The effect of four reaction parameters including the amount of the catalyst, the amount of hydrogen peroxide oxidant and pH on the drug removal was studied. In the optimal conditions, the removal efficiency of the DS with a concentration of 50 mg/l reached more than 90% at 33 min; with 15 mg of the catalyst, 1.5 mL of H_2O_2 at pH 7. The results show that the magnetically separable catalyst can be used efficiently in the Fenton process for the treatment of pharmaceutical wastewaters.

Keywords: Wastewater treatment, catalyst, Fenton, magnesium ferrite

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New zinc(II) mixed ligand coordination polymers at nano and bulk size, precursor for preparation of ZnO nanoparticles

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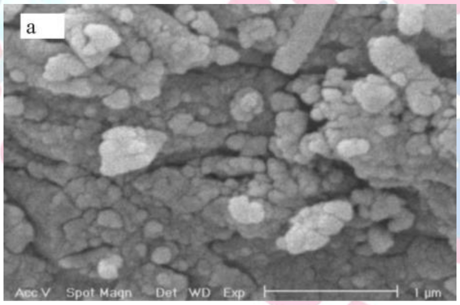
Three-Dimensional ZnII coordination polymer containing 4,4´-bipyridine (4,4´-bipy) and benzene 1,4-dicarboxilic acide (BDCA), [Zn2(μ-4,4´-bipy)(μ-BDCA)$_2$]n has been synthesized and characterized by elemental analysis, IR spectroscopy, Raman and its structures studied by single Crystal X-ray crystallography. ZnO nanoparticles were obtained by calcination of compound at 500ºC under air atmosphere and were characterized by X-Ray Diffraction (XRD), Raman spectroscopy, solid state UV and Scanning Electron Microscopy (SEM) [1-2].



Reaction between mixture of 4,4´-bipy and BDCA with a mixture of zinc(II) acetate led to formation of the new zinc(II) 3D coordination polymer [Zn2(μ-4,4´-bipy)(μ-BDCA)2]n. Nanoparticles of this Nano Coordination Polymers (NCP) were obtained by ultrasonic irradiation in a Methanol/water solution and single crystalline material was obtained using a slow evaporation

$$Zn(\mathrm{OAC})_2 + 4{,}4 - \mathrm{bpyr} + \mathrm{BDCA} \rightarrow$$
$$\rightarrow \begin{cases} \xrightarrow{\text{(MeOH) in Branched−Tube}} \{\text{Single Crystal of } [\mathrm{Zn}_2(\mu - 4{,}4' - \mathrm{bipy})_2(\mu - \mathrm{BDCA})_2]_n \\ \xrightarrow{\text{Ultrasond Irradiation+MeOH}} \{\text{Nanoscale of } [\mathrm{Zn}_2(\mu - 4{,}4' - \mathrm{bipy})_2(\mu - \mathrm{BDCA})_2]_n \rightarrow \\ \qquad \rightarrow \xrightarrow{\text{Calcination at 500−600℃}} \text{Nanoparticle of ZnO} \end{cases}$$

Keywords: Zinc(II), Coordination Polymers, Nanostructure, Mixed Ligands, ZnO

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New flour link Cu-V mixed ligand-mixed metal nano coordination polymers, study of antitumor activity

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Anticancer cells and antimicrobial activity of new mixed metal $[Cu_2(BPA)_2(VOF_5)_2]_n$ Complex (BPA = 2,2-Bipyridineamine) at Bulk and Nano-sized have been studied and these new unusually structure complex characterized by elemental analysis, IR spectroscopy and its structures studied by single Crystal X-ray crystallography. Nanopowder of this compound synthesized by sonochemical method then characterized by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) [1]. These synthesized CP and NCP (CP = Coordination Polymers and NCP = Nano Coordination Polymers) of fluoride link Copper-Vanadium with 2,2-bipyridine amine, as ligand, after being subjected to biological tests, showed anticancer activity [2]. As ligand BPA is biologically active, the results of biological activity are as expected specifically, an activity was demonstrated in breast cancer cells (MCF7 and MDA MB 231) and proliferative cells (MCF7).

Keywords: Cu(II), Vanadium, Antitumor, Nano Coordination Polymers

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Synthesis, characterization, thermal and gas sensing properties of new scandium(III) nano coordination polymers

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New Scandium(III) coordination polymer at bulk and nanopowders as Scandium 1,4-benzene dicarboxylic acid hydroxide [Sc(OH)(BDCA)]n, (BDCA = 1,4-Benzene Dicarboxylic Acid) has been synthesized by the reaction of a mixture Sc(III) Nitrate and BDCA in MeOH by simple Branched tube and sonochemical method. The nanopowders of Sc_2O_3 was prepared from the calcinations of the NCP at air atmosphere. The structure of the CP and NCP (CP = Coordination Polymers and NCP = Nano Coordination Polymers) were determined by X-ray crystallography, while nano-structural materials were characterized by X-ray powder diffraction (XRPD), Thermal Gravimetric Analysis (TGA) and Scanning Electron Microscopy (SEM). These NCP and Sc_2O_3 nanostructures have been tested for CO_2 gas monitoring by depositing them as thick films on an interdigitated alumina substrate and evaluating the surface resistance of the deposited layer as a function of operating temperature and CO_2 concentrations. The gas sensitivity tests have demonstrated that the Sc_2O_3 nanopowders, exhibit high sensitivity to CO_2 proving their applicability in gas sensors. The role of the nanopowdesr on the sensing properties of NCP and Sc_2O_3 are also discussed [1-2].

Keywords: *Coordination Polymers, Sc_2O_3, Nanopowders, CO_2, gas sensing.*

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Synthesis and characterization and application of zirconate(IV) complex for C–C coupling reactions

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Carbon-Carbon bond forming reactions are among the important catalytic transformations in organic synthesis[1,2]. Heterogeneous catalysts have been highly investigated in the C-C cross coupling reactions [3]. The metal compelexs show high catalytic activities in various cross-coupling reactions of an aryl or alkenyl halide[4]. Highly efficient catalysts based on zirconium nanoparticles in C-C cross-coupling reaction were reported[5]. In this work, synthesis and characterization of the Zr(IV) complex, $[Ph_3PCH_2C_6H_4CH_2PPh_3]_2\,[ZrCl_6]$, has been reported. The prepared compound was characterized using elemental analysis and spectroscopic methods IR, ^1H, and ^{13}C NMR. Finally, this compound was investigated as an effective catalyst in Suzuki and Heck carbon-carbon coupling reactions. All products were prepared in the presence of this complex in high efficiency. The obtained compound can be recovered and it can be reused without significant reduction in its catalytic activity.

Keywords: Zirconium(IV) chloride, Suzuki reaction, Heck reaction

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Synthesis, characterization of cyclopalladated complexe and Its application as efficient catalysts for Suzuki-Miyaura and Heck-Mizoroki coupling reactions

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Palladium-catalyzed cross-coupling reactions are one of the most important carbon-carbon bond forming processes[1-2]. Nowadays, the Suzuki Miyaura cross-coupling reaction has become a standard tool in natural product synthesis[1.2]. The development of new ligands lead to improvements but also the design of new precatalyst structures can increase the catalytic activity as they initiate the formation of the catalytically active species in the cross-coupling reaction. It is often reported in the literature that the palladium complexes show a better catalytically activities. Several air-stable (NHC)-palladium(II) precatalysts have been reported. (NHC)-palladium(II) complexes with cyclometalating ligands such as N,N-dimethyl-2-aminobiphenyl and 2-Phenylpyridine and others show high catalytic activities in various cross-coupling reactions[3-4]. Herein, we prepared novel cyclometalated Pd(II) complex, [Pd(ppy)(phen-dione)]PF_6 where ppy is 2- phenylpyridine and phen-dione is 1,10-phenanthroline-5,6-dione, and characterized by elemental analyses , IR, ^{1}H, and ^{13}C NMR techniques. It was found that this compound can act as an efficient catalyst in C-C bond formation between various aryl halides with phenylboronic acid (Suzuki-Miyaura reaction) and aryl halides with n-butyl acrylate (Heck–Mizorokireaction).

Keywords:Palladium-catalyzed, Cyclometalated complex, Suzuki Reaction, Heck Reaction

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Unusual porosity behavior in a new zinc-based MOF with the heptanodal topology

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Currently, the design and synthesis of metal-organic frameworks (MOFs) attract broad attention because of the interesting structural architectures and topological features which have a key role in the final behavior of their application [1]. In order to construct porous compound networks, the common strategy is employed based on the suited selection of organic linkers and metal ions that affect the final topology of the clustered networks [2, 3]. In this work, to obtain a new topological structure of a zinc-1,3,5-benzentricarboxylate (Zn-BTC) MOF, we choose the various synthetic methods in the presence of different solvents and ratios of the Zn:BTC reagents. Herein, we report the synthesis and characterization of a new Zn-BTC MOF (**FUM-181**) with the heptanodal topology. The single-crystal X-ray diffraction (SCXRD) reveals that **FUM-181** crystallizes in the monoclinic space group $P2_1/c$. The crystal structure of **FUM-181** consists of seven independent Zn^{2+} centers, four topologically different kinds of BTC^{3-} groups (BTC-1, BTC-2, BTC-3, and BTC-4), four H_2O, two -OH groups, and three coordinated DMF molecules in the asymmetric unit. A precise examination of **FUM-181** demonstrates that it is a three-dimensional network with complicated and unusual pore structures. Furthermore, a detailed theoretical study has been carried out on the adsorption of CO_2 and CH_4 in this MOF at 298, 303, 318, and 333 K and 1-50 bar. The theoretical gas adsorption measurement predicts that **FUM-181** has a superior performance in CH_4 gas adsorption compared to CO_2. It is worth mentioning, Hong et. al have recently reported a new hexanodal zinc-BTC MOF with high CO_2 gas adsorption [4]. Interestingly, the changing gas adsorption behavior can be observed in our reported Zn-BTC MOF by changing the hexanodal to heptanodal topology.

Keywords: Zn-BTC Metal-Organic Frameworks, The heptanodal MOF Topology, Sorption behavior

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Synthesis of zinc-based metal organic frameworks modified as highly efficient and recyclable catalysts for Suzuki and Heck cross-coupling reactions

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As a unique class of porous materials, metal-organic frameworks (MOFs) are promising platforms for creating heterogeneous catalysts [1]. MOFs with a highly porous structure enable efficient access of reactive molecules to the site of the active metal and are promising as heterogeneous catalysis. Heterogeneous catalysis is superior to homogeneous catalysis because it leads to easier separation, reusability, minimized waste, and cleaner products [2, 3]. Therefore, MOFs are used as heterogeneous catalysts to accelerate coupling reactions or as support materials in various catalysts due to having active catalytic sites in the structure, high surface area, structural diversity, and tunable pore size porosity [4, 5]. The porosity of MOFs is one of the factors affecting the rate of Suzuki and Heck cross-coupling reactions. In this research, a new modified Zinc-Based Metal–Organic Frameworks (MOF-5) catalyst was synthesized using the solovthermal method with high porosity and remarkable thermal stability. The mesostructured MOF-5 is composed of the bond between metal Zn^{2+} and 1, 4-dicarboxybenzene (PTA). In order to increase the efficiency and expand the surface area of MOF-5, from surfactant was used. The MOF-5 catalyst in Suzuki and heck cross-coupling reactions was easily recovered and recycled in 6 cycles without significant leaching or loss of catalytic activity.

Keywords: Metal-organic frameworks (MOFs), Surfactant, Heterogeneous catalysis, Porosity, Suzuki and Heck

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Rational design of organic-inorganic metal halide perovskites with deep blue emission and encapsulation in metal organic frameworks as a stable platform with improve emission characters

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Organic-inorganic metal halide perovskites (OIMHPs) is one of the most interesting and exciting nanoscale optoelectronic materials that has recently received attention [1]. Having excellent optoelectronic properties, high quantum efficiency, flexible adjustment of the emission wavelength, wide and adjustable absorption range, high absorption coefficient, adjustable band gap and high charge carrier mobility have made it used in devices be used [2]. However, an important problem of Metal halide perovskites, especially OIMHPs, is their instability to light, heat, oxygen, ultraviolet (UV) radiation, and other stimuli that cause the loss of the primary crystal structure and decomposition or aggregation [3]. The synthesis of OIMHPs with deep blue emission and their stability is a great challenge for future research in various fields of application. One of the ways to overcome the unstable problem of their coating is by using protective shells such as metal-organic frameworks (MOFs) [4,5]. In this work, a new OIMHPs with deep blue emission and maximum PL emission peaks of locate at 397 nm (λex = 320 nm) was synthesized by ligand-assisted reprecipitation technique (LARP) method, then it was placed in the MOF-5 mesostructure in order to improve the stability and increase the luminescence. OIMHPs /MOF-5 composites powder resulting has stronger deep blue emission, higher photoluminescence intensity and higher thermal and environmental stability than OIMHPs.

Keywords: Organic-inorganic metal halide perovskites (OIMHPs), Metal-organic frameworks (MOFs) , Deep blue emission, Photoluminescence, Shell

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Photocatalytic degradation of methylene blue dye by nanocomposite based on Mg-Al layered double hydroxides

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With the increasing development of industries, water pollution by organic pollutants such as dyes has become a serious environmental crisis [1]. The purpose of this research is to design and synthesize an environmentally friendly nanocomposit based on layered double hydroxide (LDH) to enhance the separation of charge carriers and improve the photocatalytic performance for the decomposition of the cationic dye methylene blue (MB) under visible light irradiation. Composite prepared via hydrothermal and co-precipitation methods.Various analyses including Fourier transform infrared spectroscopy (FT-IR), field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), energy dispersive X-ray (EDX), ultraviolet-visible diffuse reflectance spectroscopy (UV-Vis DRS), Dynamic Light Scattering (DLS) and Zeta Potential and photoluminescence (PL) were conducted to characterize the synthesized samples. Additionally, various electrochemical studies such as electrochemical cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), transient photocurrent (TPC), and linear scanning voltammetry (LSV) were performed to further investigate the synthesized materials and study the fate of electrons generated under light irradiation. The effect of absorption, amount of catalyst and pH on the photocatalytic efficiency of pollutant degradation was investigated and the optimal reaction conditions were determined. Through Scavenger tests , the active agents involved in the photodegradation of MB were identified, and a photocatalytic degradation mechanism for MB was proposed. The synthetic Mg-Al LDH -based composite appears to be very promising for use in a variety of commercial domains and industries in the future. They can also be employed to photodegrade other organic contaminants.

Keywords: Photocatalyst, Layered Double Hydroxide, Methylene Blue

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Functionalization of HMTA and investigation of its catalytic activity in the reaction of CO_2 and epoxide

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In recent years, the conversion of carbon dioxide (CO_2) into valuable compounds has gained significant attention as a way to decrease the green housegas CO_2 [1]. In this study, we focused on the functionalization of hexamethylenetetramine (HMTA) with a halogen and then investigate its catalytic activity for converting CO_2 to cyclic carbonates. HMTA was converted to $HMTA^+X^-$ where X = I, Cl, Br at mild reaction conditions. The synthesized $HMTA^+X^-$ was used as a catalyst in CO_2 conversion with styrene oxide, aiming to produce styrene carbonate [2], which holds great potential as a green solvent and a useful reactant for generating biodegradable polymers [3]. The reaction conditions, including temperature, catalyst loading, and reaction time were accurately optimized through DOE to achieve the highest yields. The results demonstrated that $HMTA^+X^-$ exhibited remarkable catalytic activity and under optimized conditions, we could achieve a yield of >99% for the formation of styrene carbonate. In conclusion, our study presents a successful synthesis of a novel HMTA derivative. We investigate its catalytic activity for CO_2 conversion into styrene carbonate, highlighting its potential for sustainable CO_2 utilization. These results contribute to the development of metal-free catalysts and provide insights into the efficient transformation of CO_2 into value-added chemicals [4].

Keywords: HMTA, Carbon dioxide, Carbon Conversion, Catalysis.

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Synthesis and characterization of a nickel(II) unsymmetrical salen complex as an efficient catalyst for selective oxidation of alcohols

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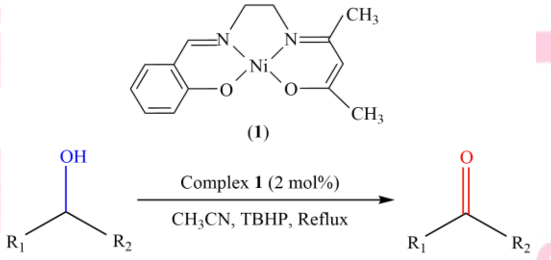
Oxidation of alcohols to the carbonyl compounds is a major transformation in organic synthesis because the carbonyl compounds such as aldehydes and ketones are versatile intermediates for synthesizing various drugs, chemicals, vitamins, and fragrances [1]. Schiff base transition metal complexes are interesting oxidation catalysts owing to their easy synthesis and their chemical and thermal stability. Unsymmetrical Schiff base ligands are important compounds and received much attention due to the bounding of central metal ions with unsymmetrical ligands in natural systems [2]. In the present work, unsymmetrical salen ligand was synthesized in good yield according to the published procedure [3], and then metallated with $NiCl_2.6H_2O$ to obtain complex **1**. The prepared complex **1** was characterized by FT-IR, UV-Vis, ^{1}HNMR, and elemental analysis. The synthesized complex **1** was successfully employed as a new and efficient homogeneous catalyst for selective oxidation of various alchols to the corresponding aldehydes and ketones in acetionitrile under reflux conditions (Scheme1). Good to excellent yields, short reaction times, and use of *tert*-BuOOH (TBHP) as a green oxidant can be mentioned as advantages of this method for oxidation of alcohols.



Scheme 1: Oxidation of alcohols catalyzed by complex **1**

Keywords: Unsymmetrical Schiff base, Nickel(II) complex, Homogeneous catalyst, Selective oxidation, Alcohol

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Oxovanadium(IV) unsymmetrical Schiff base complex as an efficient catalyst for selecive oxidation of sulfides to sulfoxides with H_2O_2

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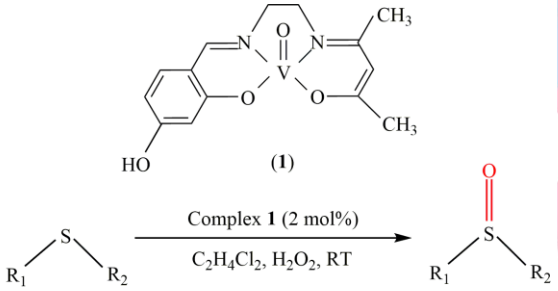
Organic sulfoxides play an essential role in the synthesis of chemically useful and biologically active compounds including drugs, flavors, germicides, and catabolism regulators. Therefore, the selective oxidation of sulfides into the corresponding sulfoxides has taken up a great part in modern synthetic chemistry [1]. Transition metal Schiff base complexes are significant and efficient homogeneous catalysts in the oxidation of organic compounds using different oxidizing agents. Good catalytic activity and selectivity have been reported as the main advantages of homogeneous metal complexes [2].In this work, the oxovanadium(IV) unsymmetrical Schiff base complex (**1**) was synthesized in good yield based on the procedure described in the literature [3]. The synthesized complex **1** was successfully used for selective oxidation of sulfides to sulfoxides with 30% H_2O_2 at room temperature (Scheme1). Good to excellent yields and use of hydrogen peroxide as a green oxidant can be mentioned as advantages of this protocol for the oxidation of sulfides.



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

Keywords: Oxo-vanadium(IV) Schiff base complex, Homogeneous catalyst, Selective oxidation, Sulfide

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Investigation of catalytic activity of oxovanadium(IV) unsymmetrical salen complex in the oxidative coupling of thiols to disulfides with UHP

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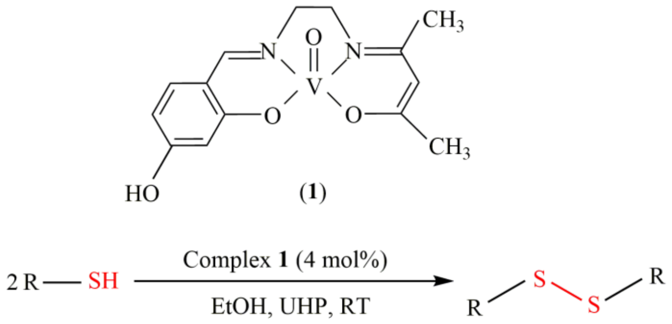
A main reaction in biological and chemical processes is the conversion of thiols to disulfides [1]. The disulfide bond formation in active biochemical molecules, peptides, and sweet oil processing is essential. Besides, disulfides, as a highly beneficial class of compounds, are applied in various industrial and biological processes such as peptide stabilization in proteins, DNA cleavage, vulcanizing agents for elastomers and rubbers, and designing rechargeable lithium batteries [2]. In the present work, the oxovanadium(IV) unsymmetrical salen complex (**1**) was synthesized in good yield based on the the literature [3]. The synthesized complex **1** was successfully applied as a new homogeneous catalyst for oxidative coupling of thiols to disulfides with urea/H_2O_2 (UHP) as oxidant in ethanol as solvent at room temperature (Scheme1). Good yields of products, mild reaction conditions and no formation of by-products can be mentioned as advantages of this method for the preparation of disulfides.



Scheme 1: Oxidative coupling of thiols to disulfides catalyzed by complex **1**

Keywords: Oxo-vanadium(IV) Schiff base complex, Homogeneous catalyst, Selective oxidation, Sulfide

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A Zn-based coordination polymer with good ability for selective detection of mercury ions in solution

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$[Zn(NCS)Cl(L)]_n$ (Zn-SCP) is a one-dimensional coordination polymer with a terminal thiocyanate group. The flexible sulfur donor ligand is bridged between metal centers by the anti-anti-anti conformation which forms an infinite 1D zigzag chain and the third and fourth coordination spheres are occupied by terminal Cl^- and NCS^- anions [1]. Considering the HSAB concept (Hard-Soft Acid Base) [2], N-coordinated thiocyanate as a Lewis base has a good potential for coordinating mercury from its free sulfur atom. In this work, we have used Zn-SCP for the detection of Hg^{2+} from water solution with different consecrations. Mercury has been coordinated to the free sulfur of thiocyanate groups as it was excepted. The IR spectrum of Zn-SCP showed a remarkable shift for the NCS peak from 2070 cm^{-1} to 2120 cm^{-1} which clearly shows the change in the coordination sphere. The white color of Zn-SCP powder was changed to grey by coordination with mercury [3]. It is worth mentioning that Zn-SCP has selectivity in the detection of mercury and there were no changes for other metals such as Pb^{2+}, Cd^{2+}, or copper. FT-IR, UV-visible, and ICP have confirmed the binding of mercury to thiocyanate. The Hg^{2+} ions which are coordinated to the Zn-SCP could be removed from the water solution by simple filtration.

Keywords: Mercury detection; Sulfur coordination polymer; Zn complex; Methimazole based ligands

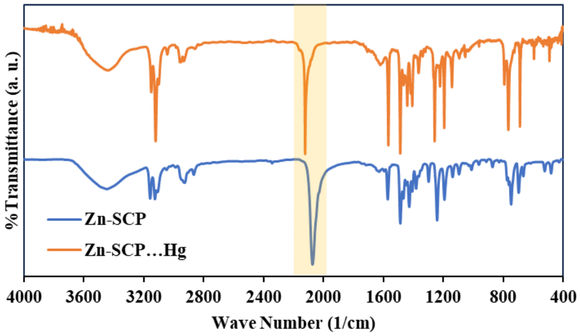

Fig 1. The FT-IR spectra of as-synthesized Zn-SCP and exposed to Hg^{2+} cations.

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Interaction of a new Pd(II)-piperidine complex with CT-DNA using fluorescence spectroscopy

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While the platinum-based anticancer agents have great therapeutic utilities [1], the types of cancer that can be cured with these agents are limited and the drugs exhibit side effects and resistance phenomena. Thus, bioinorganic synthetic chemists are continually trying to prepare non-platinum-based complexes bearing more effective, less toxic, target-specific and interact non-covalently with DNA as a target molecule in the cancer cells [2]. Recently, numerous Pd(II) complexes having higher anticancer activity and lower toxic side effects have been reported [3]. In this study, a new Pd(II) complex with the formula *cis*-$[Pd(pip)_2Cl_2]$, in which pip is the piperidine ligand, was synthesized and characterized. The interaction of the complex with double stranded calf thymus DNA (CT-DNA) was studied by a competitive binding fluorescence experiment using ethidium bromide (EB) as a probe. This study was done at three different temperatures of 298, 305 and 310 K. In these experiments, the fluorescence intensity of EB bound to DNA was quenched considerably on addition of the Pd(II) complex. This indicates that the intercalated EB molecules on ds-DNA could be replaced partially by the Pd(II) [4]. The binding constant (K_b) values in the interaction of the studied complex with CT-DNA were calculated to be 4.5×10^4, 1.7×10^5 and 6.1×10^5 M^{-1} at 298, 305 and 310 K, respectively. The number of binding sites (n) on DNA for this complex was found to be about 1. The obtained results indicate a moderately strong interaction between the Pd(II) complex and CT-DNA, which is probably occur via groove binding. The thermodynamic parameters $\Delta H°$, $\Delta S°$ and $\Delta G°$ in the interaction of the metal complex with CT-DNA were also determined using the results obtained from the fluorescence spectroscopy, which indicate a spontaneous hydrophobic interaction between the Pd(II) complex and DNA.

Keywords: Palladium(II) complex, DNA interaction, Fluorescence spectroscopy Thermodynamic parameters

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Synthesis, characterization and biological study of cyclopalladated(II) complex bearing bioactive ligand

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Organometallic complexes have found numerous applications in targeted cancer treatment, due to the outstanding physicochemical properties including chemical stability and structural diversity. The coordination sphere aroun the metal center seems to have the most important factor in the successful design of potent anticancer agents. Small changes in the ligand architecture can induce particular function or significant capability in the metal complex. Cyclometallated complexes with a metal-to-carbon σ-bond stabilized by chelation, have attracted numerous attention in this field of research. [1-4] In the present study, mononuclear cyclometalated Pd (II) complex containing tyrosine amino acid, was synthesized and characterized via FT-IR and NMR spectroscopic methods. The interaction of the synthesized mononuclear complex with the deoxyribonucleic acid (DNA) and bovine serum albumin (BSA), was studied by UV-Vis absorption and fluorescence emission spectroscopies. Based on the experimental studies, an intercalating mode was proposed for the interaction between the complex and DNA. In addition, the interaction between the complex and the BSA seems to be static while the complex has bound to the hydrophobic binding site of the protein. Molecular docking theoretical calculation successfully confiremed the experimental results.

Keywords: Palladacycle, Cyclometallation, Anticancer, DNA, BSA

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In vitro assay of targeted drug delivery platform based on ZIF-67 nanocarrier containing curcumin on MCF-7 cells

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The targeted delivery of anti-cancer drugs exclusively to tumor cells presents an appealing strategy as it amplifies the therapeutic effectiveness compared to non-targeted medications [1]. To enhance the cellular uptake of chemotherapeutic agents, nanoscale delivery systems incorporating polyethylene glycol (PEG) as a surface covering, along with aptamer-conjugated nanoparticles capable of specifically binding to proteins found on the surface of tumor cells, have emerged as promising solutions. In this study, the Epithelial cell adhesion molecule (EpCAM), which is commonly overexpressed in solid cancers and has recently been identified as a marker for cancer stem cells, was utilized. Ultimately, The ZIF-67 pnanoparticles encapsulating curcumin (Ccm@ZIF-67@PEG@EpCam NPs) were fabricated in-vitro environment and characterized by XRD, SEM, TEM, DLS, TGA and BET methods [2]. Then its release was investigated at two pH of 5.4 citrate buffer and 7.4 saline phosphate buffer. Finally, the cytotoxicity of the synthetic nanoplatform was evaluated by MTT assay on human breast cancer cell line (MCF-7) [3].

Keywords: polyethylene glycol, aptamer, nanoparticle, Epithelial cell adhesion molecule, Zeolitic imidazolate framework-67

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Synthesis and modification of zeolite beta for studying aggregated species

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In this study, zeolite beta with three dimensional structure was synthesized using hydrothermal method by tetraethyl ammonium hydroxide as template[1]. The mesoporous form of the zeolite was obtained by post-synthesis method by adding a surfactant structure-directing agent into a suspention containing the previousely synthesized zeolite. Functionalizing process was done with 3-aminopropyl trimethoxysilane (APTMS) to react effectively with the silicon groups of the surface of zeolite beta in order to provide different space and environment for the loaded species [2]. Methylene blue (MB) was loaded into both in the original microporous and mesoporous zeolite [3]. The effect of functionalization and in the original and mesoporous zeolite beta in the final product were investigated in terms of the loaded amount and some structural features such as monomeric and dimeric forms of the dye (i.e. MB). The prepared materials were characterized by X-ray diffraction, scanning electron microscopy, FT-IR, BET, diffuse reflectance spectroscopy and field effect scanning electron microscopy. There are some differences in relative amount of the different monomeric or protonated forms of the dye upon the structure. we found that there is a special space in zeolite beta that convert MB^{+} to MB^{2+} which is absent in the mesoporous zeolite beta. The details will be demonstrated in the poster provided.

Keywords: Zeolite Beta, Functionalizing, dyes, Loading, Mesoporous formation

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Replacing impact modifiers based on mineral craft (mineral polymer) instead of chlorinated polyethylene in hard PVC pipes and fittings industries

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. In this article, the effect of using inorganic polymer additive IM20-80 (Kraft impact modifier) instead of chlorinated polyethylene on mechanical properties, especially the impact behavior of hard polyvinyl chloride, with the formulation of materials for PVC connection systems is studied Raw materials include PVC resin, thermal stabilizer, filler, pigment, and compared. has taken. internal and external lubricants, and impact modifiers, including two types of additives, one is IM20-80 kraft base modifier, a product of the leading Baspar Sepahan company, and the other is First, the materials were mixed in a turbo mixer and اpolyethylene. Chlorine grade A135 in China. then converted into PVC joints by an injection machine and subjected to qualitative tests in accordance with the relevant national standards in the mechanics laboratory of Azad University of The results of mechanical .Najaf Abad and the laboratory of Hamgam Manufacturing Company. impact tests (falling weight) and bending show that by keeping the rest of the formulation components constant and changing the type and amount of impact modifier used in joints (substituting IM20-80 instead of chlorinated polyethylene), the mechanical properties of The Therefore, this replacement of the opinion of the criteria of the national standards was accepted formulation in raw materials, by changing the amount of modifier consumption, can be economical in terms of economic efficiency. It should be noted that both samples meet the requirements of impact, compression, indentation and wicket tests according to the relevant national standards.

Keywords: rigid polyvinyl chloride joints, impact modifiers, mechanical properties.

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Photodegradation of some organic dyes by Nd-doped pyrotitanate nano-sponges as visible light catalysts

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$A_2B_2O_7$ mixed metal oxides are interested for their possible applications. $A_2B_2O_7$ compounds are used as photocatalyst for water splitting [1]. The compounds have an excellent power for fixing matrices of highly active radionuclides from nuclear wastes [2]. They are also used in electrochemical devices due to their ionic conductivity . Besides, $A_2B_2O_7$ compounds are known for their piezo-/ferroelectric properties, used for high temperature devices, and for their attractive photo-luminescent properties when associated with other lanthanide ions [3–4]. $Nd_2Ti_2O_7$ nano-sponges were fabricated via a conventional solid state rout at 800 ºC for 8 h when Nd_2O_3 and TiO_2 were used as raw materials. Crystal structural analyses and purity of the obtained materials were analyzed by *FullProf* program that used profile matching condition with constant scale factor. Field emission scanning electron microscope (FESEM) was applied to study the morphology of the fabricated samples. Ultraviolet – Visible (UV-Vis) spectroscopy showed that the direct optical band gap energies was 3.40 for $Nd_2Ti_2O_7$. The synthesized nanomaterials were used as heterogeneous photocatalysts for the degradation of some water pollutant organic dyes under direct visible (with fluorescent light with 40 W Power) and UVC lights illumination. Malachite green (MG) was used as a typical dye to obtain the optimum photocatalytic degradation conditions. The photocatalytic performance of the as-fabricated samples on the degradation of the pollutant dyes was studied under visible and UVC light irradiations. The optimum conditions were 35 mg of catalyst, 0.05 mL of H_2O_2 and 40 min reaction time. The photocatalytic reaction yield was 97% at the present conditions.

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Keywords: $Ln_2Ti_2O_7$, heterogeneous photocatalyst,Degradation, Malachite Green

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Synthesis, characterization and DFT calculation of naphthalene-based crystal structure with pyridylimine-binding units

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Naphthalene-based structures and imine systems have diverse multidisciplinary applications, including the assembly of cyclophanes, helicates, dimers, trimmers, and grids[1-3]. The authors synthesized a compound using 1,6-diaminonaphthalene and pyridine-2-carbaldehyde through refluxing in extra-pure ethanol. The resulting crystal was characterized using single crystal X-ray diffraction. The article describes a crystal structure consisting of two pyridylimine-binding units linked to a 1,5-naphthalene. The structure is connected by C-C, C-H, and π-stacking interactions to form a three-dimensional structure. The crystal has four units with two orientations in each unit face of the unit cell and belongs to the monoclinic space group P2(1)/c. The structure was fully verified through infrared examination. The infrared examination showed a strong peak at 1288 cm^{-1} due to aromatic amine stretching frequency, two medium peaks related to CH$_2$ and CH$_3$ deformation, and a medium peak at 1472 cm^{-1} corresponding to the symmetric bending vibration of the CH$_2$ group. The absence of hydrogen atoms bonded to highly electronegative atoms in the structure suggests that its physical and chemical properties, such as melting point, boiling point, solubility, and reactivity, are not affected. The absence of hydrogen bonding interactions can have various effects in different applications. Additionally, we included computational results for NMR, Raman, and charge distribution using the Gaussian software.

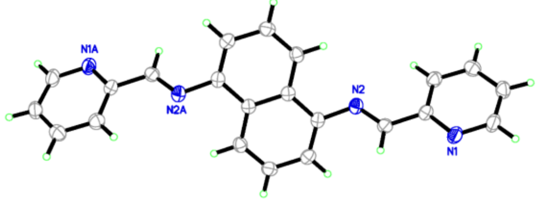

Fig.1.Molecular structure of Ligand

Keywords: Schiff-base, Aromatic, weak interaction, Crystal structure, DFT.

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Lanthanide Coordination Polymers as Heterogeneous Lewis Acid Catalysts for Glycerol Acetalization

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Coordination polymers containing lanthanide ions (LnCPs) have received relatively less attention compared to d-block metal coordination polymers, despite their potential for remarkable luminescence, catalytic activity, and magnetic properties [1,2]. LnCPs have shown promise as Lewis acid catalysts for various chemical transformations. Lewis acids are electron acceptors that can facilitate chemical reactions by accepting electron pairs from other molecules [3]. The use of lanthanide ions as Lewis acid catalysts is of particular interest, and researchers have been exploring their potential in this area [4]. $[Er_2(bpndc)_3(DMF)_2]$ (**1**) and $[Yb_2(bpndc)_3(DMF)_2]$ (**2**) were synthesized by combining Benzophenone-4,4'- dicarboxylate (bpndc2-) linker, Erbium nitrate hexahydrate, Ytterbium nitrate hexahydrate, respectively, using a facile solvothermal reaction and characterized using single crystal X-ray diffraction, Fourier transforms infrared spectroscopy, Thermogravimetric analysis, Powder X-ray diffraction, and Scanning electron microscopy. Both compounds exhibit good thermal and solvent stability. These coordination polymers were used as heterogeneous Lewis acid catalysts for glycerol acetalization. The investigation has focused largely on the effect of reaction time and temperature, and catalyst to glycerol molar ratio. Optimal conditions for these two polymers included a duration of 4 hours, a temperature of 50º C, a molar ratio of 1 to 10 catalyst to glycerol, and a conversion percentage was 77% for $[Er_2(bpndc)_3(DMF)_2]$ polymer and 72% for $[Yb_2(bpndc)_3(DMF)_2]$ polymer. The catalysts leaching, stability, and recyclability were investigated. This study shows the potential role of the $[Er_2(bpndc)_3(DMF)_2]$ and $[Yb_2(bpndc)_3(DMF)_2]$ as heterogeneous Lewis acid catalysts for glycerol acetalization.

Keywords: Coordination polymers, Lanthanides, Lewis acid catalysts, Acetalization

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Design, synthesis, properties, and applications of perovskite nanomaterials

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The structural formula ABO_3 describes perovskite oxide in general [1]. Perovskite oxides have garnered a lot of interest because of their high activity, abundance, and availability along with their optical and electrical properties, chemical stability, and lack of toxicity [2]. Perovskite oxide's ability to act as catalysts in a variety of chemical processes is one of their most significant chemical characteristics. One of the advantages that significantly contributes to the catalytic capabilities of these compounds is their durability at high temperatures as well as the presence of A and B interchangeable cationic sites [3]. This presentation provides a broad overview of recent developments in perovskite oxide applications and synthesis methods.

Keywords: Perovskite oxides, Catalysts

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Investigation of adsorption kinetics of phenobarbital on Fe_3O_4/SBA-16-NH_2 nanocomposite

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In traditional drug delivery systems, the drug is distributed throughout the body through the circulatory system, and due to the distribution of the drug throughout the body, only a small percentage of the drug reaches the target tissues [1,2]. The purpose of targeted drug delivery is to increase the drug concentration in the target tissue and decrease its concentration in other tissues [3]. To achieve this goal, the designed systems must be such that the body's defense system is not stimulated and the carriers can stay longer in the bloodstream and reach the target tissue to a greater extent [4]. In this study, the kinetics of phenobarbital drug absorption on Fe_3O_4/SBA-16-NH_2 magnetic nanocomposite as a drug carrier was investigated. For this purpose, Fe_3O_4/SBA-16-NH_2 magnetic nanocomposite was synthesized in the first step. Then, zero-order, pseudo-first-order, pseudo-second-order, and Higuchi models were investigated to find the best kinetic model of phenobarbital drug absorption on Fe_3O_4/SBA-16-NH_2 magnetic nanocomposite. The results showed that the loading process of phenobarbital in Fe_3O_4/SBA-16-NH_2 magnetic nanocomposite is consistent with the pseudo-first order model. Figure 1 shows the synthesis strategy of Fe_3O_4/SBA-16-NH_2 nanocomposite and its application in phenobarbital drug loading and release.

Keywords**:** Adsorption; Response Surface Methodology; Phenobarbital; Fe_3O_4/SBA-16-NH_2; Drug Delivery.

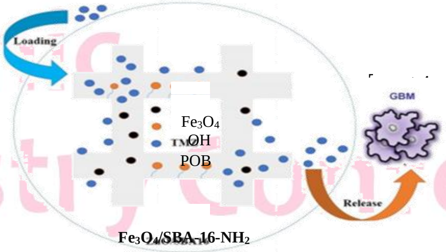

Figure 1. Synthesis strategy of Fe_3O_4/SBA-16-NH_2 nanocomposite and its application in phenobarbital drug loading and release

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Synthesis, characterization, DFT studies, and molecular docking of Fe(III) complex containing β–amino alcohol ligand

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In this project, a new complex of Fe(III), $[Fe(L)(NO_3)(H_2O)_2]^{2+}$ (L: (2-((2-((2-hydroxyethyl)amino)ethyl)amino)cyclohexane-1-ol)), was prepared and identified by elemental analysis, FT-IR spectroscopy, and DFT studies. The L unit is a potentially tetradentate ligand that can be bound to the metal atoms through two N-atoms and two O-atoms but in this complex, the ligand acted as tridentate and formed two five-membered chelate rings. As shown in the structure of the compound (Figure 1), the complex has a FeN_2O_4 environment, so the coordination number of the Fe(III) ion is 6 which proves that the geometry of the complex is octahedral. The structure was optimized with the Gaussian 09 software [1] and calculated for an isolated molecule using Density Functional Theory (DFT) [2] at the B3LYP/6-31G(d,p) and B3LYP/LanL2DZ level of theory for L and complex, respectively. However, since Gaussian provides the sum of electronic and thermal free energies, there is a shortcut: namely, to simply take the difference of the sums of these values for the reactants and the products. For example, using the information extracted from Gaussian, the Gibbs free energy of the reaction can be calculated simply by: $\Delta G = \Delta G_{products} - \Delta G_{reactants} = -0.136946$ u.a [3]. Molecular docking showed that the complex has close fitness scores (In interaction with the CatB protein) compared to doxorubicin (anticancer drug) thus we suggest that studying the anticancer activities of this compound could be interesting (Figure 2).

Keywords: Amino Alcohol, Free Gibbs Energy, DFT Calculation, Docking Study

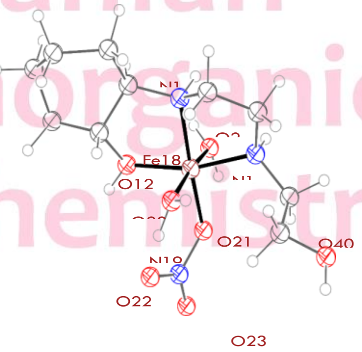

Figure 1.The ortep diagram of

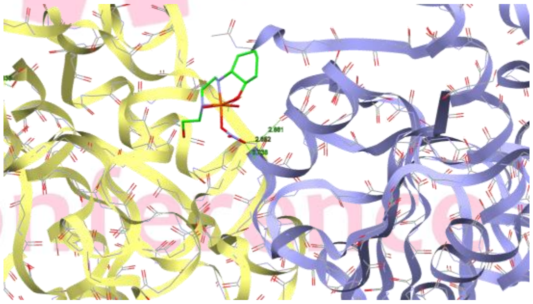

Figure 2. Docking study results, showing the interaction between the complex and CatB protein

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A new mixed-ligand Cobalt(II) complex with synthesis, characterization, and docking study

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A new mixed-ligand complex [1] has been synthesized by the reaction of Co(II) ion with 2-(2-(2-Hydroxyethylamino)ethylamino)cyclohexanol (HEAC) in the presence of pyridine-2,6-dicarboxylic acid, (PDCA), and identified by elemental analysis and FT-IR spectroscopy. In the complex, the HEAC coordinates through two N-atoms, and PDC coordinates through one N- and two O- which forms three five-membered chelate rings. As shown in Figure 1, the coordination number of the complex is 5. The τ value is calculated to be 0.10 for the Co atom, indicating a distorted square-pyramidal geometry [2]. The data obtained from molecular docking revealed that the complex has a higher docking score than the doxorubicin in reaction to CatB protein, thus we suggest that the anticancer activity of this compound will be studied (Figure 2).

Keywords: Mixed-ligand complex, Pyridine dicarboxylate, Square-pyramidal geometry, Molecular docking

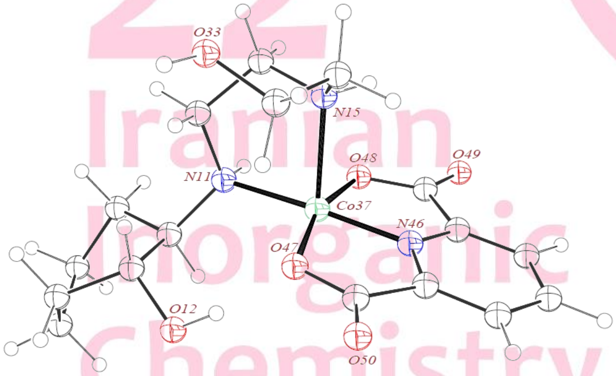

Figure 1.The ortep diagram of complex.

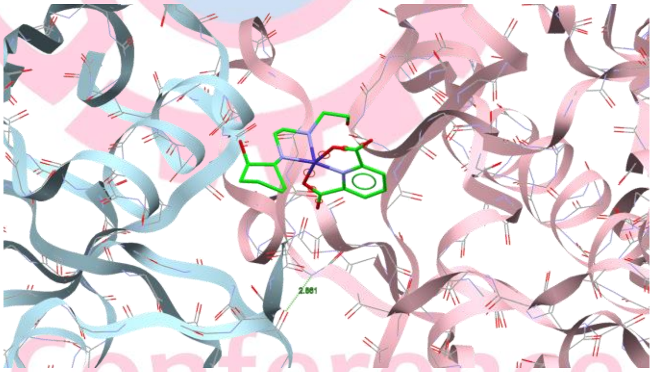

Figure 2. Docking study results, showing the interaction between the complex and CatB protein

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Review of the synthesis methods of layers of double hydroxide and their application in removing water pollutants

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In recent decades, a class of anionic clays known as layered double hydroxides (LDHs) or hydrotalcite-like compounds (HTlc) has attracted substantial attention. The structure of LDHs is the intercalation of anions in the hydrated interlayer regions. Double layer hydroxides belong to a group of clay minerals, that have physical and chemical properties very close to clay minerals and are known as anionic clays. These compounds are obtained naturally and synthetically. LDHs can be represented by the general formula$[M^{2}{}_{1-X}.M^{3}{}_{X}(OH)^{X+}]$ $(A^{n-}{}_{x/n}).mH_2O$ where M^{2+} and M^{3+} are divalent and trivalent cations, respectively; the value of x is equal to the molar ratio of $M^{3+}/(M^{2+}+M^{3+})$, whereas A is the interlayer anion of valence n. The identities of M^{2+}, M^{3+}, x, and An may vary over a wide range, thus giving rise to a large class of isostructural materials with varied physicochemical properties. LDHs exist as naturally occurring minerals, they are also relatively simple and economical to synthesize. LDHs have relatively weak interlayer bonding and, as a consequence, exhibit excellent ability to capture organic and inorganic anions. The most interesting properties of LDHs include large surface area, high anion exchange capacity (2–3meq/g) that is comparable to those of anion exchange resins, and good thermal stability. LDHs have been studied for their potential use in a wide range of important areas, i.e. catalysis, photochemistry, electrochemistry, and polymerization, considerable interest in using LDHs to remove environmental contaminants since environmental pollution has emerged as an important issue in recent decades. Significant progress has been achieved in the research and development of LDHs' application in environmental protection, such as their use as environmental catalysts in removing organic and inorganic wastes. Indeed, increasing interest has recently been diverted to evaluating the ability of LDHs to remove inorganic contaminants such as oxyanions (e.g. arsenite, chromate, phosphate, selenate, borate, nitrate.) and monoatomic anions (e.g. fluoride, chloride, bromide, and iodide) from aqueous solutions by the process of adsorption and ion exchange [1]. This review article provides an overview of LDH synthesis methods and LDH characterization techniques.

Keywords: Layered Double Hydroxides, Brucite-like Sheets, Anionic Clays

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Behaviors of electrochemical energy storage sources, based on organometallic frameworks and their composites

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Metal-organic frameworks (MOFs), which are constructed through inorganic vertices and organic ligands, have attracted the attention of a wide range of research communities due to their diversity in construction and composition. Recently, MOFs have been considered suitable substrates in the field of electrochemical energy storage (EES), and many MOFs used in electrochemical fields show unique functions. In this article, I intend to briefly introduce the synthesis strategies applications, and composites of MOFs, as well as the general and electrochemical mechanisms of MOFs in lithium-ion batteries and supercapacitors (SCS). It is expected that these investigations will play an effective role in the development of MOFs and their composites in relation to electrochemical mechanisms [1].

Keywords: Organo-metallic Frameworks (MOFs) Composites, Lithium-ion Batteries, Supercapacitors

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Isotopic effects on the hydrolysis of anticancer drug titanocene dichloride: a DFT study

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Anticancer activity of titanocene dichloride namely bis (cyclopentadienyl) titanocene dichloride, Cp_2TiCl_2, Cp = η^5-($C_5H_5)_2$) has been discovered in the 1980s, and since then it has attracted continuous attention in the experimental literature [1-7]. In this work, hydrolysis of the anticancer drug titanocene dichloride complex was illustrated using the quantum mechanical method. BP86 functional and basis sets of 6-311G(d,p) and Def2-TZVPPD for the main group element and Ti atoms, respectively, were considered. Two typical reactions involved in the complex hydrolysis include the first and second hydrolysis processes: first hydrolysis: $[Cp_2TiCl_2].H_2O$ (R1A) → $[Cp_2TiCl\ (OH_2)]Cl$ (PA1) and second hydrolysis: $[Cp_2TiCl(OH_2)]^+.H_2O$ (R2A) →$\{[Cp_2Ti(OH_2)_2].Cl\}^+$ (PA2). It was tried to show how the thermodynamic, and kinetic parameters of titanocene dichloride hydrolysis were affected by the replacing of hydrogen atoms of Cp ligand with deuterium.

Keywords: Anticancer Drug, Isotopic Effects, Hydrolysis, Titanocene Dichloride

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Synthesis and investigation of biological activity of a magnetic nanocomposite based on functionalized graphene oxide nanosheets by casein, Zn-Al LDH, and alginate hydrogel

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Due to the increasing prevalence of diseases and their effects, the field of biomedicine, especially tissue engineering and wound healing, is a rapidly growing area of research [1-3]. Researchers are adopting new strategies to promote wound healing, and nanomaterials are playing an increasingly important role in these efforts [4-5]. Regarding this, we fabricated a novel nanobiocomposite using graphene oxide (GO), casein, LDH (Zn-Al), sodium alginate, and Fe_3O_4 magnetic nanoparticles. The GO was synthesized by a modified Hammer's method, and then its surface was covalently functionalized with casein protein. The functionalized GO was then combined with the as-synthesized LDH (Zn-Al). The composite was then conjugated with alginate hydrogel via the gelation process. Finally, the nanobiocomposite was magnetized by in-situ magnetization. The nanobiocomposte (GO/CS/LDH/Alg/Fe_3O_4) was fully characterized using several techniques, including FT-IR, FE-SEM, EDX, XRD, TGA, and VSM. The cell viability method, hemolysis, and anti-biofilm assays were performed to explore the biological capability of the nanocomposite. The results of the MTT assay showed that the viability percentages of Hu02 cells treated with the nanocomposite after 24, 48, and 72 hours of incubation were 93.08%, 91.64%, and 91.19%, respectively. The hemolytic effect of the nanobiocomposite was 3.84%. The measured bacterial growth inhibition percentages of *E. coli* and *S. aureus* bacteria in the presence of the nanobiocomposite were 52.18% and 55.72%, respectively. Overall, the results of this study demonstrate that the novel nanocomposite has good biocompatibility and antibacterial and anticancer activity. It is a promising candidate for use in tissue engineering applications.

Keywords: Graphene oxide, Alginate, Nanoparticles, Layered Double Hydroxide, Biomaterial.

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Synthesis, structure, and catalytic activity of novel polyoxomolybdate $C_{22}H_{47}Mo_4N_{12}O_{15}$ in the azide-alkyne cycloaddition reaction

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A new polyoxomolybdate with a formula of $(C_7H_{15}N_4)_3[CH_2Mo_4O_{15}]$ was synthesized and then it was characterized using IR, EDX, and X-ray crystallography. The unit cell of 1 consists of three N-methyluroptropine $(C_7H_{15}N_4)^+$ cations, and one polyanion $[CH_2Mo_4O_{15}]^{3-}$ (Figure 1). In the polyanion $[CH_2Mo_4O_{15}]^{3-}$, molybdenum metals are surrounded by two terminal and two bridging μ2-oxygen atoms, one μ_4- bridging hydroxyl ligand and also one oxygen of the methanediol ligand is coordinated to each molybdenum metal. This novel polyoxomolybdate was used as an efficient catalyst for the azide–alkyne cycloaddition reaction to produce various 1,2,3-triazoles in high yields. During this cycloaddition reaction, some effective parameters on the reaction such as the amount of catalyst, reaction temperature, and time of reaction were studied [1].

Keywords: Polyoxomolybdate, Catalytic activity, Azide-alkyne cycloaddition reaction.

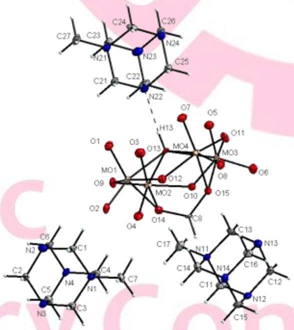

Figure 1. View of the $(C_7H_{15}N_4)_3[CH_2Mo_4O_{15}]$ with labeling of the atoms

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Synthesis of Cu-BTC@Fe_3O_4 nanocomposites for removal of arsenic from water followed by electrothermal atomic absorption spectrometry determination

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Arsenic is one of the toxic heavy metals, which is found in soil, air, and water resources [1,2]. Arsenic contamination can cause serious health problems, including skin damage, heart, liver, and bladder cancer, and death [3,4]. World Health Organization (WHO) and the Environmental Protection Agency (EPA) classified arsenic as the first priority contaminant among hazardous substances and declared that the limit of arsenic concentration for drinking water is less than 10 ppb. Accordingly, several technologies have been developed to eliminate arsenic from drinking water including reverse osmosis, chemical coagulation, membrane filtration, ion exchange, and adsorption methods. Because of its robust usage, high efficiency, and cost-effectiveness, adsorption proved to be one of the most promising and efficient remediation techniques for As removal. A wide range of adsorbents, including boehmite, alumina, activated carbon, hydrated ferric oxide, fly ash, clays, chitosan resins, activated alumina, and cation-exchange resins have been reported for arsenic removal. However, most of the established adsorbents have many limitations such as unsatisfactory capture capacity, slow kinetics, and poor selectivity increasing the need for new efficient adsorbents. In this work, Cu-BTC@Fe_3O_4 nanocomposites were synthesized by growing H_3BTC thin layers joined by carboxyl groups onto Fe_3O_4 nanoparticles for the removal of arsenic from water. The prepared sorbent was characterized using X-ray diffraction (XRD), vibration sample magnetometer (VSM), scanning electron microscopy (SEM), and Fourier transform infrared (FT-IR) techniques. Several factors that may affect the adsorption process, including sample pH, sorbent amount, and adsorption time were optimized. The adsorption isotherm indicated that As adsorption fitted best to the Freundlich isotherm model and the maximum adsorption capacity was 91.32 mg/g.

Keywords: Cu-BTC@Fe_3O_4 Nanocomposites, Removal, Arsenic

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Structural, reactivity, and optical properties of homo and hetero binuclear cycloplatinated(II) complexes with bridging cyanide

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Coordination-driven self-assembly and metallophillic interactions provide power tools to construct bi-tri-or extended supramolecular luminescent structures featuring different and rich excited states with applications in different fields([1]). Herein, we present a series of homonuclear and heteronuclear cycloplatinated(II) complexes featuring cyanide ligands. Homobinuclear symmetrical $(NBu_4)[Pt_2(C^\wedge N)_2(p\text{-}MeC_6H_4)_2(\mu\text{-}CN)]$ were prepared by reaction of the corresponding mononuclear anionic complexes $Q[Pt(C^\wedge N)(p\text{-}MeC_6H_4)(CN)]$($C^\wedge N$ = bzq, ppy, dfppy) with $[Pt(C^\wedge N)(p\text{-}MeC_6H_4)(SMe_2)]$ ([2]). By contrast, neutralization reactions with one equivalent of $TlPF_6$ provide heteronuclear Pt-Tl compounds with excellent yield. Their structures were confirmed by single crystal X-ray diffraction and, as an illustration, the structures of $(NBu_4)[Pt_2(dfppy)_2(p\text{-}MeC_6H_4)_2(\mu\text{-}CN)]$ and $[\{Pt(bzq)(C_6F_5)(CN)\}Tl(THF)]$ are shown in Figure 1a-b. The photophysical properties of all compounds were studied in powder, polymer films, and solution states. While the precursors and diplatinum complexes display in rigid media, structured emissions ascribed to typical mixed $^3LC/^3MLCT$ excited states, the heteronuclear Pt-Tl compounds, exhibit unstructured strong emissions associated to the formation of metallophillic Pt-Tl bonds. Furthermore, the Pt-Tl compounds show in solid state reversible vapochromic and vapoluminiscent response to some organic solvent such as MeOH and mechanochromic behavior by simple grinding. As an example, the solvatochromic behavior of $[\{Pt(bzq)(C_6F_5)(CN)\}Tl(THF)]$ is given in Figure 1c.

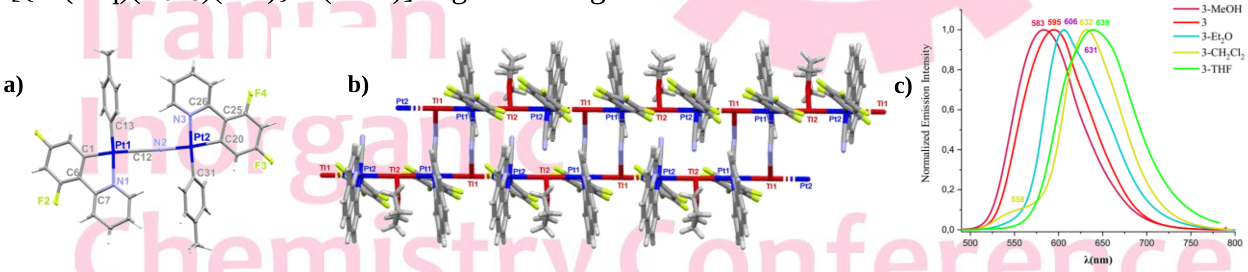

Figure 1. a) View of the molecular structure of $\mathbf{(NBu_4)[Pt_2(dfppy)_2(\mathit{p}\text{-}MeC_6H_4)_2(\mathit{\mu}\text{-}CN)]}$, b) $\mathbf{[\{Pt(bzq)(C_6F_5)(CN)\}\text{-}Tl(THF)]_n}$, c) Normalized emission spectra of the orange solid $\mathbf{[\{Pt(bzq)(C_6F_5)(CN)\}Tl(THF)]}$, and ($\mathbf{[\{Pt(bzq)(C_6F_5)(CN)\}Tl(THF)]\text{-}solvent}$). ($\lambda_{ex}$ 405, 415nm).

Keywords: CycloPlatinated, metallophillic ineractions, cyanide.

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A comparative study of Pd/Pt-cyclopropa[60]fullerenes compounds with ambidentate phosphorous ylide ligands; Synthesis and DFT calculations

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Functionalization of fullerenes C_{60} and investigation of their new properties, in particular, biological and reactivity studies of these compounds have attracted the attention of academic researchers in the past decades [1]. Although there are many reports of metallofullerenes [2], few studies have focused on the Pd/Pt-cyclopropa[60]fullerene complexes bearing phosphorus ligands [3]. Among them, the simple mono- and diphosphines are the most widely used ligands coordinated to C_{60} and neutral Pd(0)/Pt(0) core which form metallacyclopropa[60]fullerene complexes [4]. Versatile functionalized diphosphines, especially α-keto stabilized phosphorus ylides can coordinate to transition metal ions through the terminal PPh_2 group and/or formally negatively charged carbanion [5]. In this work, the reaction of C_{60} with $[Pd/Pt(dba)_2]$ (dba= dibenzylideneacetone) and phosphorus ylides $[Ph_2P(CH_2)_nPPh_2C(H)C(O)C_6H_4\text{-}m\text{-}OMe]$ (n=1, (**L^1**); n=2, (**L^2**)) gave the new Pd/Pt-[60]fullerene complexes These complexes have been fully characterized by spectroscopic methods (^{1}H, ^{13}C, and ^{31}P) and other conventional techniques such as IR, elemental analysis and mass spectrometry. Theoretical studies confirmed the P, C-chelation and P-coordination behaviors of ligands **L^1 and L^2**, respectively.

Keywords: Synthesis, Pd/Pt-[60]fullerene Complexes, Phosphorus Ylide, DFT Studies, Multinuclear NMR

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Synthesis, X-ray structural and catalytic activity of new asymmetric palladacycle complexes with bidentate (P,P- and P,O) ligands

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One of the most important research areas in organometallic chemistry is C-H bond activation in cyclopalladated complexes [1, 2]. Palladacycles have been known for over 30 years [3] and have gained great interest due to their applications in many areas including organic synthesis [4]. The interest in cyclopalladated complexes derived from *N*-donor ligands has increased considerably and it is due to their extremely high catalytic activity in a variety of important C–C coupling reactions [5]. This work reports the preparation of the mononuclear derivatives $[(K^2\text{-}C_6H_4CH_2NH_2)Pd(K^2\text{-}\mathbf{L})](ClO_4)$ (**L** = dppp and dppmo). The results of these studies including the full characterization of the obtained complexes (performed by X-ray structural, IR, and multinuclear NMR techniques and also the application of the new asymmetric cyclopalladated benzylamine as a catalyst precursor for the Suzuki reaction) are presented, and discussed in this paper. The palladacycle complexes proved to be excellent catalysts for the Suzuki reactions of various aryl halides. Therefore, in order to examine the catalytic activity of Pd(II) complexes in the Suzuki reaction, the reaction between bromobenzene with phenylboronic acid in the presence of catalyst Pd was chosen as the model reaction. Influences of different parameters such as base, temperature, solvent, and catalyst concentration have been examined to obtain the best possible combination.

Keywords: Synthesis, Palladacycle Complexes, X-ray Structure, Bidentate Ligands, Suzuki Coupling

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Graphitic carbon nitride nanotubes grown on carbon paper for efficient electrocatalytic hydrogen evolution reaction

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The growth in population and decreasing sources of energy have been a challenge in recent years. Among several energy sources, the production of hydrogen from the process of water splitting has been of interest [1]. Hydrogen reduction reaction (HER) plays an important role in various renewable energy devices and fuel cells. Currently, the state-of-the-art HER, catalyst is Pt, but their long-term availability is questionable owing to the scarcity and subsequent high cost. Therefore, substantial efforts have been devoted to developing non-noble transition-metal-based and metal-free electrocatalysts with commensurate performance. Hydrogen production from water using active semiconductor photocatalysts is an attractive solution to increasing energy demand. Recently, graphitic carbon nitride nanotubes (g-C_3N_4 NTs) have drawn considerable attention due to their unique and tunable nanostructure, good chemical stability,earth-abundant, high nitrogen content, easy synthesis, and conductivity[2,3]. To increase the photocatalytic activity of g-C_3N_4 NTs, carbon paper (CP) has been used to achieve effective photocatalytic for hydrogen production. In this work, g-C_3N_4(NTS) nanocatalyst was synthesized by precursor melamine and $Co(NO_3)_2.6H_2O$.In the next step g-C_3N_4(NTS) is used for growing upon CP. The prepared nanocatalyst was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Attenuated total reflection infrared spectroscopy (ATR-IRS). Several factors that may affect the hydrogen release rate process, including the amount of Co, and electrodeposition time were optimized. The electrochemical diagram indicated that the CP-g-C_3N_4(NTS) provides a higher specific activity than g-C_3N_4(NTS) and CP. In this study, the CP-g-C_3N_4(NTS) structure is developed as the cost-effective catalytic showing remarkable versatility for HER with high stability and activity, which originates from increased exposure and accessibility of active sites, improved vectorial electron transport capability and enhanced release of gaseous products.

Keywords: Graphitic Carbon Nitride Nanotubes, Carbon Paper, Hydrogen Evolution Reaction

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Synthesis and Characterization of $Nd_2CuFe_2O_7$ Magnetic Nanocomposites

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Multi-phase solids that have one of the components with features between 1 and 100 nm, refer to nanocomposites or structures that have repeating distances in the nanoscale between the different phases that make up the material or structures with repeating distances in the nanoscale between the different phases that make up the material [1]. The recent work reports the synthesis of $Nd_2CuFe_2O_7$ nanocomposites (NCuFO) by the Co-precipitation method. The synthesized nanocomposites were characterized by Fourier transfer infrared (FT–IR) spectroscopy, X-ray diffraction, and transmission electron microscopy. The alternating gradient force magnetometer illustrates the magnetic behavior of mixed metal oxides of $Nd_2CuFe_2O_7$ nanocomposites. The results show that uniform particles in nanometer sizes have been synthesized.

Keywords: Nanocomposites, Co-precipitation, Magnetic**,**

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Investigating the Photocatalytic Application of $Nd_2CuFe_2O_7$ Nanocomposite to Remove Organic Dyes

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Photocatalyst degradation of dyes or organic pollution in wastewater is one of the methods of removing these pollutants. These methods have advantages including the total deterioration of contaminations, being environmentally friendly, and sustainable treatment technology to protect the environment, possibly in a less expensive method. [1,2] In this work The photocatalytic property of $Nd_2CuFe_2O_7$ nanocomposites were investigated using the photodegradation of methyl violet, and malachite green oxalate and Erio chrome black T, under ultraviolet light irradiation at various parameters such as temperature, pH of the solution, dye concentration, catalyst amount and time UV radiation. The results show that these nanocomposites have applicable photocatalytic performance.

Keywords: Nanocomposites, Photocatalyst, Degradation, Methyl violet, Malachite Green

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Investigating catalytic effects of a zeolitic imidazolate framework, ZIF-8, on the phase transition and thermal decomposition of ammonium nitrate

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Composite solid propellants are widely used in space and military missions [1]. consist of two major components, i.e., a gas-producing solid oxidizer and an organic, metal fuel and Perchlorates [2]. AN, which has extensive applications in the area of nitrogen fertilizers and explosives, is of interest as a potential replacement for AP, due to its environmentally innocuous products, and positive oxygen balance (+20%) [3]. The advantages of AN-based propellants can be expressed as their low cost, smooth burning without smoke, and production of a high volume of gases [4]. Using the AN in large missile motors, despite these privileges, is restricted due to some disadvantages such as the room temperature volume changing phase transformations, adsorption of moisture, low energy, and low burning rate [5]. In this work, the phase transitions and the thermal decomposition of AN were investigated under the influence of a zeolitic imidazolate framework (ZIF-8). Different percentages of AN/ZIF-8, i.e., 0.95:0.05, 0.9:0.1, and 0.85:0.15, were prepared by the solvent methods, and their phase transition and thermal decomposition have been studied by TG-DSC. To investigate the interactions between AN and ZIF-8, the UV–Vis-DRS and XRD techniques were used.

Keywords: Ammonium Nitrate, Phase Transition, Thermal Decomposition, Zeolitic Imidazolate Frameworks, ZIF-8.

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Investigating the Catalytic Effects of MOF-199 on the Thermal Decomposition of Ammonium Dinitramide (ADN)

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Understanding the decomposition behavior and combustion products of composite solid propellants is of significant interest. Nowadays, ammonium perchlorate (AP) is extensively used in composite solid propellants as an oxidizer [1, 2]. AP has the highest effective oxygen content among the oxidizers, i.e., its oxygen balance is up to +34%. However, since AP contains Cl, the combustion of AP-based propellants generates significant quantities of HCl as a reaction product [3], which is a toxic gas and its emission is an environmental concern. Moreover, the HCl produces a large amount of smoke in the tail of the rocket [4]. In order to overcome this problem, a new green oxidizer as a possible replacement for ammonium perchlorate (AP) has been investigated in recent years. ADN is a metal-free energetic compound with the chemical formula of $NH_4N(NO_2)_2$ and is composed of ammonium cation (NH^{4+}) and the dinitramide anion ($(N(NO_2))^{2-}$), It has a high oxygen balance (+25.8%), which is used in military explosives and smokeless solid propellants or green propellants [5]. In this work, the effect of MOF-199 on the thermal decomposition behavior of ADN was studied. Different compositions of ADN/MOF-199, i.e. 98:2, 95:5, 92.5:7.5, and 90:10%, were prepared by the solvent method and their thermal behavior has been studied by DSC. Accordingly, MOF-199, in spite of its low weight, improves the thermal decomposition behavior of ADN significantly. In addition, the rapid catalytic combustion of ADN/MOF-199 (90:10) was shown in a sharp exothermic peak. The results showed that MOF-199 can be introduced as an excellent catalyst for modifying the combustion of ADN, due to its porous structure, Lewis/Bronsted acid sites, and dispersed metallic sites

Keywords: Ammonium dinitramide, Thermal Decomposition Behavior, Decomposition Temperature, Metal-Organic Frameworks, MOF-199

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Synthesis and characterization of a new green high energetic primary explosives Couper (I) with sodium 5-nitrotetrazole

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Primary explosives are sensitive than secondary explosives and propellants [1]. When the primary explosives subjected to a flame, heat, impact, electric spark or friction are generated a detonation wave .This compounds are used in small quantities in initiating devices such as detonators for military and civil applications [2-5]. In the present paper, a new green high energetic primary explosives [Cu(NT)x] using sodium 5-nitrootetrazole (NaNT) as a ligand was synthesized and characterized by applying Fourier transform infrared (FT-IR) spectroscopy, elemental analysis, Ultraviolet (UV-Vis) spectroscopy and Inductively coupled plasma (ICP) spectroscopy,. The results of spectral and characterizations showed that the structure of a new green compound is [Cu(NT)]. The sensitivity properties such as impact sensitivity, friction sensitivity and sensitivity to temperature for a new green primary high explosives has the ability to replace toxic compounds such as lead styphnate and lead azide in initiator.

Keywords: Energetic metal complex, Primary explosives, sodium 5-nitrootetrazole

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Investigating on the interaction of the new copper complex with DNA and proteins: synthesis and structural characterization

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A new complex of Cu(II), [Cu(AEAE)(L)Br], containing 2,2-aminoethylaminoethan-1-ol (AEAE) and 4,4-Bipyridine (L) as ligands were prepared and its spectral (IR), structural properties and molar conductivity were investigated. The AEAE ligand acts as an N2O- donor in this complex by forming two five-membered chelate rings. The Cu(II) ion has a CuN_3OBr environment which proves that the coordination number of the compound is 5 (Fig.1). The Geometry optimization was performed using Gaussian 09 software. The Protein Data Bank (PDB) files 4r5y, 3ai8, 5cdn, 3c0z, 2bx8, 1peo, 3qfa, 1njb, 4gfh for the nine receptors, BRAF kinase, CatB, DNA gyrase, HDAC7, rHA, RNR, TrxR, TS, Top II, respectively, used in this research were obtained from the PDB ([1]). The Hermes visualizer in the Gold Suite was used to further prepare the metal complex and the receptors for docking. The optimized complex was used for the docking studies. The results are reported in terms of the values of fitness which means that the higher fitness the better the docked interaction of the compound (Fig.2). The fitness score of the complex with CatB(Protein) is higher than the fitness score of doxorubicin([2]).

Keywords: Protein, Copper, Structural characterization, Doxorubicin

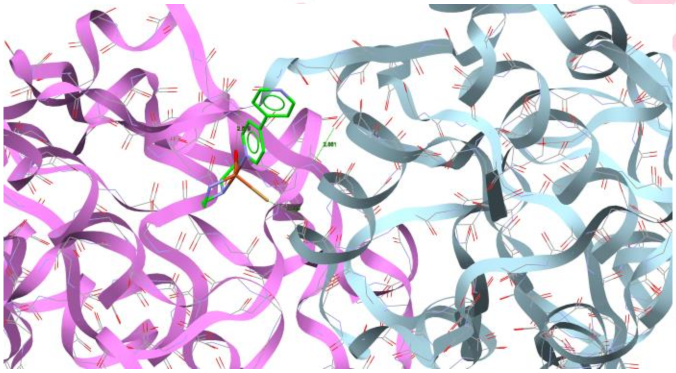

Fig.2. Docking study results, showing the interaction between the complex and CatB protein.

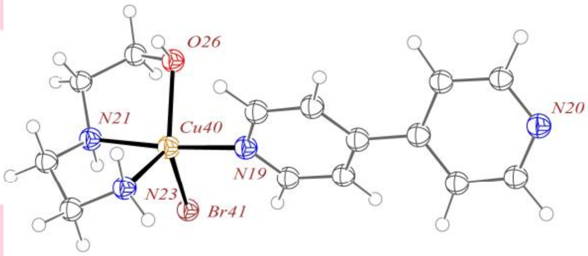

Fig.1. The ORTEP-III diagrams for the complex.

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Synthesis and characterization of the new Cobalt(II) amino alcohol complex: A combined experimental, computational, and docking studies

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In this work, a new complex of Co(II), $[Co(L_1)(L_2)(NO_3)(H_2O)]$, with 2-(2-aminoethylamino)ethanol (L_1) and 4,4-Bipyridine (L_2) was prepared and characterized by elemental analysis, molar conductivity and FT-IR spectroscopy. As it is shown in Figure 1, the coordination number of the Cobalt(II) ion in the compound is six and the geometry of the complex is octahedral. The L_1 unit which is based on Cambridge Structural Database(CSD) ([1]) is a potentially tridentate ligand that can be bind to metal atoms through two N-atoms and one O-atom. In this structure, the ligand was fully coordinated and formed two five-membered chelate rings. The structure was optimized with the Gaussian 09 software and calculated for an isolated molecule using Density Functional Theory (DFT) at the B3LYP\6-31G(d,p) level of theory for ligands and B3LYP\LanL2DZ for the complex. The predicted free Gibbs energy of the reaction is -76.5366 u.a. For predicting the biological activities of the complex, interactions of this compound with macromolecule receptors, using Gold docking software ([2]), were studied. Docking calculation showed that the complex (interaction with CatB) worked better than the anti-cancer drug, Doxorubicin, thus we suggest that studying the anticancer activities of this compound could be interesting (Figure 2).

Keywords: Biological activity, Coordination chemistry, Docking study, Gaussian, DNA

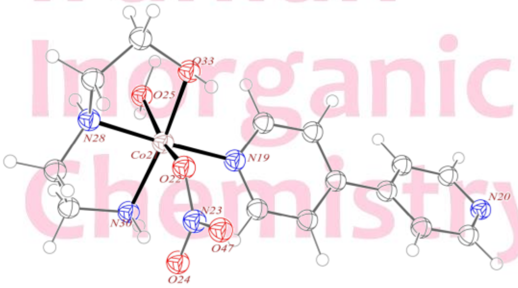

Figure 1.The ortep diagram of complex.

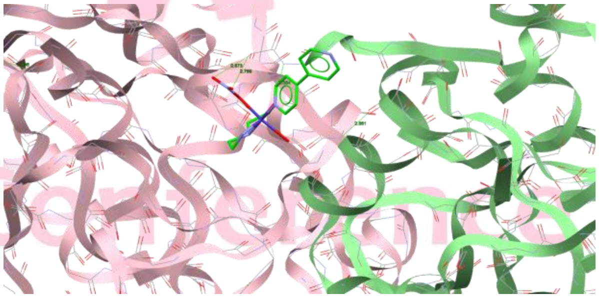

Figure 2. Docking study results, showing the interaction between the complex and CatB

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Synthesis and characterization of the copper(II) complex of a new *β*-amino alcoholic ligand in the presence of the 4,4-bipyridine supported by molecular docking

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In this work, 2-(2-(2-hydroxyethylamino)ethylamino)cyclohexanol, L_1, was prepared in solvent by the ring opening of Epoxycyclohexane with 2-(2-amino-ethylamino)ethanol [1]. Reaction of $CuBr_2$ with L_1 in methanol in the presence of 4,4-bipyridine (L_2) led to the $[CuL_1L_2Br_2]$. we elucidated the structure of Cu(II) complex prepared and identified by elemental analysis and FT-IR spectroscopy. The L_1 unit is a potentially tetradentate ligand that can be bind to metal atoms through two N- and one O-atoms, but here, it is coordinated to the central metal through one N- atom. As it is shown in (Figure 1), the coordination number of the Cu(II) ion in the compound is 4 and according to the τ value (τ =1.0), the geometry of the compound is ideal square-planer. For the accurate evaluation of the located site of the synthesized complex on biomacromolecules, the docking analysis of the interaction was performed [2]. Docking calculation (Figure 2) showed that the complex has higher fitness scores with CatB, rHA and RNR proteins compared to doxorubicin (anticancer drug), thus we suggest that studying the anticancer activities of this compound could be interesting.

Keywords: *β* -Amino alcohol, 4,4-bipyridine, Coordination Chemistry, Molecular docking

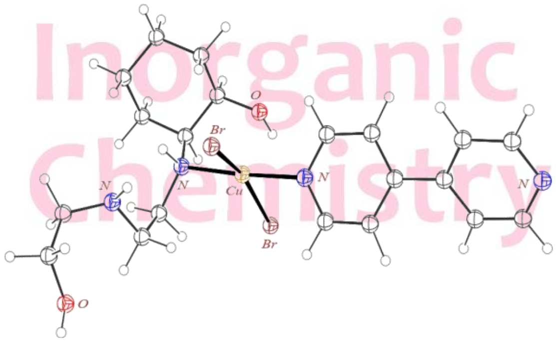

Figure 1. The ortep diagram of complex.

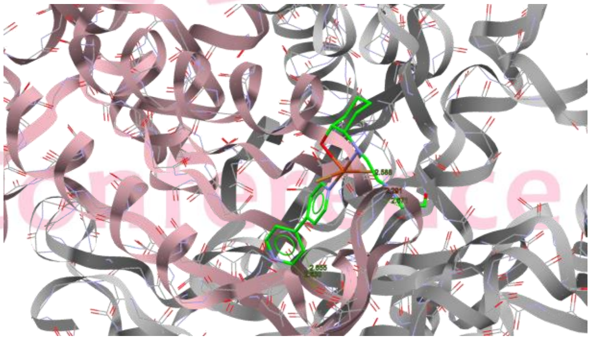

Figure 2. Docking study results, showing the interaction between the complex and RNR protein.

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A new tetra-coordinated copper(II) complex: Synthesis, characterization, DFT studies and investigating interaction with Biomacromolecules

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In the present work, the reaction of $CuCl_2.2H_2O$ with 2-(2-(2-hydroxyethylamino)ethylamino)cyclohexanol, (HEAC), in methanol in the presence of 4,4-bipyridine led to the $[Cu(HEAC)(Cl)_2(bipy)]$. The complexes were identified by elemental analysis, FT-IR spectroscopy, and DFT studies. As shown in (Fig.1), In the structure, the coordination number of the Cu(II) ion in the compound is four and the complex has a CuN_2Cl_2 environment. According to the τ value (τ =1.0), the geometry of the Cu is an ideal square-planer. As well as equation (Eq.1) illustrates Gibbs free energy changes (ΔG) at corresponding temperatures to determine the spontaneous or non-spontaneous process of the reaction([1]). The predicted free energy of the reaction is -0.157555 u.a. Molecular docking is done between a small molecule (complex) and a target macromolecule (protein and DNA) and is considered a key tool in drug design([2]). Docking calculation (Fig.2) showed that the complex has higher fitness scores with CatB, rHA, and RNR proteins compared to doxorubicin (anticancer drug), thus we suggest that studying the anticancer activities of this compound could be interesting.

$$\Delta G_{reaction} = \Delta G_{products} - \Delta G_{reactants} \quad (1)$$

***Keywords*:** Bio Macromolecule, Geometry, DFT, Gibbs Free Energy

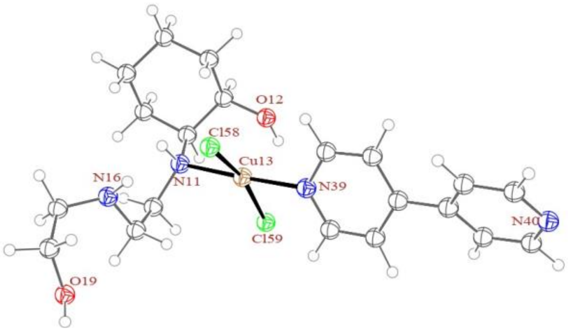

Figure 1. The ortep diagram of complex.

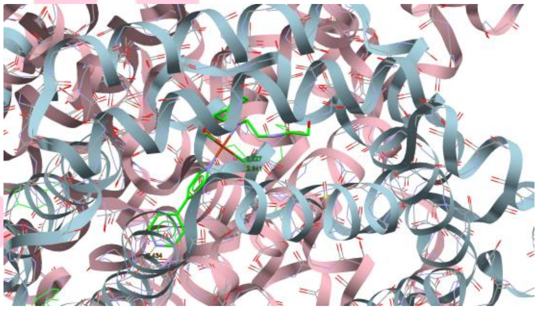

Figure 2. Docking study results, show the interaction between the complex and rHA protein.

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MIL-101(Cr)@EDTA-Zn$^{(II)}$ complex as an Effective Heterogeneous Catalyst for the synthesis of polyhydroquinolines

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Multicomponent reactions (MCRs) are of importance in synthetic organic chemistry as they can produce complex molecules with greater efficacy and atom economy from three or more starting materials in a one-step without isolation of intermediate [1]. MCRs have been shown to be environmentally friendly as they minimize the number of synthetic steps and workups and eliminate isolation of unstable intermediates. In addition, the synthesis of a broad range of complex products can be achieved by MCRs such as the Hantzsch reaction [2]. A simple, efficient method for the one-pot synthesis of polyhydroquinoline derivatives via a one-pot four-component reaction of aromatic aldehydes, Ammonium acetate, ethyl acetoacetate, and dimedone in the presence of a catalytic amount of EDTA-Zn$^{(II)}$ complex –supported on the amine-functionalized MIL-101(Cr) MOF in ethanol at reflux conditions is reported (Fig. 1). The process proved to be simple, environmentally friendly, efficient and high to excellent yielding. Accordingly, the process in question can be given the label of "green chemistry".

Keywords: MIL-101(Cr)-NH_2 MOF, EDTA-Zn$^{(II)}$, Post-Synthetic Modification, Hantzsch Reaction, Polyhydroquinolines

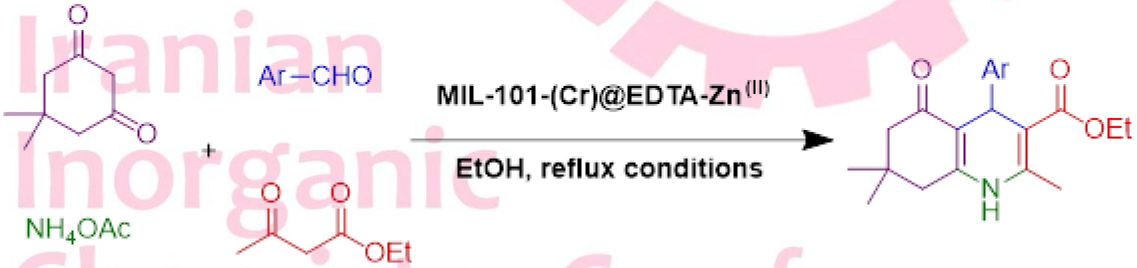

Figure 1. Synthesis of polyhydroquinolines over the catalysis of MIL-101(Cr)@EDTA-Zn$^{(II)}$ complex.

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Nanomagnetic Phosphotungstic acid-catalyzed Chemoselectivity esterification of Carbonyl bond of alpha-chloroacetic acid

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Esterification of alpha-chloroacetic acid with water-soluble alcohols in the liquid phase using sustainable methods is the first challenge in the way of the total synthesis of polymer solar cells (PSCs) [1]. Carboxylic acid esterification is one of the basic reactions in organic chemistry, the speed of which can be increased by increasing the acidic catalyst in the reaction medium [2,3]. In the reaction of esterification, both homogeneous and heterogeneous catalysts can be used. Among the heterogeneous catalysts that can be used, phosphotungstic acid stabilized on nanomagnetic Hercynite as a spinel normal catalytic support used to esterification alpha-chloroacetic acid with different water-miscible and immiscible alcohols to prepare the corresponding esters in excellent yields, and without removing the chlorine group at the alpha position through substitution reactions. The advantage of this is the very easy separation of the catalyst from the reaction medium by the magnet. In fact, the application of magnetic nanoparticles in the catalysts as a catalyst base has been considered due to the good spread, the surface-to-volume ratio, the ease of surface modification, and the very easy and effective separation of the reaction medium.

Keywords: Hercynite@SiO_2-PTA, Fischer Esterification, Alpha-chloroesters, Solid Acid Catalyst

12 Examples
30-120 min (87-98%)

Figure 1. Synthesis of alpha-chloroesters through fisher esterification over the catalysis of Hercynite@SiO_2-PTA.

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Phosphomolybdic Acid Hydrate Encapsulated in Mil-53 (Fe): A New Heterogeneous Heteropoly Acid Catalyst for Friedel–Crafts acylation

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Phenyl ketones show a significant family of intermediates commonly used in the synthesis of industrial chemicals, medicines, cosmetics, and food additives [1]. Acetylation is one of the most applicable, beneficial, and essential reactions in organic chemistry setting chemists to introduce reagents for this reaction [2]. In organic synthesis, this functionality is normally introduced on aromatic rings by acylation with anhydrides or acyl chlorides in the presence of Lewis or protonic acids and solid acids [3]. Some of the reported methods for the C-acetylation of phenols suffer from one or more drawbacks such as toxicity, cost, drastic reaction conditions, hygroscopicity, thermal stability, and the explosiveness of reagents. Given those drawbacks, new, efficient, and eco-friendly methods are still in demand. Herein, A simple, efficient method for the one-pot acylation of 4-fluorophenol via acyl chloride in the presence of a catalytic amount of PMA@ MIL-53(Fe). (Fe) MOF is reported (Figure 1). This heterogeneous catalyst showed advantages such as being very simple and eco-friendly due to the high reusability of the catalyst, excellent yield, and mild reaction conditions.

Keywords: Friedel–Crafts Acylation, 4-fluorophenol, Heterogeneous Catalyst, PMA@MIL-53(Fe).

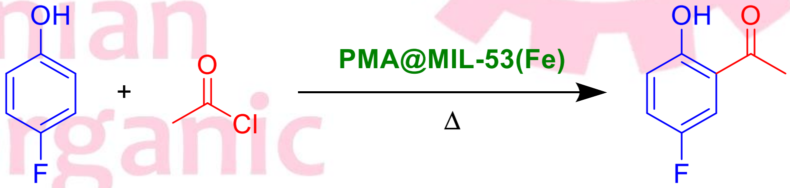

Figure 1. Friedel–Crafts acylation of 4-fluorophenol over the catalysis of PMA@MIL-53(Fe).

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Adsorptive removal of Rhodamine B from aqueous solution by a zirconium fumarate metal-organic framework (MOF-801)

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Various pollutants such as dyes following the arrival to ecosystems lead to serious global environmental pollution. Due to global strict regulations, it is obligatory to treat the wastewater before being discharged into the environment [1]. One of the common, reliable, and useful techniques employed for the removal of synthetic dyes from industrial effluents is an adsorption process [2]. In this study, the zirconium-fumarate metal-organic framework (MOF-801) was synthesized using solvothermal method [3]. The synthesized MOF-801 was characterized by XRD, SEM, IR, TGA, and BET techniques. XRD result was shown the highly crystalline nature of the MOF-801. BET surface area analysis verified the highly porous nature of the MOF-801. morphology of the obtained MOF-801 was examined by the scanning electron microscope (SEM). The SEM images showed an octahedral structure, the average diameter of which is about 300 nm. Pollutant adsorption tests were conducted over Rhodamin B (RhB) dye as an organic pollutant. The maximum equilibrium adsorption capacity was 19.1 mg g^{-1} with RhB dye having an initial concentration of 30 mg L^{-1}. Langmuir isotherm model was the best fit for adsorption data based on linear regression analysis. The best kinetic model for the adsorption was pseudo-second-order kinetics (R^2 = 0.9981). The effect of dye concentration, contact time, and MOF dose on the adsorption of dye was also investigated. The study showed that MOF-801 is an efficient adsorbent for the removal of RhB dye from aqueous solution. Therefore, MOF-801 could be regarded as a promising adsorbent for the removal of dye pollutants due to its high adsorbent activity, good reusability, and easy preparation. MOF-801 can be reused at least five times.

Keywords: MOF-801, Solvothermal, Absorption, Rhodamin B.

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Synthesis of MXene/MIL-101 nanocomposite high adsorption capacity for Methylene blue dye removal

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Water is an essential resource for life, but the increase in population and industrialization has led to contamination of natural water resources [1]. Therefore, water purification is an essential need for society, and researchers are constantly looking for new and efficient methods of water purification [2]. One of the common and useful techniques employed for removal of synthetic dyes from industrial effluents is an adsorption process [3]. In this study, novel MXene/MIL-101 nanocomposite synthesized through the solvothermal method and characterized by x-ray diffraction (XRD), infrared spectroscopy (IR), and field-emission scanning electron microscopy (FESEM) analyses. Pollutant adsorption tests were conducted over Methylene blue (MB) dye as an organic pollutant. The maximum equilibrium adsorption capacity was 23.18 mg g^{-1} with MB dye having an initial concentration of 50 mg L^{-1}. Langmuir isotherm model was the best fit for adsorption data based on linear regression analysis. The best kinetic model for the adsorption was pseudo-second-order kinetics ($R^2 = 0.999$). The effect of dye concentration, contact time and MOF dose on the adsorption of dye was also investigated. The study showed that MXene/MIL-101 is an efficient adsorbent for the removal of MB dye from aqueous solution. Therefore, MXene/MIL-101 nanocomposite could be regarded as a promising adsorbent for the removal of dye pollutants due to its high adsorbent activity, good reusability, and easy preparation. MXene/MIL-101 nanocomposite can be reused at least four times.

Keywords: MIL-101, MXene, Solvothermal, Nanocomposite, Methylene Blue

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Lacunary Keggin-type Polyoxometalate-Based Framework: Design of a Heterogeneous Catalyst for Efficient Degradation of Dye from Aqueous Solution

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In the past decades, serious water pollution due to organic dyes and pigments affected the earth's environment, and animal and human health. Catalysts based on polyoxometalates (POMs) have been extensively studied in water treatment due to their superior removal capacity in heterogeneous and homogeneous processes [1]. It is well known that lacunary derivatives are more reactive than the original Keggin anion due to the presence of multiple labile terminal oxo ligands. Lacunary POMs with a set of remarkable properties such as high coordination reactivity, rigidity, oxidative and thermal stability are an important sub-class of POMs. The lacunary species with high negative charge and nucleophilic oxygen-enriched surfaces can interact with various cations [2-4]. In this work, a new hybrid based on lacunary polyoxotungstate ($K_8[SiW_{11}O_{39}]$), Copper(II) nitrate trihydrate ($Cu(NO_3)_2•3H_2O$) and chelidamic acid ($C_7H_5NO_5$) was synthesized. Furthermore, the synthesized hybrid showed high catalytic activity in the degradation of methylene blue (MB) as an organic pollutant and degradation efficiency reached 93.83% within 120 min.

Keywords: Polyoxometalate, Lacunary, Keggin, Catalysis, Methylene Blue.

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Synthesis and Characterization of nano γ-Alumina/β -Cyclodextrin as Adsorbent for Heavy Metal Adsorption

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Nano alumina is available in various forms, most of which are γ and α-Al_2O_3. The nano γ-Al_2O_3 is used often as an adsorbent than α form due to its higher porosity and is called active alumina. In addition to the special properties of alumina, nano γ-Al_2O_3 has been more effective than other metal oxides as an adsorbent for toxic metals [1]. Nonetheless, the poor adsorption of toxic metals onto the nano γ-Al_2O_3 limits its use as a desirable adsorbent. The nano γ-Al_2O_3 was used as an adsorbent to remove toxic metals such as cadmium, zinc, lead, and copper. Water insoluble β-cyclodextrin is used as an adsorbent for the removal of organic pollutants and heavy metals in water due to their solubility in water (1.85g per 100ml) and high tendency to hydrogen bonding [2]. In a study, Pourshadlou et al [3] reported the uptake of magnesium from water by bentonite/γ-Al_2O_3 nanocomposite, and the effects of various parameters including γ-Al_2O_3 content, initial ion concentration, and adsorbent dosage were investigated. Verma et al [4] synthesized β−cyclodextrin−ethylenediaminetetraacetic acid−chitosan (β−CD−EDTA−CS) polymer was synthesized for the removal of heavy metals and organic dyes from aqueous solution and investigated the effects of different parameters such as pH, time effect, initial concentration, and reusability. They stated that the absorption of heavy metals is faster than dyes. In the current work, we synthesized nano γ-Alumina/β -Cyclodextrin as an Adsorbent for Cd (II) Adsorption. The FT-IR and XRD SEM of nano γ-Al_2O_3 and γ-Al_2O_3/β-cyclodextrin composite were evaluated. The results showed good size and morphology for nano γ-Al_2O_3 and γ-Al_2O_3/β-cyclodextrin nanocomposite. So, the results indicated the efficiency of nano γ-Al_2O_3/β-cyclodextrin to remediate Cd(II) from aqueous solutions in our study [5].

Keywords: Adsorption, Co-precipitation, Nano γ-Alumina/β –cyclodextrin, Toxic Metals

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A Bioactive Rhenium(I) Tricarbonyl Complex Bearing a Bidentate Nitrogen Ligand: Experimental and Theoretical Calculations

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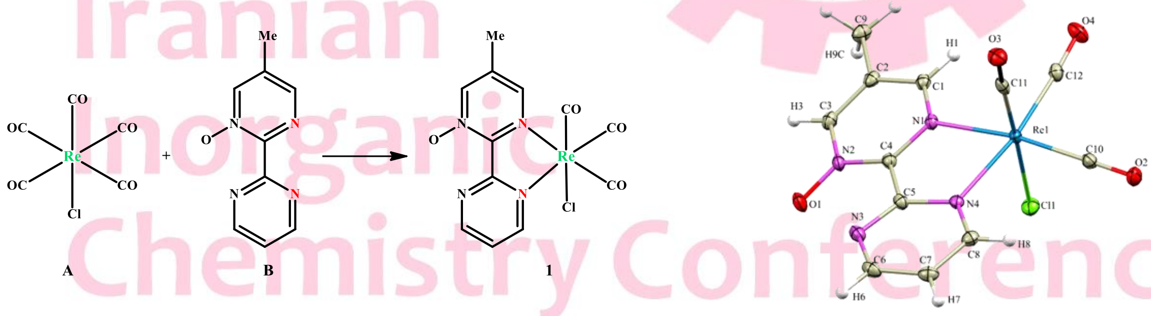
Cancer continues to be one of the world's leading causes of mortality, despite the rising corpus of research. The majority of cancer treatments include photodynamic therapy and chemotherapy, with chemotherapy continuing to be the most successful method for increasing patient survival. On the other hand, chemotherapy uses non-selective cytotoxic substances that cause cell death in both malignant and healthy tissue[1]. Platinum-based chemotherapy is used to treat more than 50% of cancers. Nevertheless, these medications suffer from serious flaws that hinder their effectiveness and show physiological side effects, such as toxicity toward healthy, non-tumorigenic cells and innate or acquired chemoresistance[2]. In this regard, organorhenium complexes possess several intrinsic properties advantageous for the development of novel anti-cancer drug candidates. As shown in Scheme 1, the reaction of [Re(CO)$_5$Cl], **A**, *via* 5-methyl-[2,2'-bipyrimidine]-1-*N*-oxide (bpyNO) ligand afforded a new Re^I complex [Re(CO)$_3$(bpyNO)Cl], **1**. The crystal structure of **1** was obtained, and this complex was characterized by means of several spectroscopic and analytical techniques, such as NMR and HR ESI-Mass. Also, theoretical calculations were carried out on this complex, and the *in vitro* cytotoxicity effect of **1** was investigated against a panel of cancer cell lines.

Keywords: Re(I) tricarbonyl complex, Nitrogen donor ligand, Theoretical elucidation, Biological investigation.



Scheme 1. Synthetic route for the preparation of **1** (left) and its crystal structure (right).

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Synthesis of substituted porphyrins for use in the structure of perovskite solar cells

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This study has focused on a series of zinc porphyrins that have been used as hole-transporting layers in perovskite solar cells. Hole-transport layers play a significant role in perovskite solar cells for attaining favorable photovoltaic performance with durability. Meanwhile, this series is brominated by NBS(N-bromosuccinimide) which can affect to modulate redox potentials, and also it can complement the enhancement of other electronic properties. Brominated is a part of the halogenation reaction which can significantly increase the excited state lifetime of a Zn porphyrin relative to the unsubstituted complex when it happens in appropriate conditions. A series of zinc-brominated meso-tetraphenyl porphyrins, H2TPPBrx (x = 2, 4,8) have been synthesized. All these series of porphyrins were characterized by chemical analysis, UV-Vis spectroscopy, Photoluminescence spectroscopy, and cyclic voltammetry (CV) studies. It has been observed that all the derivatives of brominated porphyrins represent prominent redshifts in both the Soret and Q bands of their electronic spectra compared to their nonbrominated form. As a result, it can be intelligible how these derivatives of porphyrin improve the power conversion efficiency of perovskite solar cells [1].

Keywords: Bromoporphyrins, Hole-transport Layers, Perovskite Solar Cells

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Decolorization of MB dye by Cobalt(II, III) oxide QDs linked to silver molybdate as an impressive heterojunction photocatalyst under the irradiation of visible light

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Environmental pollution has become the main concern to humans [1,2]. From the point of view of numerous and permanent solar energy, photocatalysis has attracted much attention worldwide in environmental improvement and energy generation in the last years [3-5]. Herein, the synthesis of cobalt(II, III) oxide QDs-Ag_2MoO_4 heterojunction was reported by hydrothermal method and identified by different techniques such as FT-IR, XRD, FE-SEM, EDS, TEM, DRS, PL, and UV–Vis spectroscopy. The SEM images illustrate that silver molybdate particles and cobalt(II, III) oxide QDs-AMO have a morphology of 3D-hexagons and nanosheets collected on the surface of 3D-hexagons with an average size of 36 and 28 nm, respectively. The cobalt(II, III) oxide QDs-silver molybdate photocatalyst was used toward the decolorization of MB with a conversion rate of 91%, which is 15 times faster than pure AMO. The higher photocatalyst activity of cobalt(II, III) oxide QDs-AMO should be attributed to its lower charge recombination rate compared with pure silver molybdate. The stability of this photocatalyst was determined by reusing it for five times without a remarkable decline in its activity. In addition, a postulated mechanism by the hydroxyl radical way was suggested.

Keywords: Conversion of Dyes, Heterojunction Photocatalyst, Semiconductor Quantum Dots

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Boosted photocatalytic decolorization of MB, RhB, and MO by perovskite-based heterojunction structures

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The entry of water contaminated with organic dyes causes raised toxicity levels of water and damage to organisms [1]. During the last years, inorganic perovskite oxides, have attracted significant research interest due to their specific physical and chemical properties [2,3]. Cerium oxide has the eligibility of high dielectric constant, natural plenty, inexpensive, and variable valence states between Ce^{3+} and Ce^{4+} [4]. The investigation on Ce-based perovskites is barely up to now [5]. In addition, the effect of Ce doping on the $PbTiO_3$ physical properties has not been studied. However, it is known that semiconductors with a heterojunction structure are one of the most effective procedures to increase the active sites of catalysts and decrease the charge recombination rate [5]. Here, the $CeCoO_3/MoS_2$ heterojunction and co-doped perovskite Ce-Co-$PbTiO_3$ were successfully synthesized by the hydrothermal method. Their morphology and photocatalyst performance were considered in detail. The result in optimal conditions was compared to that of pure perovskite. Because of the decrement of charge recombination rate and fast charge transfer between perovskite and nanoparticles, the heterojunction structure illustrated a higher photoactivity on decolorization of MB, RhB, and MO than pure perovskite. These photocatalysts could supply a qualified method using them as an impressive candidate for the conversion of organic dyes in the water.

Keywords: Photocatalyst, Perovskite, Conversion of Dyes, Heterojunction

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Innovative p–n semiconductor heterojunction as a nanophotocatalyst toward the C(OH)–H bond activation

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Nowadays, using semiconductors for photocatalytic treatment of pollutants has been broadly scrutinized due to their eco-friendly and low cost [1-3]. Nanomagnetic heterostructure was prepared by solvent-free thermal procedure and was characterized by various techniques. The pure copper bismuth oxide and a semi-hard ferrite (cobalt ferrite) illustrated poor photoactivity because of their high charge recombination rate and slightly visible light absorbance, respectively. The average size of the synthesized heterojunction was approximately 20 nm, which displayed almost twofold higher photoactivity than pure $CoFe_2O_4$ and $CuBi_2O_4$ toward the C(OH)–H bond activation. This nanocomposite exhibits photocatalytic efficiency as high as 98% with very high stability. The enhanced photoactivity could be attributed to the efficient Z-scheme mechanism of charge carrier separation between p–n semiconductors, which decreases the electron–hole recombination rate. The results supply a promising approach to the preparation of p–n heterostructured photocatalysts for organic reactions.

Keywords: Semiconductors, Z-scheme, Cobalt Ferrite, Copper Bismuth Oxide, C(OH)–H Bond Activation

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Self-assembly of L-cysteine–Ag–Au Nanoparticles for catalytic reduction of 4-nitrophenols

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Rapid industrialization in recent years is primarily one of the main causes of environmental concerns, especially water pollution. Various industries have caused many dangerous diseases for humans and aquatic animals. Among organic pollutants, Nitrophenol compounds as common carcinogenic pollutants demonstrate adverse effects on human beings and aquatic life. Chemical reduction of nitrophenols is known as the advanced removal methodology for such hazardous dyes from aqueous reservoirs. In recent years, researchers have used different nanocatalytic systems for the chemical reduction of nitrophenols to a useful reduction product of aminophenol using sodium borohydride ($NaBH_4$) as the reducing agent. The hierarchically organized particles (Hops) are inorganic or hybrid particles with hierarchically organized nanostructures such as spiky, sheets, and helices. In addition, Au and Ag Hops which are gold, and silver complexes with cysteine as a ligand have been shown to have structurally ordered and porous structures and are beneficial for recycling. In this study, hierarchical self-assembly of Au-Ag fractal patterns was achieved using a hydrothermal method using L-cysteine as an environmentally friendly reducing and stabilizing reagent. Here, free thiol groups of cysteine molecules electrostatically immobilized gold and silver nanoparticles (NPs). Polymeric material-supported bimetallic nanoparticles were used as catalysts for the degradation of 4-nitrophenol to 4- 4-aminophenol.

Keywords: Gold; Silver; L-cysteine; 4-nitrophenol; Sodium Borohydride.

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Central Composite design (CCD) optimization and characterization of removal of Entacapone drug using copper zinc cobalt ferrite nanoparticles modified by cetyltrimethylammonium bromide ($Cu_{0.3}Zn_{0.3}Co_{0.4}Fe_2O_4$@CTAB) nanoparticles and Adsorption Characterization

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Copper zinc cobalt ferrite nanoparticles modified by cetyltrimethylammonium bromide ($Cu_{0.3}Zn_{0.3}Co_{0.4}Fe_2O_4$@CTAB NPs) are used as an efficient adsorbent to remove Entacapone (En) drug from aqueous solutions. The characterization of adsorbent is investigated by field emission scanning electron microscopy (FE-SEM), X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectroscopy, energy dispersive X-ray spectroscopy (EDX), and the vibrating sample magnetometer (VSM) technique. To optimize the effective factors, response surface methodology (RSM) through using Central Composite design (CCD) is applied. By proper running of the Desirability function option in MINITAB software, the optimum conditions were found as pH 3.0, adsorbent mass (m) 10 mg, and initial dye concentration (C_d) of 77 mg L^{-1}. Isotherm studies of the adsorption process are carried out where the Langmuir isotherm shows the maximum monolayer capacity (q_{max}) is 224 mg g^{-1}. The kinetic studies including pseudo-first-order, pseudo-second-order, and intra-particle diffusion models indicate that the pseudo-second-order kinetic model describes better the adsorption kinetic behavior. This study shows that $Cu_{0.3}Zn_{0.3}Co_{0.4}Fe_2O_4$@CTAB NPs have excellent potential for the removal of Entacapone (En) drug from an aqueous solution.

Keywords: Adsorption; Mixed Magnetic Oxides Nanoparticles; Removal; Drug; Response Surface Methodology

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Synthesize $Ni_{0.1}Cu_{0.1}Zn_{0.8}Fe_2O_4$ nanoparticles by gel-auto combustion and microwave-assisted methods and investigate their photocatalytic activity

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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 systems, and magnetic hyperthermia), catalysis, information technology, telecommunication and environmental remediation, destruction of organic pollutants, etc [1,4]. In this work, it has attempted to synthesize $Ni_{0.1}Cu_{0.1}Zn_{0.8}Fe_2O_4$ by both gel-auto combustion [5] and microwave-assisted [6] methods, and productions were characterized by types of spectroscopic analyses, involving XRD, IR, DRS, SEM, EDS, VSM, and UV-Vis spectra. The effect of samples was investigated on the absorption and destruction of methyl orange at three different concentrations (5, 10, and 15 ppm). The average crystalline size of MNPs synthesized by gel-auto combustion and MW-assisted, obtained by x-ray diffraction analysis were 77.9 and 44.1 nm, respectively. The hysteresis magnetization curves exhibit the saturation magnetic values which, were 20.64 and 52.89 (emu/g) for MNPs obtained by gel-auto combustion and MW-assisted, respectively. Finally, both ferrites showed high absorption of methyl orange dye in water under UV-Vis irradiation ($\lambda > 400$ nm) but the sample obtained by the MW-assisted method had better function [2].

Keywords: Magnetic Nanoparticles, Photocatalyst, Gel-auto combustion, Microwave-assisted.

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Study of the effect of Ag promoter over cobalt-based catalysts in CO hydrogenation reaction

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Fischer–Tropsch synthesis can produce hydrocarbons using syngas derived from coal, natural gas, or biomass. Supported cobalt catalysts are preferred due to their high activity, high selectivity to long-chain paraffin, low water–gas-shift activity, and high resistance to deactivation[1-3]. For these catalysts, the support not only provides a large surface area for the cobalt dispersion but also has significant effects on the FT performance due to metal–support interactions, porosity, and mass transfer limitations. Conventionally, silica, alumina, and titanium can be used as Co supports [4,5]. In this research, we studied the influence of Ag promoters on cobalt-based catalysts. The catalyst was prepared incipient wetness impregnation method. The catalyst has been characterized with XRD, BET, and H_2-TPR ICP techniques and then tested in a fixed-bed reactor under pressure of 27 atm, temperature of 210 ºC, H_2 to CO ratio of 2, and GHSV of 2 l/h/gcat. The result was shown 56.3 % CO conversion, 14.6 % CH_4, 9.3 % C_2-C_4, and 76.1 % C_5^+ selectivity.

Keywords: Fischer–Tropsch Synthesis, Cobalt Catalyst, Ag Promoter, Product Distribution.

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Preparation of cobalt-based Fischer-Tropsch Synthesis

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Fischer-Tropsch Synthesis is a process for obtaining second-generation biofuels i.e. the BTL process as well as for producing chemical feedstock or motor fuels without the production of the environmentally harmful compounds encountered in direct hydrogenation [1,2]. It has been found that several metals such as nickel, cobalt, ruthenium, and iron can be activated for FT reaction [3]. Fe and Co catalysts are the most common commercial FT synthesis catalysts. The Co catalysts are preferred due to their high FT synthesis activity, high selectivity to long-chain hydrocarbons, better catalyst stability in hydrogen-rich environments, and lower selectivity to oxygenated compounds [4,5]. In this study, a cobalt-based catalyst was prepared by the incipient wetness impregnation method. The catalyst was characterized using XRD, BET, H_2-TPR, and ICP techniques. The catalyst was tested in a fixed-bed reactor under FTS conditions. The results were shown 70.6 % CO conversion, 12.4 % CH_4, 6.5 % C_2-C_4, and 82.1 % C_5^+ selectivity.

Keywords: Cobalt Catalyst, CO Hydrogenation, C_5^+ Products.

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Study of parameters affecting the assembly of linker-based gold nanoparticle core spherical nucleic acids (AuNP-core SNAs) for colorimetric detection

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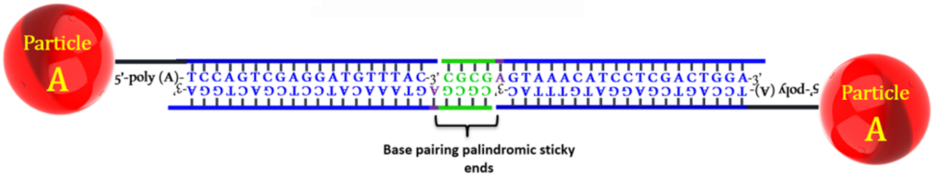
Spherical nucleic acids (SNAs) are multivalent nucleic acid structures made up of a layer of tightly packed oligonucleotide shells on the surface of a nanoparticle core. Since the first report of SNA by Mirkin et al. [1], there has been great interest in SNAs as they offer new opportunities in the field of gene and drug delivery. The DNA shell allows specific molecular recognition with much higher binding affinity for complementary sequences compared to their linear counterparts which can be programmed to recognize and bind DNA targets. Upon binding, aggregation of AuNP-core SNA red-shifts the surface resonance plasmon (SPR) band, and a visible color change of the particles in solution from red to purple is observed. The change in the optical property of gold nanoparticle suspension can be easily monitored with UV-Vis absorption spectroscopy. Colorimetric detection systems based on SNA conjugates have been used for visual detection of nucleic acids with the naked eye [2,3]. In this study, the kinetics of the self-assembly process of gold nanoparticles modified with phosphorothioate-capped oligonucleotides and complementary linker strands with palindromic tails were investigated. The engineered mixture of palindromic DNA linkers and SNA resulted in significant time-dependent spectral changes of the AuNP plasmon band due to self-assembly formation in the presence of the DNA linker. Spectral changes were monitored by tracking the plasmon band of the AuNP core SNA in UV-Vis spectra over time. A series of experiments and a theoretical model were developed to study the assembly kinetics of SNA using 24 linkers of different lengths and GC content. The kinetics of assembly formation in linker-based single-component systems was found to depend on the length and GC content of the palindromic tail. The result showed that the 4-nucleotide palindromic linker with 100% GC content was suitable for colorimetric purposes due to its faster assembly rate and greater color change in SNA solutions.



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Synthesis and modification of KIT- 6 with Zn doped CdS nanoarchitecture and its application in photocatalytic degradation of methyl green

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In this study, the mesoporous silica KIT-6 modified with Zn-doped CdS nano architectures was prepared for efficient photocatalytic properties, and the degradation of methyl green in aqueous solution under visible light was taken as a photocatalytic test. The prepared nanocomposite was characterized by X-ray Diffraction (XRD), nitrogen adsorption-desorption analysis (BET), FT-IR, field effect scanning electron microscopy (FE-SEM), and UV−Vis spectroscopy. The results show that CdS with a small amount of Zn doping can lead to an enhanced photocatalytic activity of Zn-CdS/KIT-6. We found that The mesoporous silica KIT-6 with high surface area and three-dimensional connections with a network of interconnected channels is a suitable choice of support for these nano architectures [1,2]. The obtained data from UV-Vis studies shows that 5mg of the prepared photocatalyst containing 4.8% of Zn doped CdS species can degrade 50 ml of methyl green solution with a concentration of 18 mg/l within 45 min under visible irradiation. The stability of the prepared photocatalyst was checked and it can be used several times without losing much of its activity.

Keywords: CdS, KIT-6, Methyl Green, Photocatalysis

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The effect of TPP concentration on levothyroxine release from nano clay/chitosan nanocomposite

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A nanoparticle polymer has been developed as a potential platform for drug delivery. Nanoclay/Chitosan nanocomposite was prepared with tripolyphosphate (TPP) by the ionic crosslinking method. The particle size of Nanoclay/Chitosan nanocomposite was in the range of 190-250 nm and encapsulation efficiencies of levothyroxine were 85%. A non-invasive way to deliver drugs to the deepest parts of the human body is ultrasound. To study how ultrasound causes levothyroxine to be released from chitosan nanoparticles, cumulative release was examined. In this report, we explore the effect of ultrasound on the release behavior of levothyroxine from Nanoclay/Chitosan nanocomposite. The drug release from chitosan nanoparticles was enhanced using the ultrasound wave.

Keywords: Nanoclay, Chitosan, TPP, Nanocomposite

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Evaluation of the relationship between intensity and effluent temperature in a solar still

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In this research, the exit treated wastewater from the gravity filtration unit, mechanical and chemical treatment unit, biological treatment unit and finally UV disinfection treatment unit enters to a solar desalination unit. Wastewater evaporation process is performed in this unit. In this study, in order to increase the UV waves in solar energy, nano-flooring has been used on the floor of the solar pond. The laboratory results show that the average difference between the experimental data and the theory for simple coating, coating made of zinc oxide nanoparticles and coating made of aluminum oxide nanoparticles is equal to 2%, 2.3% and 1.6%, respectively. The laboratory results show that the maximum and minimum temperature difference of the first layer and the last layer of wastewater are in April and March, respectively[1].

Keywords: Radiation Intensity; Temperature; Saline Wastewater; Nanoparticles

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Cs@Resorcinarene network as an organocatalyst for the three-component reactions

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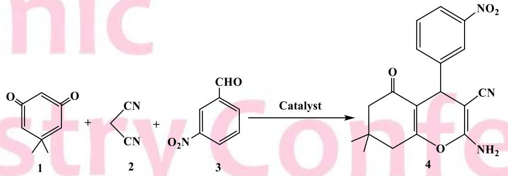
In recent years, nanoparticles have attracted considerable research interest due to their potential applications in catalysis science and technology in alignment with the principles of green chemistry. One of the green approaches for designing and applying heterogeneous catalytic systems is the use of biopolymers as appropriate biodegradable catalytic systems or supports. In this regard, chitosan and Calix, as economic biopolymers, have received considerable attention to be used in catalytic systems, as well as drug delivery and adsorbents [1]. Herein, we report the green synthesis magnetic poly calix[4]resorcinarene of cobalt ferrite by the immobilization of EDTA and free amines of chitosan as the nucleophilic functional groups that are attacking the carbonyl in EDTA to form network polymer layer on the magnetic poly calix[4]resorcinarene surface. The synthesized compound was used as a magnetic catalyst in the three-component condensation reactions of 2-amino-4-(3-nitrophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4h-chromene-3-carbonyl. Easy separation of catalysts and products, efficiency and proper reaction time, mild conditions, and reuse are some of the advantages of catalysts used [2]. In this work, 2-amino-4-(3-nitrophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4h-chromene-3-carbonyl 4 via a three-component condensation of aromatic aldehydes, malononitrile, and dimedone were synthesized in the presence of CS@Resorcinarene catalyst under optimal conditions with excellent efficiency. The resulting nanocomposite was studied by EDX, FESEM, and FT-IR techniques.



Scheme 1. Synthesis of 2-amino-4-(3-nitrophenyl)-7,7-dimethyl-5-oxo-5,6,7,8-tetrahydro-4h-chromene-3-carbonyl in the presence of catalysts

Keywords: Magnetic Nanoparticles, Catalyst, Chitosan

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Potential electrospun Chitosan/Polyvinyl alcohol/Cyclophosphamide nanofibers for anticancer applications

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Recently, electrospun polymeric nanofibers have proven to be an interesting strategy for drug delivery systems application. The high surface-to-volume ratio of the fibers can improve some processes, such as, drug loading. One of the most important and studied areas of electrospinning is in the drug delivery field, for the controlled release of anticancer agents. Different drugs can be easily incorporated into electrospun materials and their release profile can be controlled through changes in the fiber's morphology, porosity, and composition. Therefore, nanofibers can be promising materials for many biomedical applications such as anticancer drugs [1]. Chitosan (C.S) has proven challenging to electrospun. Polyvinylalcohol (PVA) is a polymer that has been studied intensively because of its good film forming and physical properties. To improve mechanical properties, C.S/PVA composite by electrospun method has challenging [2, 3]. requirement in the fields of medicine and drug deliveryCyclophosphamide (CP) is an important anticancer drug that belongs to the class of alkylating agents. (CP) is mostly used in bone marrow transplantation, rheumatoid arthritis, lupus erythematosus, multiple sclerosis, neuroblastoma, and other types of cancer [4]. By combining the advantage of electrospun nanofibers (PVA/C.S) and CP, we synthesize a new carrier system consisting of nanofiber (C.S/PVA/CP). The physicochemical properties of nanofiber were characterized by Infrared spectroscopy (IR), Scanning Electron Microscopy (SEM-EDX), Ultraviolet-Visible spectroscopy (UV-VIS), and X-ray diffraction. Finally, the results showed that the drug was loaded on the nanofibers in a nanoscale with a spherical morphology.

Keywords: Chitosan, Polyvinyl Alcohol, Nanofiber, Electrospinning, Cyclophosphamide

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Two Novel Triaza Quinoline Schiff base Ligands and Their Metal Complexes as Antibacterial Compounds: Synthesis, Characterization, structural elucidation and Thermodynamic Studies

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In this project, two new tridentate Schiff base ligand and their Zinc(II) and Nickel(II) complexes have been synthesized and characterized using various spectroscopic techniques such as elemental analysis, magnetic susceptibility, conductivity, ^{1}HNMR, IR, UV-Vis spectra, Mass spectrometry powder XRD and EDX. Then their antibacterial effects are described. These new ligands behave as tridentate triaza through quinolone moiety nitrogen, azomethine nitrogen, and amine nitrogen. The SQUAD program [1, 2] explained the trend of complex formation of metal complexes $Zn^{2+} > Ni^{2+}$ and sequence $[ML^1] > [ML^2]$. The metal (II) complexes show more potent activities than their free ligands. The stability constant and Gibbs free energy calculations show that the tetradentate Schiff base complexes of this series are more stable than the tridentate Schiff base complexes[3]. All the synthesized compounds were tested for their antibacterial activity in vitro against the Gram-positive bacteria and Gram-negative bacteria indicating that the metal complexes are more biologically active than the ligands.

Keywords: Quinoline Triaza Schiff Base Complexes, Thermodynamic Studies, Antibacterial Compounds

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An experimental study of the effects of graphene oxide (GO) nanoparticles in enhanced oil recovery (EOR)

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Over the past decade, the use of nanoparticles to improve the process of enhanced oil recovery (EOR) has received much attention from researchers. Most nanoparticles are described as an EOR chemical process in which wettability conditions are altered, interfacial tension is lowered, and viscosity is altered to aid oil recovery[1-3]. The main goal of this work is to investigate the effect of graphene oxide nanoparticles in EOR. So first, Graphene oxide was synthesized by the modified Hummer method and nanofluid was prepared using it. Nanofluid effects on surface tension, interfacial tension, wettability, viscosity, density, and recovery factor at 50 ppm and 100 ppm were examined. Graphene oxide nanoparticles are stable in water due to the electrical charge being negative of nanoparticles in water. However, adding salt nanofluids decreases stability. To stabilize the graphene oxide salt water, Several methods were used, but the best way is adding a stabilizing agent. The results of the study showed that graphene oxide nanoparticles reduce interfacial tension, reduce the contact angle of a drop of oil and a slight increase in viscosity and density. Reducing the interfacial tension increases the recovery factor. The results of the waterflooding show an increased recovery factor when injecting graphene oxide nanofluids with salt 10000 PPM. In nanofluid injection, due to the lack of stability of nanoparticles in porous media pressure increases. the methods required for the stabilization of the nanoparticle in the reservoir oil and should be further investigated.

Keywords: Graphene Oxide, Nanoparticle, EOR

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Immobilization of copper complex on the surface of SBA-15: As an efficient nanocatalyst for the synthesis of pyranopyrazole derivatives

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Copper nanoparticles as a catalyst are gaining immense interest due to their catalytic properties for a variety of organic reactions. However, metal-nanoparticle catalysts are still having limited uses, because of the problem associated with their separation from the products by traditional methods [1,2]. One of the currently adopted strategies is the immobilization of metal nanoparticles on solid supports, such as inorganic materials [3,4]. Among different supports, SBA-15 has been extensively applied as a heterogeneous support for the immobilization of homogeneous catalysts. Because SBA-15 is useable at high temperatures due to its thermal stability. Moreover, SBA-15 has a large specific surface area a large specific, high pore volume which allows supporting of huge organic ligands and metal complexes into its channels. In this study, a new nanocatalyst was prepared by the immobilization of Cu complex of 2-hydroxybenzonitrile as ligand on ordered mesoporous silica (SBA-15). The proposed catalyst (SBA-15@HBN-Cu) was characterized by FT-IR, XRD, BET, TGA, EDX, and SEM and was successfully applied in the synthesis of pyranopyrazole derivatives. Pyranopyrazoles exhibit significant biological properties such as anticancer, antimicrobial, anti-inflammatory, and antiviral [5, 6]. These catalysts can be recovered and reused for several runs without significant change in their catalytic activity or copper leaching.

Keywords: SBA-15, Copper, Green Catalyst, Pyranopyrazole

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A brief comment on salt-thermal methods to recycle lithium-ion batteries

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Ion-lithium batteries are an essential raw material for the production of most future and current products. Therefore, it is necessary and necessary to recover and recycle them at a low cost. Among the different methods of recycling, salt-thermal method is an efficient and effective method. Salt-thermal methods by producing salt or oxides with lithium defects enable the reuse of lithium ion batteries [1]. In this article, a descriptive and analytical method has been compiled using library resources, which states how the latest recycling technologies work by thermal salt methods. It also examines the advantages and disadvantages of using various methods. in order to take an effective step towards the development of this method in the coming years.

Keywords: Thermal salt methods, lithium batteries, recycling, green chemistry

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Less-lead $FAPbI_3$ (100) Surfaces, A theoretical Study

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Hybrid organic-inorganic perovskite solar cells (PSCs) have recently become one of the most efficient materials for photovoltaic applications [1]. Formamidinium lead triiodide ($FAPbI_3$)perovskites possess high light absorption and stability, making them strong candidates for efficient solar cells, yet they suffer from toxicity. The optoelectroniccharacteristics of environmentally friendly alkaline earth metals substituted $FAPbI_3$(100) surfaces,in various percentages, with PbI_6 and PbI_5 terminations has been investigated using density functional theory (DFT) as implemented in the Vienna ab initio simulation package [2], (VASP 5.4.4). We have created14 stable doped structuresaccording to the Goldsmith tolerance factor [3],in the form of $FAPb_{1-x}AE_xI_3$,(AE= Be, Mg, and Ca). Different terminations showed a negligible influence on the optical features, although their effect on the electronic properties is significant. Due to the conduction band (CB) shifting of the PbI_6 termination to the higher energies, an increase of about 0.3 eV in the bandgap of this termination was obtained compared to that of PbI_5, and suitable bandgaps of 1.623 and 1.309eVwere calculatedfor them, respectively. In doped systems, Mg and Ca substitutionmadebroader bandgaps, while two different decreasing and increasing trends on the bandgap of $FAPb_{0.95}Be_{0.05}I_3$ and $FAPb_{0.96}Be_{0.04}I_3$ structures were observed. Promising optical activitysuch as appropriate extinction coefficient and light harvesting efficiency for plain and doped (100) surfaces in the visible and UV windows and also the high capacity of all structuresto absorb more photons,especially in the near UV region for doped counterparts, altogether, indicate the capability of the (100) surfaces for optoelectronic applications.

Keywords: alkaline earth metals, $FAPbI_3$, perovskites,doping, density functional theory

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Fabrication and charaterization of PAN/Zn-MOF fibrous composites for dye removal

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The existence of dyes as contaminants in wastewater sources from the textile industry can lead to serious health problems if not treated properly. Furthermore, the release of dye effluents into the aqueous environment can pose serious problems for human health and the environment [1-3]. Herein, the separation of dyes over two isoreticular nanoporous Zn(II)-MOFs known as TMU-17 and TMU-17-NH2 owing to the effect of amine groups on the adsorption capacity was investigated, which can effectively and selectively adsorb Methyl Orange (MO) and Congo Red (CR) as anionic dyes. In addition, polyacrylonitrile (PAN) polymer was used to fabricate metal-organic framework (MOF) nanofibrous mat as a membrane to remove organic pollutants. To verify the structures, the samples were investigated by FTIR, XRD, SEM, and TGA measurements. Liquid phase adsorption experiments were performed to determine the maximum adsorption capacity. Varied conditions such as initial dye concentration, contact time, pH, and temperaturewere assessed. The Langmuir and Freundlich adsorption models were utilized to explain the equilibrium isotherm and isotherm constant computation. Three kinetic models such as pseudo-first-order, pseudo-second-order, and intra-particle diffusion equations were employed to investigate the adsorption performance. The adsorption results completely fitted the pseudo-second-order kinetic model. Additionally, CR and MO adsorption isotherms have fitted with the Langmuir model. Maximum equilibrium adsorption capacities of 143.27 and 877.19 mg g^{-1} for MO and CR were determined. High selective adsorption for MO and CR over other dyes is also represented. Over 90% of adsorption ability was preserved after five adsorption-desorption cycles. This work shows that the samples could be used as efficient adsorbentsfor removal of pollutants dyes from wastewater.

Keywords:Metal-Organic Framework; Electrospun membranes; Adsorption; Separation

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Preparation of chitosan-coated Zn-MOF@PDMS nanocomposites sponge for antibacterial activity

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Nanocomposite sponges composed of biocompatible polymers and inorganic materials have attracted much attention within various fields such as biomedicine, pharmaceutics, and food packaging [1-3]. In this study, we have fabricated some novel nanocomposites with a combination of salt leaching for fabrication of PDMS sponge, *in situ* synthesis of Zn-MOF, and dip coating process for coating Zn-MOF@PDMS sponge with chitosan. Chitosan stabilizes Zn-MOF particles and promotes the biocompatibility of the as-obtained composites. The surface morphology of PDMS and its nanocomposites was investigated by scanning electron microscope (SEM). X-ray diffraction was conducted to study the microstructure of the prepared Chitosan@Zn-MOF@PDMS sponge. The nanocomposite sponge, Chitosan@Zn-MOF@PDMS, was also studied by elemental EDS mapping technique.The antibacterial activity of the as-prepared sponges was also evaluated. Chitosan and Zn-MOF improved the antibacterial properties of the PDMS sponges against *Escherichia coli* and *Staphylococcus aureus*. The Chitosan@Zn-MOF@PDMS sponge hasthe potential for antibacterial and tissue engineering purposes owing to their biocompatibility, porosity, and good mechanical stability.

Keywords:Metal-organic framework; Polydimethylsiloxane; Biocompatibility

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Investigation of Porphyrin-Based Porous Organic Polymers for Enhanced Ciprofloxacin Adsorption from Water

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In recent times, the contamination of groundwater has emerged as a significant environmental concern, primarily due to the presence of diverse pollutants resulting from improper personal usage. Antibiotics, being a class of organic substances, possess inherent resistance to biodegradation. Unfortunately, their widespread and irregular usage has led to the pollution of groundwater, contributing to concerns such as bacterial resistance and elevated toxicity levels within underground reservoirs[1]. Among the various antibiotics, Ciprofloxacin, a commonly prescribed Fluoroquinolone antibiotic, stands out as one of the most extensively used. Unfortunately, this antibiotic exhibits a prolonged presence in municipal wastewater and even low concentrations of it can have toxic effects.In response to this concern, numerous methods have been developed to remove antibiotics from groundwater or wastewater[2]. One such approach involves the adsorption of antibiotics using porous materials. Porous Organic Polymers (POPs) have garnered significant interest due to their distinctive properties. These materials feature interconnected porous structures held together by covalent bonds, offering advantages such as a large specific surface area, exceptional chemical stability, and low skeleton density[3]. This study focuses on the application of a Porphyrin-based Porous Organic Polymer (POP) for the removal of Ciprofloxacin from wastewater. The synthesized porous organic polymer incorporates Porphyrin groups and exhibits a notable specific surface area of $594 m^2g^{-1}$. Iron is coordinatedto the POP to produce poly iron porphyrins. Experimental findings demonstrate that the optimal adsorption of Ciprofloxacin (>40%) takes place under acidic conditions, specifically at a pH of 3. Overall, this research highlights the potential of utilizing a high-specificsurface-area porous organic polymer as a green and cost-effective adsorbent for the removal of antibiotics from water. The polymer demonstrates promising performance, particularly in acidic solutions.

Keywords:Porous Organic Polymers, Adsorption, Ciprofloxacin.

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Theoretical Study of Effects of Changing the Metal Inos on Glyoxalase II Reaction Mechanism

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Metal ions are essential for the catalytic action of some enzymes. The most common role of metal ions is their ability to orient the substrate correctly for the reaction, exchange electrons in redox reactions, and stabilize negative charges.Glyoxalase II (GlxII) is a binuclear metalloenzyme with Zn(II) as the most frequently observed metal ion. However, cytosolic and mitochondrial GlxII from *Arabidopsis thaliana* contains varying ratios of Zn(II), Fe(II), and Mn(II)[1,2]. Human GlxII has also been shown to contain a mixed binuclear center with Zn(II) and Fe(II), although the mononuclear Zn(II) reconstituted enzyme is also active. This enzyme converts*S*-D-lactoylglutathione to D-lactic acid. In this study, using quantum mechanics/molecular mechanics (QM/MM) calculations, the effect of changing the metal ions on the reaction mechanism of GlxII was investigated.A model of the active site of GlxII was constructed based on the crystal structure of the human GlxII (1QH5 PDB ID) [3]. Besides, by changing the zinc ions of the active site with Fe^{2+} or Fe^{3+} ions, we constructed other eight active site models.The reaction mechanism of GlxII was investigated by using these active site models and obtained energy profiles (cf. Figure 1). Our results showed that the reaction mechanism of GlxII with two zinc ions in its active site has the lowest energy barrier which is in line with the higher preference of GlxII for zinc ion pairs in the active site.

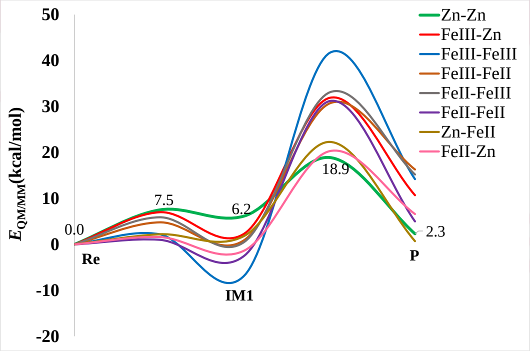

Figure 1. The energy profile of the reaction mechanism of GlxII different active site models.

Keywords: Metalloprotein,GlxII, QM/MM, DFT

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Molecular Dynamics Approach in the Comparison of Wild-Type and Mutants of D-hydantoinase

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Pregabalin (PGB), has already shown great potential in clinical applications as an analgesic, anticonvulsant, and anxiolytic drug [1].A suitable reaction for the production of PGB is the enzymatic desymmetrization of 3-isobutyl glutarimide (IBI) to *R*-3-isobutyl glutaric acid monoamide (*R*-IBM), which can be converted to *S*-PGB by the Hofmann rearrangement. PGB is a chiral compound and *S*-PGB exhibited a much greater level of anticonvulsant activity than *R*-PGB [2]. Therefore, *R*-selective enzymes are being researched for the asymmetric hydrolysis of IBI to yield *R*-IBM.An enzyme that can be used is D-hydantoinase, which belongs to the family of cyclic amidohydrolases and hydrolyzes bulky cyclic imides into their corresponding half-amides [3]. Molecular docking indicated that three residues, Met-63, Leu-65, and Cys-317, may affect the substrate binding [4]. In this work, we did molecular dynamics (MD) simulations on both wild-type and mutant enzymes (cf. Table 1) to determine the effects of the mutations on the local structure of the active site and the overall structure of the enzyme, as well as whether there is a relationship between these changes and *ee* and k_{cat}.Based on the RMSD, RMSF, and Rg analysis of MD simulations results, M63AL65AC317T was determined to be the best mutant of this enzyme. This result is in good agreement with the experimental results, which indicate that this mutation has 96.52% ee_p [5].

Table 1.The ee_p value and the average Rg, RMSF, and RMSD values (in Å) over the 200 ns production simulations from the MD simulations.

	ee_p (%)	Rg	RMSF	RMSD
WT	38.77 ± 0.95	21.80	14.55	1.53
M63A	89.83 ± 0.10	21.72	13.33	1.46
M63AL65A	93.99 ± 0.24	21.81	14.90	1.56
M63AL65H	95.66 ± 0.16	21.75	15.12	1.51
M63AL65AC317T	96.52 ± 0.27	21.77	12.54	1.37
M63AL65HC317T	97.00 ± 0.54	21.80	19.15	1.72

Keywords:Pregabalin, D-hydantoinase, Molecular docking, MD simulations

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Design and synthesis a highly selective chromogenic prob based on hydrazide schiff base reagent for naked eye detection of CN^- and AcO^- ionsand its application in real samples

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A new azomethine chromogenic probe, **HL**,based on hydrazide shiff base has been synthesized and used as a colorimetric sensor for naked-aye detection of CN^- and AcO^- ions in organic and semi-aqeouse media.The probe **HL** has been characterized using standard spectroscopic methods (IR, ^{1}H NMR, UV-Vis) as well as elemental analysis. The anion recognition ability of **HL** was evaluated using UV–Vis spectroscopy and ^{1}HNMR technique.The results exhibited that the **HL** acts as a highly selective chemosensor for the detection of CN^- and AcO^- in pure DMSO and DMSO: H_2O(90:10 v/v) media over other anions such as F^-, Cl^-, Br^-, I^-, SO_4^{2-}, SO_3^{2-}, PO_4^{3-}, $H_2PO_4^-$, HSO_4^-, NO_2^- and NO_3^-.Fig .1.as well as, In order to examine the potential applicability of the prepared chemosensor, **HL** was used for detection Sodium diclofenac (**SD**) in aqeous media. As shown in Fig. 2, a diagnosable color change was observed from colorless to pale yellow after addition of **SD**.The ability of **HL** for rapid colorimetric sensing of SDwas studied using UV–Vis spectroscopy, and ^{1}H NMR titration methods.

Fig 1

Fig 2

Keywords:Schiff base, Chemosensore, Anion sensing,Organo-aqueousmedia, Naked eye

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A newCe-Schiff base complex on modified KIT-6 as a reusable nanocatalyst for the synthesis of tetrahydrobenzo[b]pyrans and sulfoxides

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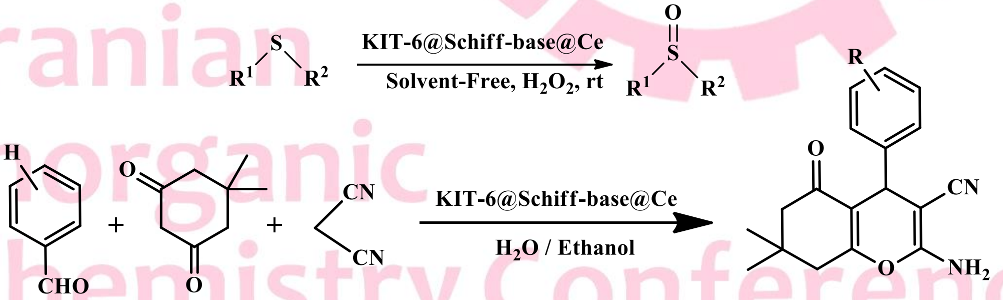
In this work, KIT-6@Schiff-base@Ce was synthesized and identified using different techniques including BET, FT-IR, WDX, SEM, EDX, and TGA. KIT-6@Schiff-base@Ce was found to be a novel and recyclable catalyst for the synthesis of sulfoxide and tetrahydrobenzo[b]pyran derivatives. Conversion of organosulfur compounds such as sulfides into sulfoxides is a topic of interest in several chemical areas, due to their applications in biological, medical, synthetic and petroleum industry. For example, pantoprazole, omeprazole, lansoprazole and pesticide fipronil are typical examples of the pharmaceutically important sulfoxide derivatives in pharmaceutical and fine chemical industries [1].Tetrahydrobenzo[b]pyrans have belonged to the class of oxygen-containing heterocycle compounds which can be used in the biological and pharmaceutical fields. They have possessed significant attention in the biological properties such as spasmolytic, diuretic, anticoagulant, anticancer, antianaphylactic, antitumor, antifungal, antiallergic, antibacterial,antileishmanial, hypotensive, antiviral and insulin-sensitizing activity[2, 3]. These compounds are synthesized from the condensation of aldehydes, malononitrile, and dimedone in the presence of various catalysts[4].



Scheme 1. Catalytic efficiency of KIT-6@Schiff-base@Ce in oxidation of sulfides and synthesis of tetrahydrobenzo[b]pyrans

Keywords: Mesoporous KIT-6,nanocatalyst, cerium, sulfoxides, tetrahydrobenzo[b]pyrans

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Preparation and characterization of MCM-41@Schiff-base@La as a recyclable heterogeneous nanocatalyst for the synthesis of tetrahydrobenzo[b]pyran derivatives and oxidation of sulfides

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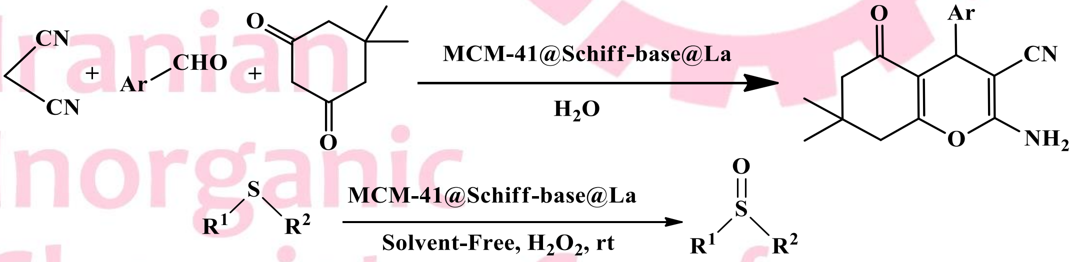
In this paper, MCM-41@Schiff-base@La as a novel, green, heterogeneous, and extremely efficient nanocatalyst was successfully synthesized by the immobilization of La complex on MCM-41 modified mesoporous silica. The prepared catalyst was characterized by TGA, FT-IR, ICP, BET, SEM and EDX techniques. The synthesized nanoparticle was sused as a recyclability catalyst for synthesis of tetrahydrobenzo[b]pyran and sulfoxide derivatives. Tetrahydrobenzo[b]pyran derivatives are an important class of heterocyclic compounds with many applications. These compounds are synthesized from the condensation of aromatic aldehydes, dimedone and malononitrile in the presence of various catalysts. 4H-pyran derivatives have pharmacological and biological activities, such as anticancer, antifungal, antibacterial, antioxidant, anticoagulant, antianaphylactic, spasmolytic, antiviral, antileishmanial, antiallergenic and diuretic [1, 2]. Beside, sulfoxides play as therapeutic agents such as anti-hypertensive, anti-fungal, anti-ulcer, anti-bacterial, anti-atherosclerotic, and psychoactive. Also, sulfoxides are good intermediates in the synthesis of some vitamins and drugs [3,4].



Scheme 1. Catalytic efficiency of MCM-41@Schiff-base@La in the Synthesis synthesis of tetrahydrobenzo[b]pyran derivatives and oxidation of sulfides

Keywords: Mesoporous KIT-6, nanocatalyst, lanthanum, tetrahydrobenzo[b]pyrans, sulfoxides.

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Micorelectrochemical sensing and deposition within bubble film

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We describe a novel electrochemical cell design with a thickness of about 30 µm that comprises a carbon fiber electrode (10 µm diameter) placed through a bubble wall (or stable surfactant film) which serves as the solution. To create a durable surfactant film,we employeda solution infused with non-ionic Triton-X100 surfactants. To do electroanalysis, a modified carbon microelectrode with nanosheet graphene oxide(as a sensing electrode) was placed through a soap bubble wall along with a 1 mm diameter silver wire as the counter/reference electrode [1]. By using this strategy, the proposed sensing system has demonstrated successful detection of NO_2^- both on the hand and dissolved in Triton-X100 surfactants film [2-3]. This technique holds particular significance in criminal investigations, as the presence of NO_2^- ions on the hand is indicative of gunshot residue and can aid in identifying suspects. Therefore, this method is a rapid analysis with a low limit of detection of 28 µM and proves functionality for on-site sensing. To do electrodeposition in a bubble wall, different ions such as silver and palladium ions were dissolved within the bubble film, a bare carbon microelectrode is placed inside the bubble wall , and the suitable cathodic potential is applied. The deposited metallic film was analyzed by scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy. The images obtained from the analysis revealed that the thickness of the bubble wall or electrochemical cell imposes limitations on the electrodeposition area at the microscale level. Furthermore, the lifespan of the bubble wallplayed a crucial role in controlling the duration and thickness of the deposited film from nanoscle to microscle [3].

Keywords: Microelectrochmeistry, Microdepostion, Thin film, Nitrite detection, Bubble film.

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Dye removal from aqueous solution using ferrite-based nanocompositein the photocatalytic process

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Lack of pure water is the one of the major barriers in the global socio-economic development. The industrial discharge and other human activities release different kinds of chemicals into the natural environment, contaminating available resources of water [1]. Dyes are one of the largest polluting groups of textile wastes and other industrial processes. Due to the adverse effects of organic dyes on human health, several technologies have been used to treat dye-containing wastewaters, including coagulation- flocculation, biological treatment, electrochemical treatment, membrane filtration, ion exchange, absorption, chemical oxidation, and advanced oxidation processes.Photocatalytic oxidation is one of the effective and well-known techniques for reducing the negative effects of environmental pollutants [2]. The photocatalytic process involves the acceleration of a chemical reaction in the presence of substances called photocatalysts, which can absorb quantum light with the appropriate wavelength, according to the band structure of their orbitals. In this research, the efficiency of $MgFe_2O_4/MoS_2$ nanocomposite in the photocatalytic oxidation of acid blue 113dye was investigated. The effects of three parameters, including contact time, pH value and the amount of catalyst on the dye degradation were studied.The optimum conditions for degradation of 20 mg/l acid blue113 were found at 10.07 min, and catalyst dose of 20.95 mg under visible light irradiation. The results show that by photocatalytic oxidation process using the synthesized nanocomposite, 93.91% of the dye degradation can be achieved.

***Keywords*:**Nanocomposite; Acid Blue113; Optimization; Wastewater;Photocatalyst.

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Investigation of the effect of surface functional groups on iodine sorption properties of a 2D zinc (II) coordination polymer

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In this work, a two-dimensional zinc(II) coordination polymer (Zn-CP, **1**) has been selected for consecutive post-synthetic modifications. In the first step, the coordinated solvent was removed to create the solvent-free structure Zn-CP-df (**2**) with open-coordination or Lewis acid sites. Then, the solvent-free structure **2**was functionalized by ethylene diamine and 1,3-diamino propane to obtain amine functionalized structures Zn-CP-en (**3**) and Zn-CP-DAP (**4**), respectively containing Lewis base sites. Finally, Zn-CP-en was reacted with chlorosulfonic acid ($ClSO_3H$) to obtain Zn-CP-SO_3H (**5**) with Bronsted acid sites. The capability of compounds **1-5** in iodine sorption in both vapor and liquid phases was investigated in detail. The results show outstanding iodine capture for both amine functionalized structures Zn-CP-en (100% wt) and Zn-CP-DAP (204%) [1-4].

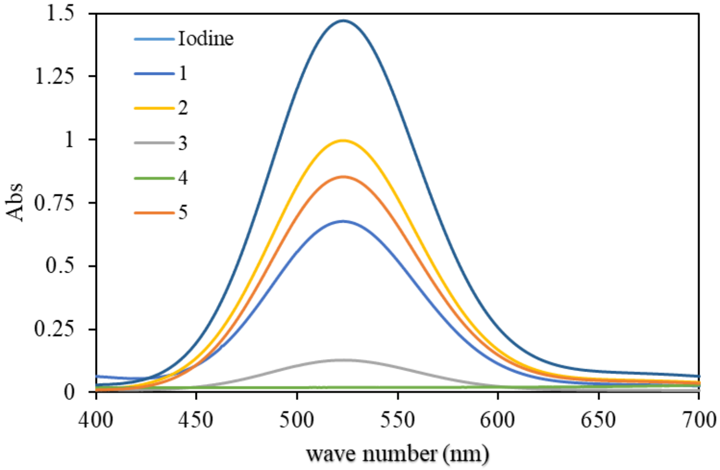

Fig. 1: Iodine sorption of compounds 1-5.

Keywords:Coordination polymer,Surface group, Post-synthetic modification, Iodine sorption.

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Evaluation the Performance of Polyaniline Graphene Oxide Nanocomposite Coating toward Corrosion Protection of Carbon Steel in Acidic and Saline Environments

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Majority of industries are inherently faced with the problem of corrosion and steps for protection of materials from corrosion have been of large interest to them. In this research the potential of graphene oxide nanosheets (GO) dispersed in polyaniline (PANI) network as an efficient coating for corrosion prevention was investigated [1]. GO was synthesized from natural flake graphite by the modified Hummers method. Also, polyaniline was chemically synthesized by oxidation of aniline monomer under acidic condition (0.5 M H_2SO_4) using potassium permanganate and potassium iodate as an initiator of oxidative polymerization [2]. GO was dispersed in a PANI solution which was dissolved in tetrahydrofuran (THF) with the aid of ultrasonic agitation and the obtained dispersion denoted as PANI-GO that was used as a thick film for coating the corten steel. Characterization of the PANI-GO by scanning electron microscope (SEM) revealed that GO nanosheets were well dispersed in PANI network. Anodic polarization curves were used to evaluate the corrosion rate of bare and PANI and PANI-GO coated electrodes in 3.5% NaCl, HCl 0.1 M and seawater [3]. The results showed that the presence of GO in coating significantly increased the corrosion potential and drastically reduced the corrosion current and corrosion rate of corten steel. The highest protection efficiency was achieved when a PANI film containing 0.005 g GO was used as coating on the metal surface.

Keywords:Corrosion; Corten steel; Polyaniline; Graphene oxide nanosheets; Polarization curve.

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Mesoporous KIT-6 as a support for the immobilization of a palladium organometallic nanocatalyst and its application in C–C coupling reactions

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Many Pd complexes have been used as homogeneous catalysts incross-coupling reactions [1]. Although some of the Pd complexes have potential for recycling [2,3], most of them haveproblems such as deactivation and difficult separation from the solution. Thus, it is necessary to develop heterogeneous catalysts which can easily be recovered from the reaction system and reused [4, 5]. Recently, Ryoo and co-workers reported a new cubic mesoporous silica material named KIT-6, which was prepared using triblock copolymer (P123) as the mesopore directing agent. KIT-6 possesses large readily tunable pores with thick pore walls, high thermal stability, high specific surface area and large pore volume. Therefore, mesoporous KIT-6 can be used as a support for the synthesis heterogeneous catalysts. In this work, a new Schiff base complex of Pd(II) was fabricated on the surface of KIT-6. For this purpose Schiff-base ligand was synthesized from condensation of diethylenetriamine (DETA) and salicylic aldehyde (SA). In the next step, Schiff-base ligand was reacted with (3-iodopropyl)trimethoxy silane (IPTMS). Then, Schiff base complex of palladium was synthesized using a complexation reaction of $Pd(OAc)_2$. Finally, the obtained palladium complex was fixed on KIT-6 (Pd@SA-Schiff base@KIT-6) as a new reusable and practical catalystin Suzuki reaction. This catalyst was characterized using IR, BET, EDS, SEM, and TGA methods.

Scheme 1. Carbon-carbon coupling reaction in the presence of Pd@SA-Schiff base@KIT-6.

Keywords:Mesoporous silica materials, Nanocatalyst, Suzuki reaction, KIT-6, Schiff base complex, Palladium.

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Design, preparation and characterization of Zr(O)@Creatine@KIT-6 nanoparticles as a nanocatalyst for the synthesis of various tetrazole derivatives

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In the last few years, immobilization of homogeneous catalysts on various solid supports with the advantage of catalysts separation and recycling have been widely studied in many divergent areas of research [1,2].Among different nanoparticles, mesoporpus silicais commonly employed as a heterogeneous support for the immobilization of homogeneous catalyste [3].KIT-6 is a relatively new structure of mesoporous silica with thick expanded walls, thermal stable, open porosity and very accessible to guest species and metal complexes.Therefore, due to the mentioned unique properties of mesoporous KIT-6, it can be used as a suport for the synthesis heterogeneous catalysts. In this work,the synthesized KIT-6 was modified by 3-chloropropyltrimethoxysilane (CPTMS). Then creatine was immobilized on its surface (creatine@KIT-6). Finally, zirconium dioxide was fabricated on creatine@KIT-6 (Zr(O)@creatine@KIT-6). The obtained catalyst was identified by IR, BET, XRD, EDS, SEM and TGA methods and further it was investigated in the synthesis of tetrazole derivatives. All products were obtained with high yield and purity which indicates the high catalytic activity of this catalyst.

Scheme 1. Synthesis of 5-substituted 1H-tetrazoles catalyzed by Zr(O)@creatine@KIT-6 nanocatalyst.

Keywords: KIT-6, Heterogeneous catalysts, Mesoporous materials, Tetrazole, Creatine.

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Modified Sol-Gel Processing of $NiCr_2O_4$ Nanoparticles; Structural Analysis and Optical Band Gap

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Nickel Chromite nanoparticles were successfully synthesized via a modified sol-gel method using nickel acetate and ammonium dichromate in melted stearic acid as a complexing agent. The diffractograms of the nanoparticles confirmed a pure formation of $NiCr_2O_4$ spinel without any minor phase. The coordination structure of as prepared nanoparticles shows a series of absorption bands below 1,000 cm^{-1} were evidenced the M-O (Cr-O, Ni-O) bond in the sample. Optical band gap, magnetic properties and color parameters (L*.a*.b*) indicates that the final nanoparticles are optically and magnetically active. The particle size of $NiCr_2O_4$ was calculated using Scherrer equation at about 24 nm. Optical band gap obtained at 1.7 eV indicating that $NiCr_2O_4$ nanoparticles are semiconductor material and can be used in electrical devices.

Keywords: $NiCr_2O_4$ spinel, optical band gap, sol-gel, nanoparticles.

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Synthesis, X-ray crystallography, and Hirshfeld surface analysisof a New Carbacylamidophosphate

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Carbacylamidophosphates (CAPh) with moiety –C(O)NHP(O)– are important inorganic ligands in the synthesis of metal complexes such as transition metals, lanthanides, and Sn(IV) with biological and pharmacological activities [1,2]. Besides, the biological activity behavior of CAPh, its seemed efficient ligands in coordination chemistry either as O,Ó-bidentate chelates in neutral and deprotonated form or in a monodentate fashion *via* oxygen of the phosphoryl group [3,4]. $Cl_2HCC(O)NHP(O)[NHC_6H_{11}]_2$ was synthesized and characterized by IR spectroscopy and elemental analysis. The structure of CAPh was determined by single-crystal X-ray crystallography technique. The compound crystallizes in triclinic system, space group $P\bar{1}$, unit cell a = 4.8182(3)Å, b = 11.6693(6) Å, c = 16.3611(9) Å, α = 84.171(4), β = 86.836(4)°, γ = 85.947(4)°, Z=2. In the crystalline lattice of CAPh, there are Op...NH_{amine} and Oc...NH_{amide} hydrogen bonds between adjacent molecules led to one dimentional polymer along the c-axis. There are also weak intramolecular hydrogen bonds CAPh adopts a 3D supramolecular structure.The main non-covalent intermolecular interactions were also studied by Hirshfeld surface analysis and fingerprint plots.

Keywords: Carbacylamidophosphate, X-ray crystallography, Hirshfeld surface analysis.

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The interaction of Phosgene gas with the pristine and B-doped $Si_{12}C_{12}$ nanocluster: A DFT, TD-DFT, RDG and AIM

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Fullerenes are also a well-known class of carbon-based and SiC nanostructures with a cage-shaped configuration, employed in diverse applications, including superconductors [1], gas storage [2], nano-electronic magnetic devices, biotechnology [3–4], In this project, we investigated the effects of B doped, and phosgene adsorption on the structural and electrical properties of SiC nano cluster by using density functional theory method. At the first time, we examined different configurations for adsorbing phosgene on the outer surface of nano cluster, after optimizing all models; we selected 15 stable models for this study. From optimized models the quantum parameters, RDG, NMR, HOMO-LUMO orbitals and thermodynamic properties are calculated by using cam-B3LYP/6-31G(d,p)level of theory. The calculated results indicated that the bond angle and bond length of nanocluster around doping and adsorbing position increase significantly from original values. The result of NMR graphs reveal that the chemical shielding parameters with doping (B atoms) and adsorbing phosgene increase. The quantum parameters such as gap energy and global hardness of system decrease significantly from pristine models, and so the reactivity and conductivity of system increase. The reduced density gradiant and atom in molecule theory results demonstrated that the nature ob bonding between SiC nanocluster with phsogen is van der Walls type and the doped nano cluster is a good candidate for adsorbing phosgene molecule.

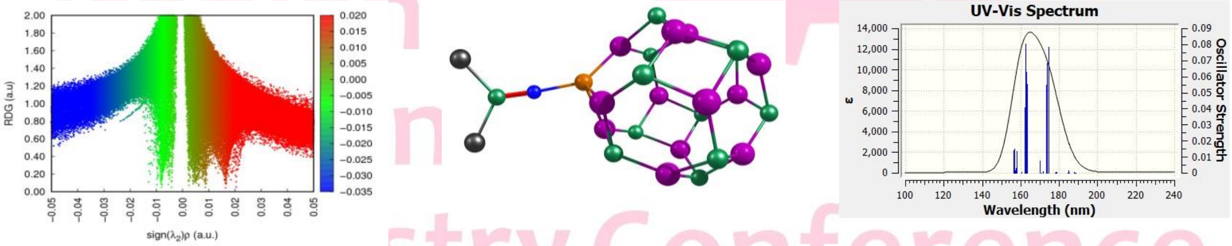

Figure: The optimized structure and RDG and UV-visible spectrum of $Si_{12}C_{12}$ nanocage@Ph complex

Keywords:$Si_{12}C_{12}$ nanocage, Phosgene, DFT, AIM.

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Investigation the impact of surfactant on the stability of nanofluids in the presence of aluminium oxide as an additive in ignition engines

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Nanotechnology refers to the ability to manipulate, measure, produce, and fabricate particles within the range of 1-100 nanometers in size[1]. The study of materials and their properties is a fundamental aspect of many academic disciplines. Nanotechnology is a field of study that encompasses various disciplines, such as toxicology, medicine, physics, chemistry, biology, mechanics, and engineering, among others. It is an interdisciplinary area of knowledge[2].The proper implementation of physical and chemical techniques for achieving uniform dispersion of nanoparticles in base fuels and preventing agglomeration is a crucial aspect in the context of ignition (CI) engines. A dual-stage methodology was employed in the production of nano-additive fuels. Initially, the production of nanoparticles involved the utilisation of surfactants to facilitate the separation of particles, minimise agglomeration, and enhance the chemical stabilisation of the suspension.The steric stabilisation mechanism is responsible for the ability of surfactants to stabilise suspensions, which is a noteworthy observation[3]. In this study, ϒ-Al_2O_3 nanoparticles was used as the additive for reducing the ignition delay time in the present of the Dimethylaminoethyl azide(DMAZ), and then the effects of surfactant on droplet burning rate are discussed.Therefore sorbitan monooleate(sp-80), sorbitan trioleate (sp-20), Polysorbate 80(tween-80), poly ethylene Glycol-200 (KEPEG 200), polysorbate 60 (tween-60=KEPS 60), polysorbate 20 (tween-20=KEPS 20), Cetyl Trimethyl Ammonium Bromide (CTAB), and combinations of these surfactants were examind. the obtaind results confirm tween-20 ,tween-60, and CTAB have accaptale efficency.

Keywords: Surfactant , Tween, ϒ-Al_2O_3, Nanoparticles.

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Evaluation of the Specific Ignition Delay Time for the DMAZ with Nanoparticles for the Rocket Engine

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Hydrazine, monomethyl hydrazine (MMH), and unsymmetrical dimethyl hydrazine (UDMH), either individually or in combination, have been widely utilised in space programmes[1]. The utilisation of hydrazine-based fuels presents a significant peril to the well-being of individuals engaged in the handling, storage, and conveyance of said fuels, due to their acute toxicity and potential carcinogenic properties. As a result, it is preferable to substitute them with alternative hypergolic liquid fuels that exhibit comparable ignition and combustion performance, but are not carcinogenic and possess significantly lower toxicity levels than hydrazine-based fuels[2].Numerous studies have been conducted in the pursuit of viable alternative hypergolic fuels. Notably, amine azides have garnered significant interest in this regard. One example of a representative amine azide is DMAZ, which stands for dimethyl amino ethyl azide.According to the LD50 acute toxicity, DMAZ exhibits approximately thirty times lower toxicity than MMH. Additionally, DMAZ outperforms MMH in various other performance measures[3].Dimethylaminoethyl azide, sometimes known as DMAZ, is an excellent alternative to the hydrazine group in the aerospace sector. However, with the liquid oxidizer, white fuming nitric acid (WFNA), it has a reasonably long ignition delay period, and it is nonhypergolic when used in conjunction with inhibited red fuming nitric acid (IRFNA). In this study, the ignition delay periods of DMAZ were reduced by the incorporation of several nanoparticles, including metal oxide (including Fe, Zr, B, Al, Cu, and Ce), carbon nanostructures, multi-walled carbon nanotubes (MWCNT), graphene, and graphene oxide without surfactant.According to the findings, the ignition delay time of DMAZ was reduced from 90 milliseconds to just 11.9 milliseconds when ϒ-Al_2O_3 was added.

Keywords:Metal Oxid, Nanoparticles, ϒ-Al_2O_3, DMAZ.

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Investigating the effect of time on the morphology and crystallinity of MIL-125 in the solvothermal synthesis method

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The use of metal-organic frameworks(MOFs) is constantly expanding. MIL-125 is one of the most important and widely used cases [1]. Several methods have been reported for the synthesis of this framework, such as the use of reflux and autoclave in solvothermal synthesis [2]. Synthesis time is one of the most important parameters in synthesis, which includes energy consumption and time, which are two important parameters in research. In this research, the synthesis of MIL-125 was done by solvothermal method, and in an autoclave, we specifically investigated the effect of time on morphology and crystallinity. Our results showed that the 24-hour synthesis had the best results among the times of 6, 12, 18, and 24h. These results were also checked with 72-hour time and reflux conditions, which most of the syntheses are reported in the reports with this method, and it was shown that 24-hour time with autoclave had a favorable and acceptable result[3]. This means that there is an acceptable improvement in time and energy.

Keywords:MIL-125, Metal-organic frameworks (MOFs), Synthesis, Solvothermal.

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Copper-Decorated Core–Shell StructuredOrdered Mesoporous Containing Cobalt Ferrite Nanoparticles as High-Performance Heterogeneous Catalyst toward Synthesis of Tetrazole

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The present work describes the synthesis of copper immobilization on $CoFe_2O_4$/MCM-41 as a catalyst, which is created by attaching copper and ligand (N-phenyl anthranilic acid (PA)) on the surface of $CoFe_2O_4$/MCM-41 ($CoFe_2O_4$/MCM-41/PA/Cu). The synthesized $CoFe_2O_4$/MCM-41 support and immobilized copper were identified by FTIR, TEM, VSM XRD, and nitrogen adsorption–desorption analysis. The results showed that MCM-41 silica was coated with magnetite nanoparticles and copper was successfully immobilized on this structure. The catalytic performance of synthesized catalyst was tested in the synthesis of tetrazole. It was shown that the solid catalyst exhibited a strong magnetic response and showed good catalytic activity in the synthesis of tetrazole. The catalytic test showed that copper supported on $CoFe_2O_4$/MCM-41 hybrid showed much better catalytic activity than copper supported on $CoFe_2O_4$, indicating that MCM-41 plays an important role in $CoFe_2O_4$/MCM-41 hybrid for the synthesis of tetrazole.Separation of the solid catalyst from the reaction mixture was easily performed by external magnetism without apparent mass loss. And the catalyst could be reused six times for the synthesis of heterogeneous tetrazole [1-3].

Keywords:$CoFe_2O_4$/MCM-41, N-phenyl anthranilic acid (PA), Copper, Synthesis of tetrazole.

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The computational study of the interaction of Hydroxycarbamide molecule with pristine, Ni-doped C_{20} nanocage: AIM, NBO, DFT, and TD-DFT

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After the discovery of carbon nanoparticles, great attention focused on other nanoparticles and nanocages such as C_{20} nanocage due to thermal stability, high conductivity, high hardness, gas sensing, hydrogen storage, electronic devices [1], and other adsorption properties[2–3]. This study aims to investigate the adsorption of hydroxy carbamide (HCA) drugson the surfaces of the pristine and Ni-doped C_{20} nanocage. For this purpose, at the first step, we consider different configurations for adsorbing HCA on the surface of nanocage, and then all considered structures are optimized at the cam-B3LYP / LanL2DZ level of DFT theory by using Gaussiansoftware (09). The quantum parameters, thermodynamic parameters, molecular electrostatic potential, TD-DFT parameters, UV-visible spectrum, the density of state (DOS), and MEP graphs are calculated and all calculated results are analyzed. The Uv-visible results demonstrate that with adsorbing HCA drug and functionalizing Ni atom, the adsorption frequency increased significantly from the original state. The HOMO-LUMO and MEP results show that the charge density transferred from the HCA drug towered nanocage surface and so the nucleophilic properties of nanocage surface increase. The quantum parameters show that the gap energy of the system after adsorbing HCA alters silently from the original state, and so the C_{20} nanocage is not a good sensor for detecting drugs. On the other than the values of thermodynamic parameters such as enthalpy and Gibbs free energy for all adsorption models are negative and favorable in the thermodynamic approach. These results confirm that the pristine and Ni-doped C_{20} nanocage can be used as adsorbed for HCA molecules.

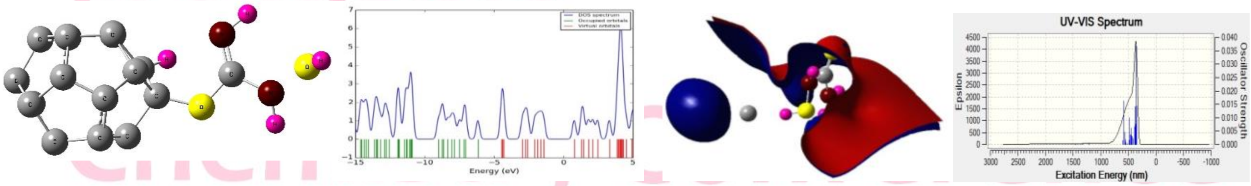

Figure 1: The optimized structure, DOS, MEP, and UV-visible plot of C_{20} nanocage with HCA drug complex.

Keywords:C_{20} nanocage, Hydroxycarbamide, Ni, NBO, DOS.

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Co-(PYT)$_2$@boehmite as anefficient and reusable nanocatalyst in the synthesis of tetrazole derivatives

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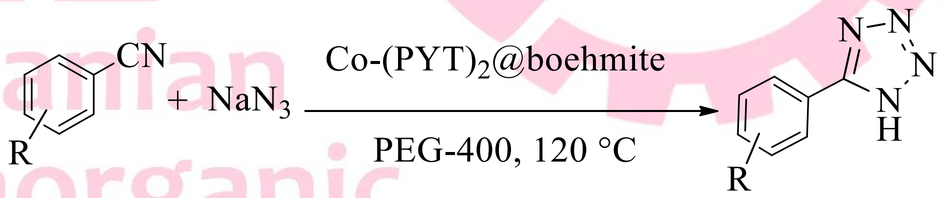
Boehmite is γ-AlOOH and it is the most stable phase of alumina after gibbsite [1], which contains high aggregation of hydroxyl groups on its surface [2]. Therefore boehmite nanoparticles can be used as an excellent support for fabrication of heterogeneous catalysts [3]. Consequently at first part of this work, boehmite nanoparticles were modified using 3-choloropropyltrimtoxysilane and then 1,3-bis(pyridin-3-ylmethyl)thiourea ((PYT)$_2$) was anchored on its surface. Then, cobalt complex was immobilized on its surface (Co-(PYT)$_2$@boehmite). The final obtained nanoparticles were characterized by FT-IR, TGA, SEM, WDX, EDS, and XRD techniques. At second partof this work, Co-(PYT)$_2$@boehmite was used as an efficient, stable, and selective nanocatalyst for the synthesis of tetrazole derivatives. Because tetrazoles are an important group of medicinal and organic compounds which possess many uses in several fields such as coordination chemistry, synthetic organic chemistry, drugs, medicinal chemistry [4, 5].Co-(PYT)$_2$@BNPs can recovered and reused again for several consecutively runs without any re-activation.



Scheme 1. Synthesis of tetrazoles in the attendance of Co-(PYT)$_2$@boehmite

Keywords: Boehmitenanoparticles, tetrazoles, cobalt, homoselectivenanocatalyst.

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A La-Schiff base complex on MCM-41 as a recyclable nanocatalyst in the homoselective synthesis of tetrazoles

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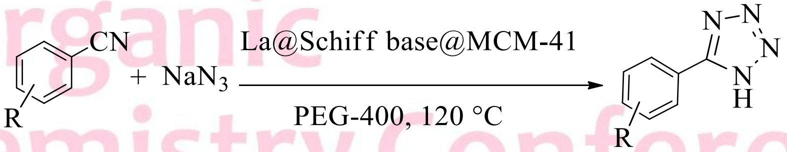
Recyclable and high efficient catalysts are one of the principles of green chemistry [1]. Therefore difficult recovering of the homogeneous catalysts and low catalytic activity of the heterogeneous catalysts are main challenges chemists [2]. To overcome on these problems, the nanostructure catalysts emerged as ideal catalysts because nanocatalysts have a heterogeneous nature with high surface area [3]. Therefore, nanocatalysts exist as a border between heterogeneous and homogeneous catalysts because they have advantages from both, such as efficiency, selectivity and reusability [3,4]. Therefore, various nanoparticle have been employed in catalysis applications. Amongst them, mesoporous nanomaterials especially MCM-41 were widely used as a support for immobilization of various catalysts [5]. Because MCM-41 has unique properties e.g. excellent stability, high surface area, easy surface modification, homogeneous hexagonal channel structure, large pore volumes, and easy separation from the reaction mixture [6]. Therefore, we investigated a new lanthanum-Schiff-base complex on MCM-41 (La@Schiff base@MCM-41) as an efficient, stable and reusable nanocatalyst in the homoselective synthesis of 5-substituted 1H-tetrazoles.La@Schiff base@MCM-41 was characterized by ICP, CHN, XRD, TGA, BET, FT-IR, SEM, EDS and WDXtechniques. This catalyst has good stability and heterogeneity nature which can easily recovered and reused for several times without significant loss in catalytic activity.The recovered La@Schiff base@MCM-41 catalyst was characterized by FT-IR, SEM and AAS techniques.



Scheme 1. Synthesis of 5-substituted 1H-tetrazoles in the presence of La@Schiff base@MCM-41.

Keywords: MesoporousMCM-41, tetrazoles, lanthanum, selective catalyst, Schiff-base complex.

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Boehmite magnetic nanoparticles as a practical and magnetically recoverable nanocatalyst in the synthesis of tetrazoles

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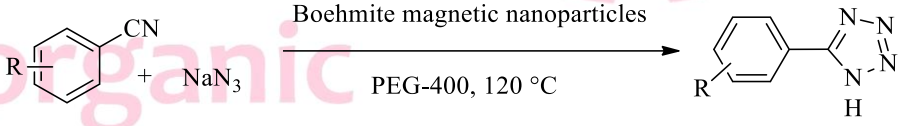
High catalytic activity is usually observed in the homogeneous catalyst systems[1]. However, purification of the products and recovery of the catalyst is often difficult and time consumingin the homogeneous catalyst systems [2]. In the other hand, clean technology and green chemistry require the use of recyclable catalysts [3]. While we need to a catalytic systems which have recyclability and high activity. This goal is achieved by nanocatalysts which are the bridge between heterogeneous and homogeneous catalysts [4]. However, nanoparticles (NPs) are not fully recycled by conventional methods such as centrifugation or filtration. All of these problems can be overcome using magnetic nanoparticles (MNPs) [5], which are quickly, easily and completely recovered using an external magnet [6,7]. In this work, boehmite MNPs were synthesized from a hybrid of boehmite and Fe_3O_4 nanoparticles. At first, boehmite nanoparticles were prepared. Then, these nanoparticles were magnetized using Fe_3O_4 NPs. Boehmite MNPs was characterized by TEM, SEM, EDS, WDX, ICP, FT-IR, Raman, XRD and VSMtechniques. Then, boehmite MNPs were applied as a homoselective, highly efficient, and recoverable nanocatalyst in the synthesis of tetrazoles. Boehmite magnetic nanoparticles was recycled for several runs in the synthesis of tetrazoles.



Scheme 1. Synthesis of 5-substituted 1H-tetrazoles in the presence of Boehmite magnetic nanoparticles.

Keywords: Boehmite NPs, magnetic NPs, heterogeneous nanocatalyst, reusable nanocatalyst.

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Nd-LArg-5BrSalen@MNC as a practical and reusable nanocatalyst in the synthesis of tetrazoles with antifungal properties in agricultural

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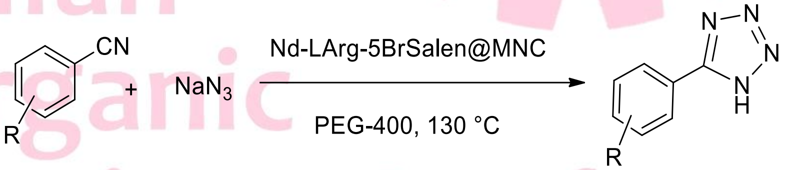
This project reports a simple procedure for the synthesis and characterization of neodymium on MCM-41 magnetic nanoparticles (MCM-41 MNC) as a reusable nanocatalyst. Firstly, MCM-41 MNC prepared by Fe_3O_4-dopping into mesoporous MCM-41 channels. Then, a novel neodymium Schiff base complex was immobilized on MCM-41 MNC. Finaly, this catalyst (Nd-LArg-5BrSalen@MNC) was used as magnetically recoverable nanocatalyst in the synthesis of tetrazoles. This nanocatalyst was characterized *via* TGA, TEM, SEM, FT-IR, SEM-EDS, VSM, ICP, XRD, WDX, and BET techniques. All tetrazole products were synthesized with high yield in short time and were identified by ^{1}H NMR, FT-IR and physical properties. Nd-LArg-5BrSalen@MNC nanocatalyst can be isolated and reused for several times consecutively without considerable loss of its catalytic activity. The recycled catalyst was characterized by SEM, EDS, WDX, XRD and FT-IR techniques. Also, the antifungal activity of the some tetrazole derivatives was studied against *Fusarium oxysporum*(rot disease of chickpea root) and *Botrytis cinerea* (gray mold of strawberry) using the paper disk method on PDA culture medium.



Scheme 1. Synthesis of tetrazoles catalyzed by Nd-LArg-5BrSalen@MNC nanocatalyst.

Keywords: Mesoporous MCM-41, magnetic nanoparticles, tetrazoles, antifungal, neodymium.

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One-step synthesis of titanate microstructures as efficient light scattering layer for dye-sensitized solar cells

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Non-renewable energy sources such as fossil fuels are still the first choice in energy resources. However, in order to maintain energy security and avoid the environmental problems caused by these energies, such as the greenhouse effect and air pollution, the focus should be shifted to renewable energy sources. These renewable energies have many advantages, such as harmlessness to the environment, abundant sources, and the ability to renew them because they are unlimited [1,2].Dye sensitized solar cells (DSCs), a third generation photovoltaic technology, are one of the most promising photovoltaic technologies for generating renewable, clean, and affordable energy. They are generally made from cheap and non-toxic components [3].As a crucial component of DSSC, the photoanode must perform several functions, such as a large BET surface area for dye adsorption, a suitable band gap for electron transport, and a suitable size for light scattering effect [4]. Researchers have claimed that the energy conversion efficiency (PCE) is closely related to the intrinsic properties of the photoanode materials, as the photoanode plays a key role in DSSCs [5].Herein, we report a simple, environmentally friendly hydrothermal process for large-scale fabrication of sodium titanate architectures in a NaOH solution medium to be used as a light scattering layer (LSL) in DSSCs. we use titanate as an oxide semiconductor in DSSCs due to its excellent optical and electronic properties (as a wide bandgap semiconductor) as well as its long-term stability, low cost, and nontoxicity. Titanate is used as LSL in the photoanode because LSL is important to prevent or reduce light loss during the DSSC process, which can lead to a decrease in power conversion efficiency (PCE). The more light captured on the sensitized photoanode, the more dye molecules are excited and the more voltage and current are generated, leading to an increase in the PCE of the DSSC device. Thus, the addition of LSL leads to a decrease in the recombination effect and an increase in the light scattering effect to improve the DSSC performance

Keywords: renewable energy, solar cell, DSSCs, light scattering layer, titanate.

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Investigation and optimization of the n-heptane isomerization reaction over the Pt-Zr-HMS catalysts with RSM method

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Since the isomerization process plays an important role in various industries, increasing the efficiency of these processes is an inevitable necessity [1]. In this research, using platinum catalyst, we tried to obtain the efficiency by changing the numerical value of temperature parameters, weight percentage of zirconium and hydrogen flow. The process of n-heptane isomerization on platinum catalysts with the effect of different numerical values of the following parameters in response surface methodology (RSM) software; T: temperature (200-500 °C), WZ: weight percentage of zirconium (5 to 35%), and TOS: time on hydrogen flow (1-6 h).As can be seen, the selectivity has a downward trend and then an upward trend. In this reaction, the minimum selectivity is between 320 and 440 °C, and the lowest value (27.3%) refers to 350 °C. At a temperature of 200 to 260 °C, this reaction has the maximum selectivity, which is 55.3%, happened at 200 °C and TOS of 3.5 h. The highest selectivity is related to 200 °C and 3.5 h, and the weight percentage of zirconium is 35% and 5%, respectively.

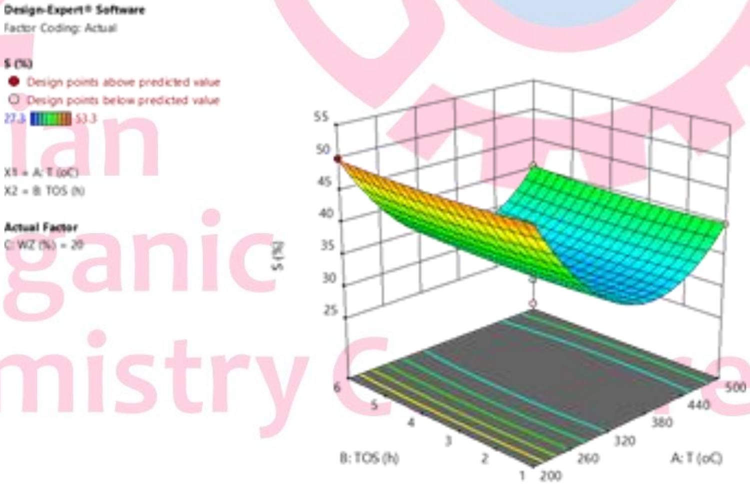

Figure 1. Surface response for the n-heptane isomerization as a function of reaction temperature and time on stream at a weight percentage of zirconium (20%).

Keywords: Isomerization, Catalysts, Response surface methodology, Zirconium.

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The kinetic study of toluene hydrogenation with response surface method over three Pt-supported catalysts

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Toluene is one of the unsaturated hydrocarbons. Breathing a high concentration of toluene leads to death, and lower concentrations affect the nervous system and lead to dizziness, unbalanced behavior and organ failure. Exposure to these volatile organic compounds causes harmful effects on the organs. Therefore, researchers are searching for new methods to replace these compounds with less dangerous substances. One of the methods presented in this process is the hydrogenation of toluene in the presence of suitable catalysts [1, 2].In this process, the catalyst that has the highest efficiency is suitable for toluene hydrogenation. Before the experiment, the reduction of the catalyst was done, and in the next steps, toluene was injected into the reactor tube at different speeds. The flow of hydrogen gas was adjusted to the optimal value, and the kinetic study of hydrogenation was carried out continuously at one-hour intervals. The fixed bed micro reactor at 130-190 °C using 1 g of each catalyst, three parameters were reported as temperature, flow rate of hydrogen and toluene. The results show that with increasing the toluene flow, the reaction rate has a relatively upward trend. The highest value of the rate was reported at 190 °C and a toluene flow of 120 cc/min. The lowest rate was reported at 130 °C and a toluene flow of 62.4 cc/min.According to the obtained results, the amount of hydrogen and toluene flow rates are effective and determine the amount of reaction rate. Among these three catalysts tested in a certain temperature range, toluene with a flow rate of 4.8 cc/min and hydrogen with a flow rate of 45 cc/h, among the data obtained from the above reaction, the Pt/HMS and Pt/SiO_2 catalysts have the highest reaction rates.

Keywords: Hydrogenation, Toluene, Flow rate.

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A Sm@Schiff-base@MCM-41 as a reusable and practical nanocatalyst for the synthesis of tetrazoles

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In recent years, nanoparticles have been used as supports for the stabilization of homogeneous catalysts [1,2]. Among them, mesoporous silica materials, such as MCM-41, have high stability in aqueous solution, air atmosphere and high temperature. Large specific surface area of MCM-41 (>1000 m^2/g) including a lot of silanol groups leads to ease modification of its surface [3]. High stability of MCM-41 allows the application of MCM-41 in harsh condition of the organic reactions [4]. Moreover, the large specific pore volume of MCM-41 which is up to 1.3 ml/g allows supporting of huge organic ligands and metal complexes into its channels [5-7]. In this regard, we are reporting asamarium Schiff-base complex on MCM-41 (Sm@Schiff-base@MCM-41) as an efficient and heterogeneous nanocatalyst for the synthesis of tetrazole derivatives. Sm@Schiff-base@MCM-41 was characterized by various techniques such as BET, TGA, XRD, FT-IR, SEM, EDS, WDX, and ICP. Sm@Schiff-base@MCM-41can be recovered and reused for several runs without significant change in its catalytic activity

Scheme 1. Synthesis of tetrazoles in the presence of Sm@Schiff base@MCM-41.

Keywords: MesoporousMCM-41, tetrazoles, samarium, Schiff-base, homoselective catalyst.

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A novel complex of samarium on boehmite nanoparticles as an efficient and reusable nanocatalyst for the synthesis of tetrazoles

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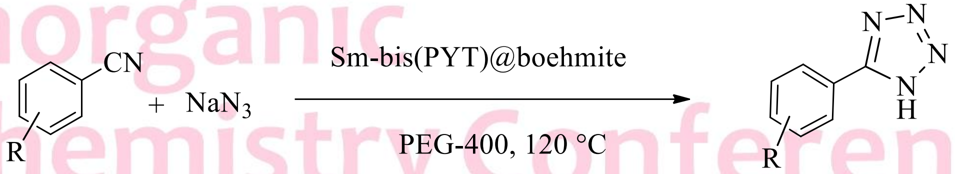
Boehmite is one of the attractive mineral materials, which was recently employed as support in the synthesis of heterogenous catalysts [1]. Boehmite consists of double layers of octahedron structure from oxygen and a central aluminum atom with a cubic orthorhombic unit cell [2]. Boehmite nanomaterials have unique properties such as excellent surface area, nanometer size of crystallite, easy availability, non-toxicity, and thermal stability [3]. Beside, samarium has rarely been reported as a catalyst for the synthesis of organic compounds. Regarding the fact that selective and reusable catalysts are the main principles of green chemistry, herein a new samarium complex on boehmite nanoparticles (Sm-bis(PYT)@boehmite) was investigated as a selective and recyclable nanocatalyst in the synthesis of 5-substituted 1H-tetrazole derivatives in PEG-400 as a green solvent. Because, tetrazoles are an important group of organic compounds which can be used in various fields such as coordination chemistry, drugs, synthetic organic chemistry, medicinal chemistry [4]. Sm-bis(PYT)@boehmite was characterized using thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET), wavelength dispersive X-ray spectroscopy (WDX), energy dispersive X-ray spectroscopy (EDS), scanning electron microscope (SEM), dynamic light scattering (DLS), Inductively coupled plasma mass spectrometry (ICP-MS), Fourier transform infrared spectroscopy (FT-IR), and X-ray diffraction (XRD) pattern. Notably, Sm-bis(PYT)@boehmite is stable and has a heterogeneous nature. Thus, it can be reused for several runs without any re-activation.



Scheme 1.synthesis of tetrazoles in presence of Sm-bis(PYT)@boehmitenanocatalyst.

Keywords: Green Solvent, Boehmite Nanoparticles; Reusable Catalyst; Environmentally Friendly Catalyst, Homoselective Catalyst, Tetrazole.

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Investigation of the interaction of boron nitride nanosheets (h-BN) with cyanogenfluoride (FCN) by density functional theory method

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Among various nanomaterials, carbon-based nanostructures are one of the major types of DDC, utilized in various configurations like nanoparticle, nanotube, graphene and graphene oxide [1–3].The aim of this work was to investigate the adsorption and detection of cyanogen fluoride (FCN) molecule on a boron nitride nanosheet marked with hydrogen ion (H^+) in the presence and absence of an electric field. Calculations were performed using density function theory (DFT/WB97XD) and 6-31G(d,p) base set by Gaussian 16 software. After calculations, quantum and thermodynamic parameters, absorption energy, UV spectra, HOMO and LUMO orbitals, DOS and RDG diagrams, optical properties and other results were extracted. The values of enthalpy and adsorption energy are negative for all absorption models, indicating that the adsorption process is exothermic in all models. Gibbs free energy is negative in most absorption models, which indicates that the adsorption process is spontaneous in these models. The results of AIM, RDG and NBO show that the adsorption of cyanogen fluoride on the boron nitride nanosheet is hydrogen and van der Waals type. Applying an electric field and adding hydrogen ions to the nanosheet reduces the absorption energy, gap energy and hardness of the nanosheet, which can lead to stronger adsorption, increased conductivity and reactivity of the nanosheet. These results suggest that boron nitride marked with hydrogen ions in the presence of an electric field can be a good choice for the adsorption and detection of cyanogenfluoride.

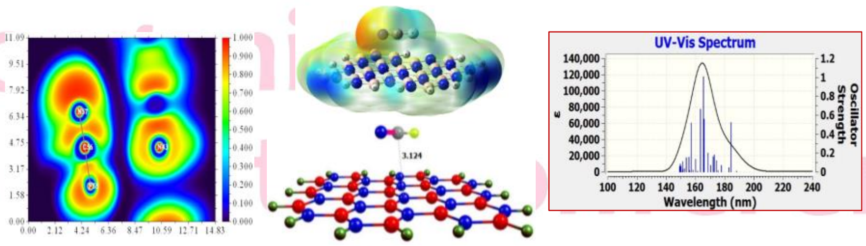

Figure 1: The ELE , MEP, UV-visible and optimized sturctures of FCN@h-BN nano sheet.

Keywords: *h*-BNanosheet, Cyanogen Fluoride, Hydrogen Ion, Electric Field, DFT.

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Immobilization of tris hydroxyaminomethyl methane on hercynite MNPs as a magnetically recoverable organocatalyst in the synthesis of tetrahydrobenzo[b]pyran derivatives

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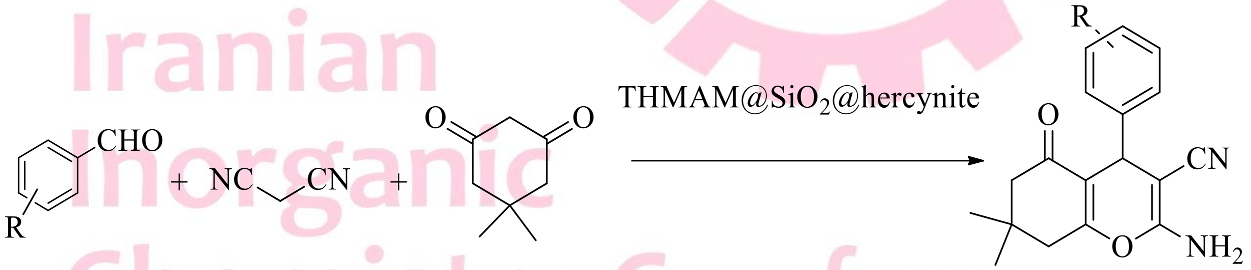
Recently, heterogeneous catalysts have been used in organic reactions and modern organic synthesis [1,2]. In this regard, hercynite magnetic nanoparticles have high density of hydroxyl groups on its surface, which could be available for immobilization of various catalysts [3]. Therefore, hercynite magnetic nanoparticles have attracted great attention, especially in the synthesis of heterogeneous catalysts, due to their feasible recovering and reusing by an external magnet [4]. More addition, hercynite nanoparticles is composed from Al, O and Fe, which have several unique properties such as easy availability, high surface area, non-toxicity, and low cost [3,4]. In this work, hercynite magnetic nanoparticles were synthesized and its surface was coated by a silica layer. Then its surface was modified by 3-choloropropyltrimtoxysilane. Finally, tris(hydroxymethyl)amino methane was immobilized on the surface of modified hercynite nanoparticles (THMAM@SiO_2@hercynite NPs). In the next step, THMAM@SiO_2@hercynite NPs was characterized by by SEM, EDS, WDX, TGA, XRD, VSM, and FT-IR techniques. The catalytic activity of tetrahydrobenzo[b]pyran NPs was studied in the synthesis of tetrahydrobenzo[b]pyran derivatives.



Scheme 1. Synthesis of tetrahydrobenzo[b]pyran in the attendance of THMAM@SiO_2@hercynite

Keywords:Hercynitenanoparticles, magnetic nanoparticles, trishydroxyaminomethyl methane, tetrahydrobenzo[b]pyran, recoverable organocatalyst.

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Fabrication of Core‒Shell-Structured Organic‒Inorganic Hybrid Nanocatalyst for the Synthesis of polyhydroquinolines

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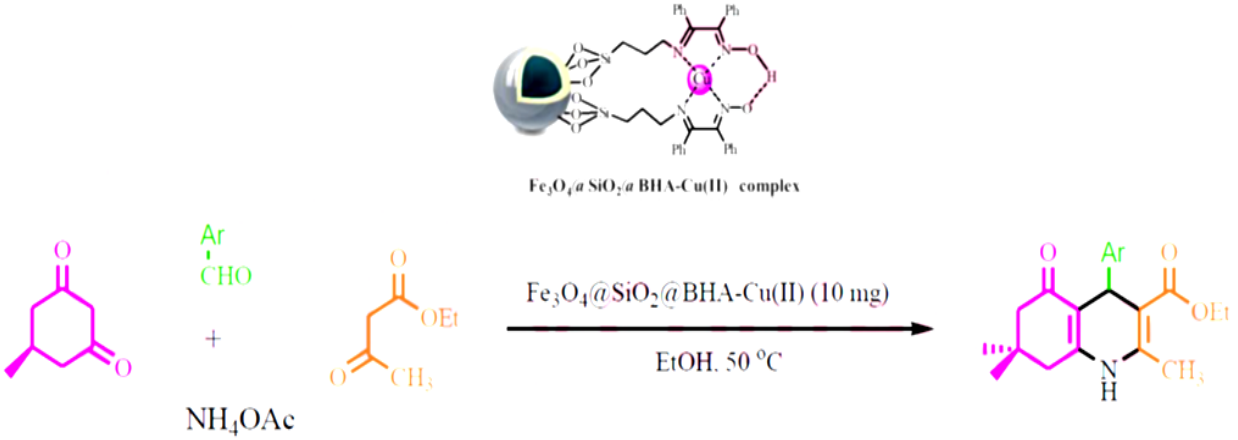
Modern state of the art of catalysis science and research reveals that the introduction of novel nanotechnologies has enabled the generation of solid-supported heterogeneous nanoscale catalysts, which are effective tools for controlling chemical reactivity as well as conferring the synergistic benefits of facile recovery [1]. By collectively integrating the key advantages of homogeneous as well as heterogeneous catalysts, they offer great prospects of meeting the sustainability criteria consistent with the goals of green chemistry [2-3]. Mgnetic nanoparticles play the role of a bridge between heterogeneous and homogeneous catalysts and have emerged as promising catalysts due to their low-cost, efficient and reusable properties [4]. A magnetically recoverable heterogeneous $Fe_3O_4@SiO_2@BHA$-Cu(II) nanocomposite was prepared by immobilizing a novel Cu(II) complex on the nanoparticles. The catalyst was characterized by FT-IR, TGA, VSM, FESEM, XRD, ICP and EDX techniques. The catalytic activity of this nanocatalyst in the synthesis of polyhydroquinoline derivatives were investigated.



Scheme 1. Synthesis of Polyhydroquinoline in the attendance of $Fe_3O_4@SiO_2@BHA$-Cu(II).

Keywords: Magnetic Nanoparticles, Polyhydroquinoline, Immobilized Copper Complex, Recoverable Nanocatalyst.

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New phosphorus-nitrogen compounds: synthesis, spectroscopic characterization and fungicide studies

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The phosphorus-nitrogen compounds, such as phosphoramides and thiophosphoramides were studied in viewpoint of their agrochemical delivery [1-4]. In the presence work, new phosphorus-nitrogen compounds were synthesized and used for the study of antifungal properties. The compounds, including (R)-$[(2,3\text{-}F_2)C_6H_3C(O)NH]P(O)[NHCH(CH_3)C_6H_5]_2$ (1), (S)-$[(2,3\text{-}F_2)C_6H_3C(O)NH]P(O)[NHCH(CH_3)C_6H_5]_2$ (2), and $P[S][NHCH_2C_6H_4\text{-}4\text{-}F]_3$ (3) were used in this study. Characterization was done by CHN analysis, Mass, IR and NMR spectroscopy.The ^{31}P signals are revealed at 4.01 and 4.10 ppm for the phosphoramides 1 and 2, respectively and at 65.40 ppm for the thiophosphoramide 3. In the ^{1}H NMR experiment, the broad signals at 9.42 ppm for 1 and 9.26 ppm for 2 associate to the N_{CP}—H unit (N_{CP} is the nitrogen atom of the C(O)NHP(O) segment), and the two other N—H protons appear as pseudo triplets at 4.88 and 5.06 ppm for 1 and 4.91 and 5.06 ppm for 2. For compound 3, the NH signal appears as a multiplet at 4.82 ppm. The ^{19}F signals of compounds 1 and 2 are revealed as doublets at –138.52 and –140.26 ppm for 1 and –138.51 and –140.26 ppm for 2. For 3, the fluorine signal appears at –116.73 ppm. The antifungal properties of these compounds against phytopathogenic fungi such as *Rhizoctonia solani*and*Fusarium culmorum* were studied, which showed their effectiveness against both fungi.

Keywords: phosphorus-nitrogen compounds, NMR spectroscopy, antifungal properties, phytopathogenic fungi.

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The computational study of adsorption of cyanide ion on the surface of Pristine and Al doped boron phosphide nanotube: AIM, NBO, RDG, TD-DFT

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Controlling and monitoring the HCN and CN ions concentration under the threshold limit value in bothindustrial and residential environments are of special interest. For detecting HCN gas and CN ion in the atmosphere, gassensors have been considered promising alternatives for environmental measurements due to their low cost, highsensitivity, fast response and direct electronic interface [1–4]. In this project, we investigate the CN ion adsorption on the surface of pristine and Al&S doped (4,4) armchair and (8,0) zigzag models of boron phosphide nanotubes (BPNTs) by using Gaussian 16 software, at the wb97xd/ 6-31G(d, p) level of theory. The results showed that adsorption energy in the all adsorption models are negative, and all adsorption models are favorable in view of thermodynamic approach. The positive value of NBO analysis indicate that the charge transfer is occurred from the cyanide ion toward the nanotube, for this means the electrical properties of nanotube change significantly from original state. The quantum results show that with doping Al&S doped the activity of nanotube for adsorbing CN ion increase. The reduced density gradient and atom in molecule theory results confirm that the bonding nature of nanotube with CN ion is electrostatic and partial covalence. The computational results demonstrate that the pristine and Al&S doped BPNTs can be a suitable adsorbent for cyanide ion in the environmental system.

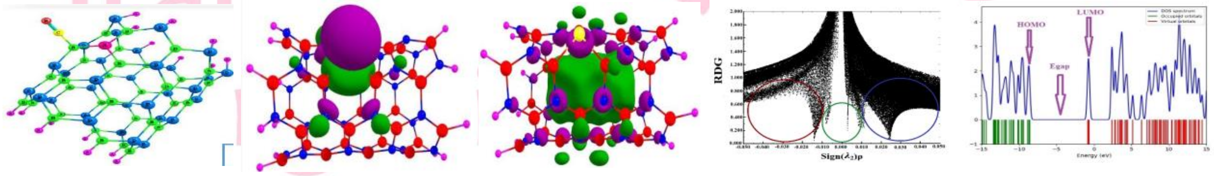

Figure 1: The RDG, DOS, HOMO-LUMO, and optimized sturctures of CN ion with BP nanotube**.**

Keywords: *BPNTs, Al&S doped,* Cyanide ion, Static Electric Field, DFT.

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New insights into the intrinsic cooperativity of intermolecular or intramolecular bonds

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There are some well-known methodologies for evaluating the cooperativity of intermolecular noncovalent bonds [1,2]. However, in this work, we report our methodology for study on the intrinsic cooperativity of both intermolecular noncovalent bonds and intramolecular metal–ligand bonds. Indeed, we improve and extend the methodology proposed in our research group [3] and show that the quantitative evaluation of the impact of chemical bonds on the strength of each other is not restricted to the intermolecular noncovalent bonds. New equations are proved for calculating the total stabilization and interaction energies as well as the cooperative energies of bonds in any system that can be considered as three fragments and two chemical bonds. We report also the calculation of the cooperativity of bonds in some metal complexes of the type LML′, where L and L′ represent a single ligand or a group of ligands. The results show that both the M−L and M−L′ bonds will strengthen or weaken depending on the degree of cooperativity or anticooperativity of bonds.Thus, the rational design of a system with a very weak or a very strong bond is possible, where we know the type and degree of cooperatvity of bonds.

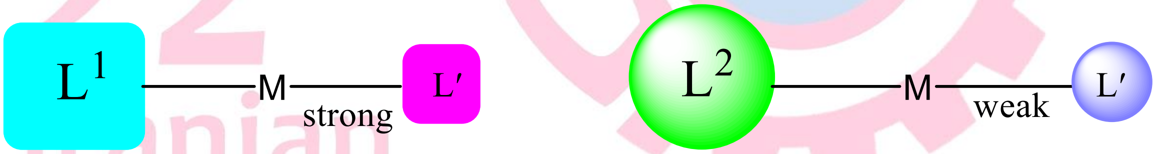

Figure 1. Changing the strength of M−L′ bond due to the existence of cooperativity and anticooperativity with M−L^1 and M−L^2 bonds, respectively.

Keywords: Theoretical study, Cooperativity of bonds, Noncovalent bond, Metal−ligand bonds.

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Nature and cooperativity of metal−ligand bonds in groups 5, 7, 9 and 11 half-sandwich cyclopentadienyl complexes

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Half-sandwich complexes that have an metal center attached to a cyclopentadienyl ligand have attracted much attention due to their unique electronic and chemical properties. The term sandwich compound was introduced in organometallic nomenclature in 1956 in a report by Dunitz and co-workers who confirmed the structure of ferrocene by X-ray crystallography [1]. In this work, we investigate the electronic structure and bonding interactions in a set of half-sandwich complexes using advanced computational methods and recently developed methodolgies [2, 3]. The aim of this project is to provide a detailed theoretical investigation of the nature of bond, and cooperativity of bonds for half-sandwich complexes containing cyclopentadienyl and carbonyl ligands with the general formula $[M(\eta^5–Cp)(CO)_n]$ ($M=Cu^+$, Au^+, Ag^+, n=1, M= Co^+, Ir^+, Ru^+, n=2, Mn^+, Re^+, Tc^+, n=3, V^+, Nb^+, Ta^+, n=4). The geometries of all complexes were fully optimized at the B3LYP, B971, M06-D3, M06L and MP2 levels with the def2-TZVP basis set using the GAUSSIAN-09 program without any symmetry restrictions. Vibrational frequency analysis, calculated at all levels of theory, indicates that the optimized structures are at the stationary points corresponding to local minima without any imaginary frequency.The results indicate that the type and degree of cooperativity of bonds in the series of these complexes depend highly on the type and nature of central metal ion.

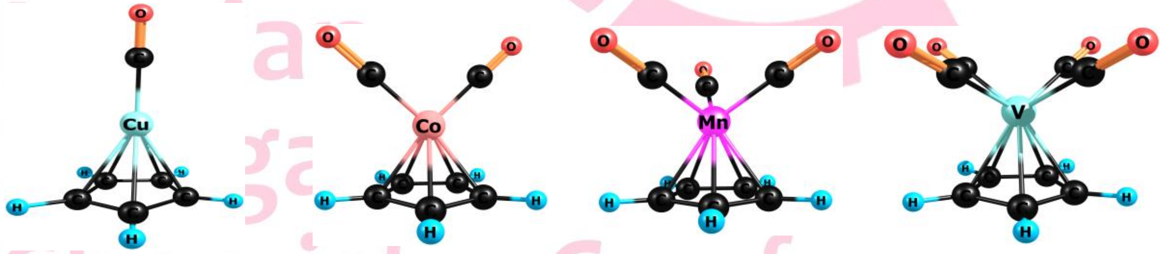

Figure 1. Optimized structure of selected complexes, $[Cu(\eta^5–Cp)(CO)]$, $[Co(\eta^5–Cp)(CO)_2]$, $[Mn(\eta^5–Cp)(CO)_3]$ and $[V(\eta^5–Cp)(CO)_4]$, at M06L/def2-TZVP level of theory.

Keywords: Theoretical study, Half-sandwich compounds, Cooperativity of bonds, Nature of bonds

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The effect of light on manganese porphyrin catalyzed oxidation of olefins with periodate under different conditions

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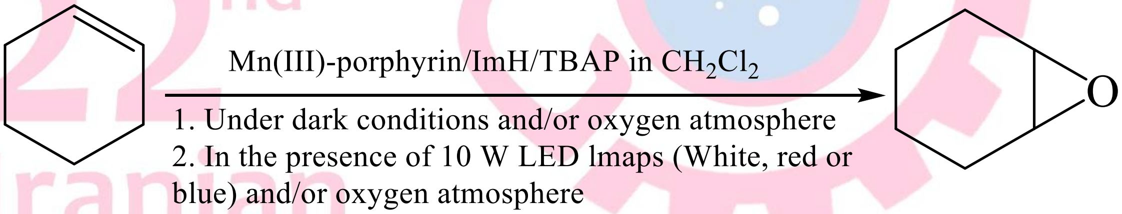
Most metal catalyzed oxidation of organic compounds with different terminal oxidants are conducted in air under exposure to sunlight or laboratory light [1-4]. However, little attention was paid to the possible influence of light and molecular oxygen on the efficiecy of the catalytic reactions. In the present study, the oxidation of cyclohexene with periodate catalyzed by manganese porphyrins was studied in dark, under the irradiation of various LED lamps and in the absence or presence of molecular oxygen to investigate the possible contribution of the excited states of manganese porphyrins and autoxidation [5] pathway in the mechanism of the oxidation reaction. The results of this study shows a meaningful difference between the conversions achieved under different reaction conditions, although no change in the product distribution was observed.



Keywords: Manganese porphyrins, Oxidation of olefins, Periodate, Autoxidation conditions, Light exposure.

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Evaluation of central-metal effect on anticancer activity and mechanism of action of isostructural Cu(II) and Ni(II) complexes containing pyridine-2,6-dicarboxylate

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Two Cu(II) (C1) and Ni(II) (C2) complexes were designed through the one-pot reaction of pyridine-2,6-dicarboxylic acid and2-aminobenzimidazole respectively with copper(II) nitrate hexahydrate and nickel(II) nitrate hexahydrate. Both complexes were characterized by single-crystal X-ray diffraction and the distorted octahedral geometry was recognizedfor them. The MTT assay indicated that the complexes have a significant antiproliferative effect on BEL-7404 cells. IC_{50} values confirmed that C1 (IC_{50}= 0.56 μM) is several times more potent than C2 (IC_{50}= 5.13 μM). The similar cellular uptake of the complexes in mentioned cells led to this proposal that the production of ROS with different values can be the main reason for different cytotoxicity of the complexes. In this study, C1 and C2 caused BEL-7404 cells arrest at the G2/M and S phases, respectively. The expression of p53, Bax up-regulation, and Bcl-2 down-regulation and also activation of procaspase-9, and 3 indicated that apoptosis through a caspase-dependent mitochondrion pathway is a remarkable pathway in BEL-7404 cells treated by C1 while mechanistic studies proved that C2 induce death of BEL-7404 cells through the activation of RAGE/PI3KC3/Beclin 1 autophagic cell signaling pathway, more specifically. The cytostatic effect of the complexes in the BEL-7404 3D spheroid model was depicted.

Keywords: Cu(II) and Ni(II) complexes, Anticancer effect, Production of ROS, Apoptosis, Autophagy.

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γ-Al_2O_3 catalysts synthesis with different aluminum sources for methanol dehydration to dimethylether

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Dimethyl ether (DME) is a versatile multi-source multi-purpose chemical being projected to become one of the main chemical feedstocks in the 21st century. It is a non-toxic, eco-friendly and easily condensable gas that can be used both as a fuel or as a chemical feedstock [1]. DME can be produced by methanol dehydration. In this study, three γ-Al_2O_3 catalysts for methanol dehydration to DME were synthesized by the precipitation method using different aluminum sources (Table 1). The activity of the catalysts was compared with a commercially available γ-alumina catalyst. The result showed that the Al precursor strongly affected the structural properties and catalytic performance with the catalyst produced from aluminum nitrate had the highest catalytic performance under the same reaction conditions, being comparable with the commercial γ-Al_2O_3. As a general trend, catalytic performance improved significantly with increasing specific surface area and pore volume of the catalysts, which are in turn a function of the textural properties and crystallinity of the sample. These caharactristics favor the availability and accessibility of acidic active sites to methanol reactant. In contrasrt, samples with low porosity and/or smaller crystallite size are less active, most probably due to their predominant amorphous nature [2].

Table 1. Textural properties and activity of catalyst samples.

Sample name	Aluminum source	BET surface area (m^2/g)	Pore volume (cm^3/g)	Pore diameter (nm)	Methanol conversion (%) [a]	
					T=260 ˚C, WHSV=$3h^{-1}$	T=300 ˚C, WHSV=20 h^{-1}
S1	Sodium aluminate	357	0.88	49.6	79	80
S2	Aluminum nitrate	353	0.80	45.5	79	82
S3	Aluminum foil	204	0.30	29.4	14	17
Commercial	-	246	0.74	62.0	80	81

[a] The catalyst activity measurements were carried out in an isothermal fixed-bed stainless steel reactor (i.d. 10 mm) at temperatures of 260 and 300 ˚C under atmospheric pressure. Feed: pure methanol, WHSV= Weight Hourly Space Velocity.

Keywords: γ-Al_2O_3 synthesis, Methanol dehydration, Dimethyl ether, Catalyic performance.

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Influence of preparation parameters of γ-Al_2O_3catalysts on its performance inmethanol dehydration to dimethylether

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A series of γ-Al_2O_3 catalysts were prepared by precipitation of $Al(OH)_3$ from aluminum nitrate solutions, using NaOH as precipitating agent, followed by filtering and calcination at 500 °C. The resulting powder was formed as extrudates and tablets prior to performance test. The catalyst were tested in a fixed-bed reactor for dehydration of methanol to dimethyl ether (DME),an alternative and environmental benign fuel and chemical [1]. The effect of preparation conditions such as NaOH concentration (1-4 M) and forming on catalyst performance were examined. The results showed that higher NaOH concentrations increased the surface area (and thus catalytic activity) of the samples (Fig. 1a) due to increased supersaturation [2]. A higher NaOH concentration is of economic benefit as it reduces the size of precipitation reactor. Above 270°C the reaction was equilibrium limited, and because of a high DME selectivity (≈100%) for all samples, this temperature is the optimum one in terms of DME yield. When formed as pellets, the extruded sample showed higher conversion compared to tableted sample, due to more reduction of pore volume in the latter as a result of much higher pressure applied. The results were compared with a commercial sample and a higher yield was observed for the extrudate sample (Fig. 1b).

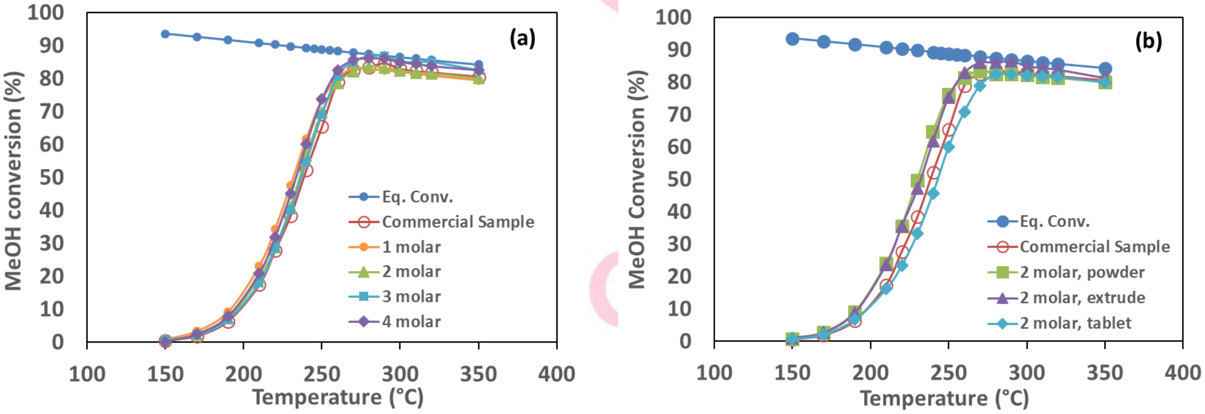

Fig. 1. Comparison of the performance of (a) powder, (b) shaped catalysts versus temperature**.**

Keywords:Methanol dehydration**,** dimethyl ether, γ-Al_2O_3 Catalyst, precipitation,catalyst forming

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Synthesis and Characterization of nanoClinoptilolite /cobalt oxide nanocomposite

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Zeolites, a member of the microporous crystalline aluminosilicates family, also known as "molecular sieves". Zeolite has the three-dimensional structures which are composed of the networks of $[SiO4]^{4-}$ and $[AlO4]^{5-}$ tetrahedral linked to each other with oxygen atoms .Natural zeolites are abundant in nature and have operational importance, including: clinoptilolite. mordenit [1].This worksynthesis annovel adsorbent nanozeolite/Co_3O_4(NZC) with high adsorption capacity by combining modified natural clinoptilolite nanozeolite and cobalt oxide to enhance the adsorption ability of zeolite. Characterization of the final nanocomposite was done by XRD pattern,Field Emission Scanning Electron Microscope (FE-SEM) andEnergy-dispersive X-ray spectroscopy (EDS). The XRD pattern results confirmed the correctness of the nanocomposite synthesis and SEM images and EDS reveal the appropriate particle size and element distribution. The prepared adsorbent can be used to absorb cationic pollutants and heavy metals [2-4].

Keywords:Cobalt oxide,Clinoptilolite, Zeolite, Adsorbent, Aluminosilicate.

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π- ExtendedDinuclear Ruthenium(II) Complex for Dye-Sensitized Solar Cell

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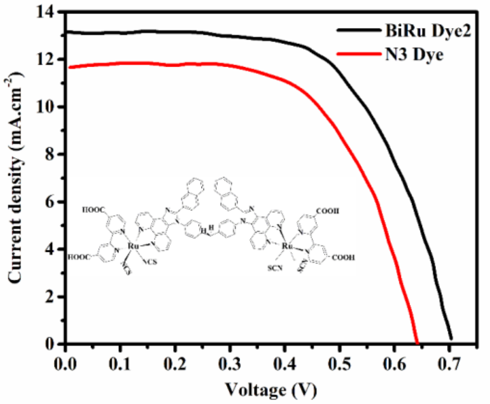

Dye-sensitized solar cells (DSSCs) have been evaluated for photovoltaic applications because of their low cost and high-power conversion efficiency [1]. Polypyridyl ruthenium complexes with ligands functionalized by thiophene, carbazole, and and π-extended moiety can be regarded as super sensitizers [1]. Herein, a new π-extended binuclear ruthenium (II) complex (BiRu2) with two naphthyl moiety was designed and synthesized and used as dye in DSSC.CV results showed that the$E_{1/2}$ oxidation of BiRu2 dye is shifted negatively by 0.02 V compared to the N3 couple, as standard dye, [2] indicating stronger electron-donating ability of the fused π-expanded ligand than H_2dcbpy. The calculated excited state oxidation potential ($E^* = -0.97$ V) for BiRu dye is close to N3 dye and sufficiently more negative than the conduction band (CB) edge level of the TiO_2 at approximately -0.7 V [1, 3] indicating energically highly favorable for electron injection from the excited dyes into the conduction band of TiO_2. Moreover, the estimated LUMO energy of BiRu2 dye (-3.3 eV) is higher than the conduction band energy level of theTiO_2 (-4.0 eV)which is desirable for more efficient electroninjection into CB of TiO_2 [4]. The DSSC based on BiRu2 achieves a conversion efficiency of 5.21%, which is 12% higher than that of the N3-sensitized solar cell under the same cell fabrication and efficiency measuring procedures (See I-V curve), which is attributed to the higher absorption coefficient in the visible region of specrum and lower $E_{1/2}$ of BiRu2 as a result of π-expanded ligand. Moreover, the improved J_{SC} and V_{OC} were caused by the avoided aggregation of BiRu2 dye, because of its bulky structure which could decrease the recombination and intermolecular charge transfer [3].In conclusion, we prepareda new sensitizer, BiRu2, by incorporating naphthyl antennas into the ancillary ligands and investigated its potential as dye in DSSC device which shows the better performance respect to the N3. The improvement performance of DSSC device based on BiRu2 reveal the great potential of this dye for DSSC application in the future.

Keywords: π-Extended ligand, Dinuclear ruthenium (II) sensitizer, Dye sensitized solar cell

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Decoration of CdS nanorods with Cu nanoparticles for photocatalytic removal of Rhodamine B contaminant

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Photocatalytic degradation of Rhodamine B by cadmium sulfide nanorods decorated with copper nanoparticles is an effective method for water treatment. In this study, Cu nanoparticles are synthesized on the surface of CdS nanorods (NRs) which act as auxiliary catalysts. Achieving the reduction of Cu ions through chemical reduction and consolidated correlation between nanoparticles and NRs has been analyzed using XRD, SEM, TEM, FTIR, and UV-Vis spectra [1]. The acquired results showed that the composition of Cu nanoparticles and CdS NRs oversees the formation of new bonds with bridging sulfur in the form of Cu-S-Cd, which leads to a substantial increase in the photocatalytic activity of CdS [2].

Keywords: Photocatalysis, Nanocomposite, CdS nanorods, Copper nanoparticles.

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Synthesis and characterization of multi-metallic electrocatalysts with graphenepencil core substrate for electro-oxidation of alcohols in fuel cells

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In this research, silver-platinum bimetallic nanoalloyselectrocatalyst was prepared on nitrogen-dop graphene pencil core (NDGPC) by electrochemical deposition method[1,2].This electrocatalyst was characterization by SEM, EDS, and EDS-mapping analysis and was used in two processes of ethanol electro-oxidation and glycerol electro-oxidation in alkaline media for use in direct ethanol fuel cells (DEFC) and direct glycerol fuel cells (DGFC)[3]. The synthesized electrocatalysts showed good results in terms of potential, current density, and stability for the mentioned alcohols. In general, electrochemical synthesis methods have advantages including easy synthesis, no need for high temperature and pressure (synthesis is done at room temperature and pressure), green and pollution-free, etc[4].

Keywords:Electrodeposition, Nitrogen-dop Graphene, Pencil Core, Electrocatalyst, Nanoalloys

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Synthesis of Zr-metal organic frameworks modified for the Suzuki and Heck reactions as an effective and heterogeneous catalyst

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Metal organic frameworks (MOFs)demonstrate an important class of crystalline porous compounds produced from organic ligands (linkers) and metal ions or clusters[1]. Functionalization of MOFs is crucial in searching their structural and chemical variety for aboundanc potential applications[2]. MOFs were commonly suitable for various reaction substrates with different substituents in both Suzuki and Heck reactions [3]. Herein, heterogeneous Zr- MOF (UiO-67) catalyst was synthesized to perform the Suzuki–Miyaura and Heck cross-coupling reactions. Nowadays,heterogeneous catalytic systems have attracted significant attention due to their facility of dissociation from liquid phase reaction matrices. Moreover, MOFs are also often utilized as the host of the catalytically active constituent [4]. The immobilized catalyst was recyclable for at least up to 5 cycles without reduction in the efficiency of the coupled product. ModifiedZr- MOF (UiO-67) was synthesis on the basis of a mixture of 4,4 -biphenyldicarboxylic acid (H_2BPDC) ligand and $ZrCl_4$ by solvothermal method.

Keywords:Zr- MOF (UiO-67) catalyst, Suzuki–Miyaura and Heck cross-coupling reactions.

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Enhanced emission intensity and stability of perovskite nanocrystals by using metal organic frameworks

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Perovskite semiconductor nanocrystals (PNCs)have appeared as a new kind of excellent optoelectronic materials for photovoltaic applications due to their remarkable optical properties[1]. Although PNCs have many significant properties, they still have problems such as poor stability. The structure of PNCs will be damaged when exposed to the environment of humidity, polar solvents or high temperature and metal‒organic frameworks (MOFs) can be used to solve this problem [2].This porous crystalline materials, possess numerous advantages including unique chemical functions (absorption/ catalyst), useful physical properties (luminescent/ magnetic), high surface area, tunable porosity, structural diversity and different coordination geometries [3]. This work reports, a facile strategy to improve the stability andphotoluminescenceof novel PNCs by encapsulating them in UiO-67 was introduced. UiO-67 is a type of MOFs thatwas synthesized using $ZrCl_4$ and 4,4-biphenyldicarboxylic acid (H_2BPDC)using a hydrothermal method.In the present study, novel synthesized PNCsusing the ligand-assisted reprecipitation technique (LARP) method.The PNCs@Uio-67 composite shows higher photoluminescence intensity and better stability compared to bare PNCs. The resulted composite powder exhibited good deep blue-luminescence(λ_{exc} = 320 nm), high PLQY (~58%), excellent thermal stabilityand long-term storage stability.

Keywords:Perovskite semiconductor nanocrystals (PNCs), UiO-67, PNCs@Uio-67 composite.

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Biochar production from agro-industrial wastes and its application in water treatments

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Human activitieslead to water resources pollution. Nitrate is one of the water pollutants thatis a significant environmental problem all around the world that provide a serious threatto human health. Also, the eutrophication is accelerated by increasing of nitrate concentration in water sources[1-2]. Hence, removalof nitrate from water and wastewater resources is important significantly. It is important to provide a simple, inexpensive, effective and environmentally-frindly methods for removal of nitrate[3]. Adsorption proccess is one of the effective methods for removal of water pollutants including nitrate, which has received more attention in recent decades. In thise regards, many natural and synthetic sorbents have been proposed, such as activated carbon, biochar, zeolites, nano composites and etc. Biochar is a charcoal-like material that is produced by decomposition of biomass (residues of agricultural and agro-industrial activities) at high temperatures. Application of biochar as a low-cost adsorbent to wastewater treatment was reported in 2009 for the first time. Since then, the application of biochar in this field has expanded rapidly and attracted increasing attention [4]. This study investigate biochar production by decomposition corn cobs at 600 °C for 2 hours. Then, magnetic biochar nanocomposites were synthesized using the co-precipitation method with different types of functional groups. The structural features of the produced sorbent was considered by XRD, FTIR, SEM and sorbtion-desorption of N_2. Finally, The produced sorbent applied for removal of nitrate from water in batch adsorption system successfully. According to the obtained results, magnetic biochar with highly porous structure, large surface area, and high ion exchange capacity is a good candidate for water and wastewater treatment.

Keywords:Water treatment, nitrate, adsorption, biochar, magnetic biochar

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Synthesis and Application of Cellulose-Chitosan Sponges for the Removal of Oil Pollution and Other Organic Pollutants from Water

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Extraction and transportation of crude oil led to extensive environmental effects such as leakage into the water resources [1, 2]. Therefore,it is very important to develop new and environmental friendly methods that can remove and separate these pollutants from water and effluent with high performance[3]. Therefore, the main objevtive ofthe present study was synthesis and application of cellulose-chitosan sponges for the removal of oil pollution and other organic pollutants from water. In this regards, firstly cellulose was extracted from the *Platanus orientalis* tree leaves, then the sponges were synthesized in combination with chitosan by different ratios of 1:10, 3:10 and 5:10 (cellulose/chitosan) and the produced sponges called C_1-CH_{10}, C_3-CH_{10}, and C_5-CH_{10}respectivly. The surface modification (hydrophobization) ofthe synthesized sponge was performedbymethyltrimethoxysilane vapor deposition. The structures and properties of the synthesised sponges were characterized by contact angle analysis (CA), SEM, N_2 sorption-desorption, TGA, XRD and FT-IR. Finaly, fro evaluation of the sponge efficiency, the absorption process was performed in a batch system on ninedifferent petroleum and organic pollutants, including crude oil, motor oil, diesel, gasoline, liquid paraffin, hexane, chloroform, kerosene, and liquid edible oil. The CA images reviled that the water contact angle on cellulose-chitosan sponge were 140, 143, and 146 degrees for C_1-CH_{10}, C_3-CH_{10}, and C_5-CH_{10} respectivly. These values indicate that the hydrophobicity of sponges increased by increasing cellulose ration. The SEM images demonstrate the porous structure of the cellulose-chitosan sponge, Which leads to an increase in the surface-to-volume ratio and consequently an increase in the absorption capacity. Moreover, the BET analysis revealed that the specific surface area were 33.2, 21.3, and 65.3 m^2/g respectively. On the other hand, according to the BJH method theaverage pore sizeof the sponges were 36.44, 21.57, and 19.71 nm, respectively. According to the absorption results, the C_1-CH_{10}sponge represent the highest absorption capacity of oil and organic pollutants and was introduced as the optimal sponge. Finally, the reusability of the sponge absorbtion was analysed, and it was used in 6 consecutive cycles without appreciable reduction in absorption capacity.

Keywords:Crude oil, Organic pollutant, oil spill, absorbent, cellulose,chitosan, sponge.

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Synthesis, identification and investigation of group 12 metal complexes based on polydentate ligands

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In this research project, a new complex of nickel chloride and cobalt chloride was prepared with the divalent ligand of {1,3-bis- pyridin-2-yl,} urea, and it was identified using spectral methods (FT-IR), melting point, and X-ray diffraction[1]. Based on the obtained structures and the examination of the resulting spectral data and the physical properties of the compound, it is proof of the formation of a triclinicand monoclinic complex of nickel and cobalt[2]. In the proposed structure of the complex, cobalt and nickel atoms have a coordination number of six and an octahedral structureAt the end, Sam and Idex complex and metal salt of each of the synthesized complexes and related metal salt were analyzed[3].

Keywords:Aminopyridine, Nickel Complex, Spectral Identification, Polydentate ligand, Urea ligand.

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[Cu(lys bipy)]Cl/GOSynthesis, Identification and Application in Oxidation of Olefine

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In this research, [Cu(lysbipy)] Clcomplex[1] was prepared. Graphene oxide was synthesized by the modified Hummers method [2] and functionalized with 3-chloropropyltrimethoxysilane andthe complex is deposited on functionalized graphene oxide ([Cu(lysbipy)]Cl/GO)[3]. [Cu(lysbipy]Cl and [Cu(lysbipy)]Cl/GO used as a catalyst in the oxidation of olefins. The synthesized complexes was identified by EDX, ICP, SEM, FTIR and XRD[4] processes. The catalytic results of the prepared complex analyzed by GC and GC–MS instrumentsandshowed that the catalytic activity of [Cu(lysbipy)]Cl/GO in oxidation reactionin of α-methylstyrene optimal conditions 4 hours,Acetonitrile solvent, 0.025 g of catalysts and using tert-butyl hydroperoxide as an oxidant 97% conversion with selectivity of 84% of acetophenone.

Keywords:Graphen oxide, Oxidation, Bipyridine, Lysine.

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Beyond Heterobimetallic Complexes: Synthesis, Characterization, and Applications

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Considering the remarkable luminescence properties and biological activities of heterobimetallic compounds, they have gained ascending and comprehensive interest in the realm of catalysis research. Additionally, the preparation of heterobimetallic complexes could be challenging and require a rational synthetic approach concerning the compatibility and stability of the ligands and metals. A stepwise synthetic pathway could yet be another alternative method for the preparation of heterobimetallic complexes. In this approach, a metal complex is prepared, and a ditopic bridging ligand (a donor ligand possessing two binding sites for the coordination of metal atoms) is bound to the first metal, which is followed by the coordination of the second metal complex. Among these linker ligands, 1,1-bis(diphenylphosphino)methane (dppm) is a suitable candidate for the coordination of various metals to form homo- and heterobimetallic complexes. We have synthesized and characterized some new heterobimetallic complexes(Figure 1), which contain two different metals such as platinum group metals (PGMs), Au, and Ag. These heterobimetallic compounds are constructed by using a dppm ligand. The biological, optical, and catalytic properties of these complexes are investigated.

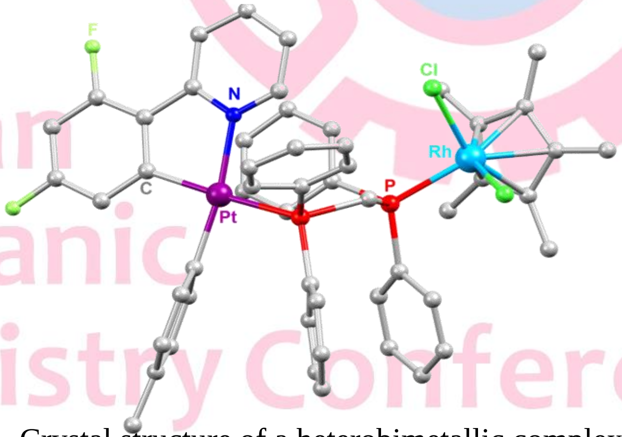

Figure 1. Crystal structure of a heterobimetallic complex.

Keywords:Heterobimetallic, Platinum group metals, Luminescence, Catalysis, Biological activity.

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Design and Ultrasound-Assisted Synthesis of an anthracene-based Cu-MOF for Hydrogen Sulfide Sensing

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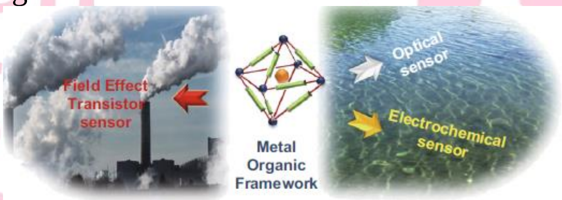
Copper metal-organic framework (Cu-MOF) fluorescent sensing is a relatively new area of research in the field of materials science and chemical sensing. Cu-MOFs are porous materials that have been found to exhibit unique fluorescence properties, which make them attractive for use in sensing applications. H_2S is a toxic gas that is commonly found in natural gas, crude oil, and other industrial processes. It poses a serious threat to human health and safety, and therefore, there is a need for reliable and sensitive detection methods. Cu-MOFs sensors have been shown high sensitivity and selectivity towards H_2S gas, making them a promising candidate for H_2S sensing applications. In addition, anthracene is a common ligand that has been used as a linker in the synthesis of Cu-MOFs for fluorescent sensing applications[1,2]. In this study, a novel anthracene-based Cu-MOF has been synthesized under ultrasound irradiation and used for H_2S detection. The Cu-MOF as a fluorescent sensor has surprising performance and has shown great promise in environmental and industrial monitoring. The ultrasonic-assisted synthesis method was found to produce smaller and more uniform crystals compared to traditional synthesis methods. Interestingly, fluorescence detection studies exhibit that Cu-MOF can detect hydrogen sulfide with high sensitivity and selectivity in the presence of interfering species and also show a quick response in a short time range in water.



Keywords:Cu-MOFs, Hydrogen Sulfide, Sensing, Fluorescence.

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Title: Synthesis of the urea-formaldehyde resin@MnO_2 core-shell nanoparticles and investigation of their performance in supercapacitors.

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Energy has been one of the important issues considered by the world powers and researchers, and many efforts has been made to invent and develop for energy storage. Capacitors as one of the storage devices has a high power density and high energy, and play a great role in the world needs. The main aim of the present research has been the preparation of the core-shell nanoparticles of the manganese dioxide and manganese disulfide with melamine-formaldehyde rsin shell as supercapacitor material. As the first step, the nanoparticles of urea formaldehyde resin were prepared and covered by the MnO_2 and MnS_2. The morphology and chemical structure of the samples has been investigated and confirmed by FT-IR, DLS, XRD and SEM techniques. The electrode prepared by using of the synthesized core-shell nanoparticles and carbon nanopowder such as Volkan were studied via cyclic voltammetry, charge-decharge technique, galvanostatic and electrochemical impedance spectroscopy. According to the results, the specific capacities obtained for the electrodes prepared by using of MnO_2, UF@MnO_2, MnS_2 and UF@MnS_2 as active electrode materials have been 358, 279, 428 and 105 $F.g^{-1}$. Electrochemical impedance spectrospy studies has indicated an almost ideal capacitive behviour for these electrodes. Also, a relatively ideal charge-decharge capacitive behavior has been observed for these electrodes.

Keywords:Supercapacitor, urea-formaldhyde resin, active carbon, specific capacity, cyclic charge-discharge

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Investigation on catalytic activity of Cu-complex immobilized on Modified Carbon Dots for Carbon-Carbon Homocoupling Reaction

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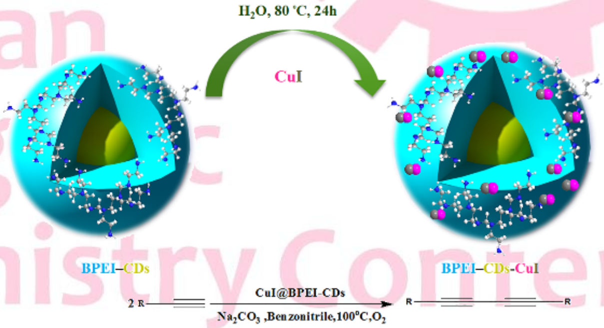
In this study attempts has been made to prepare modified carbon dots (CDs) with branch poly (ethyleneimine) (BPEI) from citric acid, as carbon source, in water at 200 ℃, followed by immobilized different Cu compounds on it and designated as Cu-BPEI-CDs nanocomposites Then it was used as catalyst for the terminal alkynes homocoupling reaction. The straight approach for the synthesis some 1,3-diynes is the coupling of two terminal alkynes, as expanded by Glayser and Hay[1-4]. Due to the high abundance, low cost and low toxicity of copper, it has been widely considered as excellent catalyst for the synthesis of 1, 3-dieynes.After characterization of the prepared heterogeneous compounds by means of XRD, FTIR, SEM, TEM and XPS, they were tested as catalysts for the oxidative homo-coupling of phenylacetylene, 4-*tert*-butylphenylacetylene, 1-ethynyl-4-flourobenzene and 1- pent-1-yn-3ol. It was found that Cu (I) I and Cu (I) bipyridene show conversion yields of 67-100 % with excellent selectivities (95–100).The catalysts were also recovered and used for four runs without significant decrease in catalytic activities.

Keywords: Carbon Dots, Couper (I) Compounds, C-C Homocoupling, Polyethylene Imine, Citric Acid



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High selective, sensitive, paper-based probe forCu(II) detection: A prospective form Nano-scale turn-on to Micro-scale turn-off states

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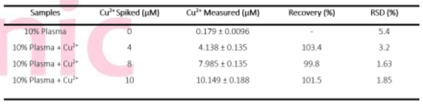
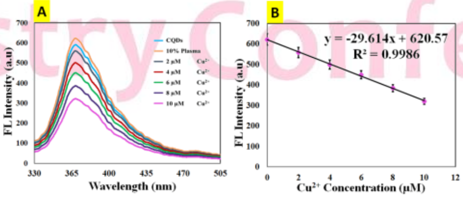
A new fluorimetric-based method has been developed for detection of Cu(II) using neocuproine-based carbon quantum dots (CQDs). When Cu(II) is adsorbed onto the surface of the CQDs, it interacts with the functional groups, resulting in either an increase or decrease in fluorescence emission depending on the concentration of Cu(II). This is the first reported method that can detect Cu(II) at both nano-molar and micro-molar levels with two different phenomena, means that 0.001-0.1 µM addition of Cu(II) caused the enhancemnet of CQDs' FL emission intensity whereas the 1-10 µM addition of Cu(II) led the FL emission of CQDs to quench. This fascinating phenomena can turn this sensing probe into promising platform for real-world applications. A low-cost, easy-to-use, highly selective and sensitive CQD-based sensing system showed a limit of detection (LOD) of 0.001 µM and a dynamic range of 0.001-10 µM. The sensing potential of the system on human serum sample has also been tested, showing the recovery of 99.8-103.4% along with the RSD of <%6. Surprisingly, the measured concentration of cupric ionsin human plasma after 2-10 µM cupric ions addition was found to be 22.157 µM, which is astonishingly well fit in the range of cupric concentration in the plasma of healthy individuals [1]. The findings indicate that the CQD-based sensor possesses high accuracy and precision toward Cu(II) detection, indicating good potential for practical use.

Keywords:Carbon Quantum Dots, Sensing Framework, Cu(II) Detection, Turn-on and Turn-off states mechanism



Samples	Cu^{2+} Spiked (µM)	Cu^{2+} Measured (µM)	Recovery (%)	RSD (%)
10% Plasma	0	0.179 ± 0.0096	-	5.4
10% Plasma + Cu^{2+}	4	4.138 ± 0.135	103.4	3.2
10% Plasma + Cu^{2+}	8	7.985 ± 0.135	99.8	1.63
10% Plasma + Cu^{2+}	10	10.149 ± 0.188	101.5	1.85



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CQD-Based Sensing Platform for Cu^{2+} Detection in Wilson's Disease

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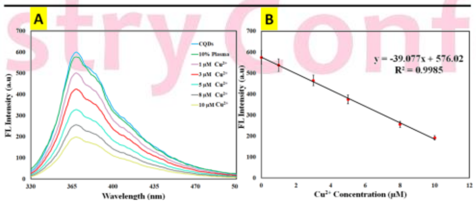
The presence of Cu(II) is strongly linked to the emergence of Wilson's disease (WD), and accurately measuring the amount of copper is a crucial step in diagnosing WD at an early stage in a clinical setting [1]. In this work, CQDs were fabricated using pollen and citric acid through a facile technique as a novel fluorescence-based sensing platform for detecting Cu(II) in the serum sample of affected individual by WD. Cu(II) ions efficiently interact with the CQDs and give rise to QDs' Flourescence (FL) emission quenching in a wide linear ranges of 1-40 µM, with the LODs of 1 µM, respectively. To the best of our knowledge, the potential of the CQD-based sensor for Cu(II) detection in the serum sample of affected individual by WD, showing the recovery of 97.2-102.9% along with the RSD of <%5, which showed high precision, applicability, accuracy, selectivity, sensitivity toward Cu(II) ions. Surprisingly, the measured concentration of cupric ions (after the addition of 1-10 µM) to the plasma sample was determined to be 8.1236 µM. It is noteworthy that this value aligns remarkably with the observed range of cupric concentration in the plasma of affected individuals by WD [2, 3]. The findings indicate that the CQD-based sensor possesses high accuracy and precision toward Cu(II) detection, making this sensor an appealing platform for monitoring the concentration of Cu(II) ions as a crucial diagnostic tool for Wilson's disease in a clinical setting.

Keywords: Wilson's diseasm, Carbon Quantum Dots, Fluorescent Sensor, Cu(II) Detection

Samples	Cu^{2+} Spiked (µM)	Cu^{2+} Measured (µM)	Recovery (%)	RSD (%)
10% Plasma	0	0.0414 ± 0.00107	-	2.6
10% Plasma + Cu^{2+}	1	0.972 ± 0.03697	97.2	3.8
10% Plasma + Cu^{2+}	3	2.841 ± 0.11649	94.7	4.1
10% Plasma + Cu^{2+}	5	5.144 ± 0.19033	102.9	3.7



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Preparation of Ni-microsphere using Ascorbic acid as coordinating ligand and study of its catalytic properties in sulfoxidation reactionsAnd synthesis of 5-substituted 1H-tetrazoles

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In this study, a novel ascorbic acid-based Ni-microsphere was prepared via the hydrothermal method.The obtained Ni-microsphere's morphology and porosity were assessed using the following techniques: XRD, FTIR, TGA, EDS, WDX, AAS, DSC, BET, and SEM. Examining the produced MOF's catalytic activity in cyclo-condensation and sulfoxidation reactions. It was found that Recycling the Ni-microsphere five times without any loss of catalytic effectiveness was simple.

Keywords:Ascorbic acid, Coordinating, 5-substituted 1H-tetrazoles, Oxidation reactions

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Synthesis and Characterization of Cu Coordinated L-Ascorbic Acid as coordination Polymer and its Catalytic Performance in the Multi-Component Reactions

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A Cu@AACP Metal-Organic Framework was synthesized and characterized by TGA, FT-IR, AAS, SEM, BET, MAP and EDX. The results of the analyses confirmed the successful synthesis of Cu@accorbic acid coordination polymer (Cu@AACP). And also show any deformation of the porous structure of the parent coordination polymer. The catalytic performance was examined in synthesizing of 2, 3-dihydroquinazolin-4(1H)-ones and polyhydroquinolines. The results show that an improved product yield is obtained between 84-95%. Recycle test of the catalyst confirmed that the heterogeneous catalyst exhibited good catalytic stability, efficiency and very high activity in successive runs because of its unique pore network.

Keywords:coordination polymer,Metal-Organic Framework, 2, 3-dihydroquinazolin-4(1H)-ones, catalyst

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Effect of ZSM-5 seeds in the synthesis of SAPO-34 catalyst in methanol to light olefins

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SAPO-34/ZSM-5 catalyst has been synthesized by using different amounts of processed ZSM-5 seeds at 100°C in order to control the selectivity of light olefins and increase the lifetime. The catalytic properties and performance of SAPO-34/ZSM-5 were different compared to conventional SAPO-34. The synthesized samples were characterized using XRD, FESEM, FTIR, BET, and NH3TPD. The effect of seed amount did not follow the same trend in the entire tested range. The XRD results showed that with the addition of seed, the crystallinity and size of the crystallites increased, at the same time, an increase in the particle size was observed in the FESEM images. The SAPO-34/ZSM-5 catalyst with 6.25wt% seeds, which has the smallest crystallitesize in catalysts with seeds, showed the highest stability (700 min) and selectivity to light olefins (89.84%) compared to other samples; Also, according to the results obtained from NH3TPD analysis in this sample, the strength of strong acid sites and the amount of total acidity is less than other samples, which has reduced the formation of coke and longer lifetime of this sample.

Keywords: Methanol to light olefin, ZSM-5 seeds, SAPO-34, SAPO34/ZSM-5

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Decolorization with magnetic ferrite magnetic nanoparticles

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MgFe2O4 nanoparticles were created using the sol-gel process to degrade organic contaminants in water, soil, and air sources, such as industrial paints.X-ray diffraction (XRD) analysis, scanning electron microscopy (SEM), and Fourier transform infrared (FTIR) spectroscopy were used to explore the structure and characteristics of nanoceramics.The Scherer equation of 11nm was used to determine particle size. The decolorization of this nanocomposite in an aqueous media under visible light and UV light was researched to learn more.Then, Vis-UV spectroscopy was used to analyze the outcome. The findings of this degradation demonstrated that ceramic nanocomposite has significant photocatalytic activity in both visible light and UV light. The findings of this study demonstrated that this technique may be applied on a bigger scale and has good effectiveness in decolorizing crystal violet contaminants from the environment by optimizing the effective operational variables.

Keywords:Decolorization,Magnetic Nanoparticles, Congo Red, Basic Red 51, Visible and Ultraviolet light

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Porphyrin Molecules Decorated on Metal-Organic Frameworks for Multi-Functional Biomedical applications.

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Metal–organic frameworks (MOFs) have been widely used as porous nanomaterials fordifferent applications ranging from industrial to biomedicals ([1]). An unpredictable one-pot method isintroduced to synthesize NH_2-MIL-53 assisted by high-gravity in a greener media for the first time.Then, porphyrins were deployed to adorn the surface of MOF to increase the sensitivity of the preparednanocomposite to the genetic materials and in-situ cellular protein structures. The hydrogenbond formation between genetic domains and the porphyrin' nitrogen as well as the surface hydroxylgroups is equally probable and could be considered a milestone in chemical physics andphysical chemistry for biomedical applications ([2]). In this context, the role of incorporating differentforms of porphyrins, their relationship with the final surface morphology, and their drug/gene loadingefficiency were investigated to provide a predictable pattern in regard to the previous works.The conceptual phenomenon was optimized to increase the interactions between the biomoleculesand the substrate by reaching the limit of detection to 10 pM for the Anti-cas9 protein, 20 pM forthe single-stranded DNA (ssDNA), below 10 pM for the single guide RNA (sgRNA) and also around10 nM for recombinant SARS-CoV-2 spike antigen. Also, the MTT assay showed acceptable relativecell viability of more than 85% in most cases, even by increasing the dose of the prepared nanostructures ([3]).

Keywords:gene delivery, CRISPR, biosensor, biomedicine, MOF, COVID-19

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N-doped carbon nanospheres as selective fluorescent probes for mercury detection in contaminated aqueous media: chemistry, fluorescence probing, cell line patterning, and liver tissue interaction

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A precise nano-scale biosensor was developed here to detect Hg^{2+}in aqueous media. Nitrogen-doped carbon nanospheres (NCS)created from the ultrasonic spray pyrolysis of melamine–formaldehyde resin were characterized by FESEM, XRD, Raman spectra, EDS, PL, UV–visspectra, and N_2adsorption–desorption, and were used as a highly selective and sensitive probe for detecting Hg^{2+}in aqueous media.The sensitivity of NCS to Hg^{2+} was evaluated by photoluminescence intensity fluctuations under fluorescence emission in the vicinityof 390 nm with a λexc of 350 nm. The fluorescence intensity of the NCS probe weakened in the presence of Hg^{2+}owing to the effectivefluorescence quenching by that, which is not corresponding to the special covalent liking between the ligand and the metal. The effectsof the fluorescence nanoprobe concentration, pH, and sensing time were monitored to acquire the best conditions for determining Hg^{2+} ([1]).Surprisingly, NCS revealed excellent selectivity and sensitivity towards Hg^{2+}in the samples containing Co^{2+},Na^{+},K^{+},Fe^{2+},Mn^{2+},Al^{3+},Pb^{2+},Ni^{2+},Ca^{2+},Cu^{2+},Mg^{2+},Cd^{2+},Cr^{3+},Li^{+},Cs^{+},and Ba^{2+}.The fluorescence response was linearly proportional to Hg^{2+}concentration in 0.013–0.046 μM with a limit of detection of 9.58 nM. The in vitro and in vivo toxicological analyses confirmed thecompletely safe and biocompatible features of NCS, which provides promise for use for water, fruit, vegetable, and/or other forms ofnatural-connected materials exposed to Hg^{2+},with no significant toxicity noticed toward different cells/organs/tissues ([2]).

Keywords:Nitrogen-doped carbon spheres, Melamine formaldehyde resin, Ultrasonic spray pyrolysis, Fluorescence probe, Hg^{2+}

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Green modified-UiO-66/MXene sandwich composites for gene chemotherapysynergistic cancer suppression: Co-delivery of doxorubicin and pCRISPR

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Advancements in material science and engineering, especially in the field of porous nanomaterialslead to new types of therapeutics and technologies. Among different types of porousnanomaterials, metal-organic frameworks (MOFs) have been considered the most promisinginorganic nanomaterials due to their significant stability and ease of functionalization. To date,very limited research has been done on developing nanocomposites based on MOFs and MXenes.The current experiment has been performed to design a novel UiO-66 MOF and MXenenanocomposite, modified with *Rosmarinus officinalis* (RO) leaf extracts for co-delivery ofdoxorubicin (DOX)/plasmid (p)CRISPR ([1]). The synthesis procedure was completed with theassistance of a high-gravity system and a rotating packed bed (RPB) device for the first time, andthe characterization results showed the successful synthesis of the nanomaterials. Based on thedrug release and loading results, the DOX payload efficiency of about 46% was recorded andsustained drug release at acidic pH values (same as the cancerous cells) was observed. However,the presence of leaf extracts slowed down the drug release and have a minor effect on the releaseprofiles, the cellular internalization results on the MCF-7 and HT-29 cell lines showedconsiderably dependent images. The gene transfections result by using two nanosystems of UiO-66@MXene@RO@DOX@pCRISPR, and UiO-66@MXene@RO@DOX@RO@pCRISPRshowed about 18.3% and 22.1% transfection efficiency on the A549 cell lines. Those resultsshowed not heavily dependent results on the presence or absence of the leaf extracts. Therefore,this study revealed that the green modification of nanocomposites does have a major effect onlyon the cellular internalizations of DOX, rather than CRISPR ([2]).

Keywords:MOF, MXene, doxorubicin, CRISPR, leaf extracts

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Application of multi-drug chemotherapy for cancer treatment using magnetic $CoFe_2O_4$nanoparticles

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Nowadays, combination therapies are used for the treatment of cancer. Patients who used chemotherapy; as a commonly used therapy for cancer treatment; may encounter side effects like drug resistance. Although increasing the drug dosage led to enhancement of its therapeutic effect, some side effects like resistance of cancer cells and toxicity to normal cells will be intensified. However, considering many problems of chemotherapy, using a multidrug dosing strategy for cancer treatment increases the efficiency via synergism of used drugs and decreases drug resistance of cancerous cells. Here, we used a combination of multi-drug chemotherapy and photothermal therapy (PTT). We synthesized a pH-sensitive and heat-sensitive nanocomposite. The nanocomposite exhibited some features like fibrous spherical morphology, typical mesoporous structure, high specific surface area, narrow size distribution, excellent superparamagnetic features and good monodispersity. This nanocomposite, cobalt ferrite ($CoFe_2O_4$), has porosity and magnetic properties that can be used for identification in MRI([1]). Doxorubicin hydrochloride could be easily loaded onto the CoFe2O4 nanoplatforms and released with pH stimuli. The mesoporous CoFe2O4 core acts as T2-weighted magnetic resonance (MR) imaging probe, PTT agent([2]). In this study, we loaded the drug DOX into these pores and coated it with chitosan-tpp, then we added ZIF-8 layer around the synthesized NPs. ZIF-8; a Metal Organic Framework; is a carrier for the delivery of anti-cancer drugs and a PH stimulus([3]). After coating NPs by ZIF-8, we load another anti-cancer drug to ZIF-8 nanospheres. We used aptamers to target only cancer cells for this nanocarrier. The size of this nanocarrier was less than 100 nanometers after synthesis and was identified using FTIR, and drug loading was also investigated. The NPs drug delivery was investigated against HT-29human colorectal adenocarcinoma cell line.

Keywords:Multi-drug chemotherapy, Cancer, CoFe2O4, Nanoparticle.

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Fabrication of Zirconium Metal-Organic-framework/Poly Triazinephosphanimine Nanocomposite for Dye Adsorption from Contaminated Water: Isotherms and Kinetics Models

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The increase in water pollution has urged industries and academia to propose effective adsorbents to deal with this issue. The present research aimed to produce, characterize, and examine the adsorption capacity of a hybrid material composed of UiO-66-NH2 and triazine-phosphanimine polymeric organic porous polymer (TPA-POP). In this respect, central composite design (CCD) was utilized to minimize the number of the reaction parameters (i.e., temperature, initial pH, and adsorbent concentration) on the removal of basic blue 41 (BB41). BB41 was adsorbed completely in 60 min with the UiO-66-NH_2/TPA-POP mesoporous nanostructure. The pseudo-secondorder model was the best equation to fit the kinetics data. Also, film adsorption and diffusion were identified as rate-limiting steps in removing the dyes. The equilibrium data were fitted by a Langmuir isotherm, and the maximum equilibrium adsorption was 260.7 mg/g. Moreover, the adsorbent was recycled for seven cycles for adsorption of BB41 dye without an obvious loss of activity.

Keywords: Metal-Organic Framework (MOF), Hybrid Material, MOF-Polymer Composite, Basic Blue 41, Central Composite Design

A novel magnetic nanocomposite based on alginate/pumice: an efficient heterogeneous nanocatalyst for synthesis of [1,2,4]triazolo[1,5-a]pyrimidines

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In this study, a facile and efficient method for the synthesis of 5-amino-7-aryl-4,7-dihydro-[1,2,4]triazolo[1,5-a]pyrimidine-6-carbonitrile based on alginate/pumicecopper-catalyzed multicomponent reaction of a triazole with aryl aldehyde is reported in the presence of malononitrile in DMF. A new heterogeneous and recyclable nanocatalyst based on copper iodide supported on functionalized pumice has been introduced for this target. The synthetic process of the mentioned nanocatalyst, Cu@Fe_3O_4/alginate/pumice, has been described[1-3].TEM, SEM, EDS, FTIR, ICP, and XRD afforded the Cu@Fe_3O_4/alginate/pumice characterization. The surface structure of the materials was confirmed using Fourier transform infrared (FTIR) spectroscopy.

Keywords:pumice, Copper Iodide, [1,2,4]triazolo[1,5-a] pyrimidines and nanocatalyst

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Overview on synthesis, Applications of Cobalt Oxide Nanoparticles

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Cobalt oxide nanoparticles are semiconducting metal oxide type that can display unusual chemical features in nanotechnology due to their tiny mass and high limit density, especially in biomedical systems, optics, and electronics. [1] Cobalt oxide NP is non-hygroscopic, non-toxic, and commonly found in organic, polar, crystalline material that has aroused interest in organic transformation, sensors, visible conductors, and surface acoustic wave devices. Transparent electronics, UV light emitters, chemical sensors, spin electronics, personal care products, catalysts, adhesives, and paint are cobalt oxide NP. Due to its unique properties, cobalt oxide NP is used in lightemitting coatings, transparent electrodes in solar cells, UV light emitters, diode lasers, varistors, piezoelectric devices, spin electronics, electronics [2], and acoustic wave propagators as an antibacterial agent as a photonic material and as a chevalier gas sensor Chevalier Biomolecules in the extract plant act as active capping agents, which assist in the production of nanoparticles. The findings revealed that the produced cobalt oxide nanoparticles had antibacterial properties against urinary tract infections, and investigated the cheap, non-toxic raw production of cobalt oxide nanoparticles by using Camellia sinensis extract to examine the efficacy of cobalt oxide nanoparticles as a photocatalyst to destroy various natural dyes such as methylene blue and methyl orange and their antioxidant activities by using Eucalyptus globulus. Cobalt oxide nanoparticles NPs are mechanically synthesized by using Azadirachta indica leaves from the Meliaceae own family [3]. According to the findings, including cobalt oxide nanoparticles in medicine has a significant impact on the membrane of biology. Cobalt oxide nanoparticles nanostructures, which resemble a 3- dimensional tetrapod, had been used to transport pEGFPN1 DNA (which carries the inexperienced fluorescent protein gene) to A375 human cancer cells [4]. Electrostatic interactions connected the plasmid DNA(plasmid DNA) to cobalt oxide nanoparticles nanostructures, and three needle-shaped legs favoured internalization of the hints for gene shipping into cells.

Keywords: Cobalt oxide, Applications, synthesis

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Investigation of nitrate removal from aqueous solution by Clinoptilolite zeolite modified with Cu and Zn

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Nitrate entered into the human body is transformed into nitrite through processes that combine with amines and cause the formation of nitrosamine, which is a carcinogenic substance. According to research, nitrate also causes Alzheimer's disease[1]. Therefore, it is necessary to remove nitrate from water. In this research work, due to the low efficiency of unmodified clinoptilolite zeolite, zinc chloride and copper acetate were used to modify the adsorbent. Various factors such as environmental pH, nitrate concentration, contact time and adsorbent dosage were investigated. The results showed that the modified zeolite is more efficient in removing nitrate from aqueous solutions due to the different adsorption sites, the simplicity of the system and the high removal efficiency compared to the unmodified zeolite. The results of the effect of contact time on the amount of nitrate removal after modification of the adsorbent by both substances show that the maximum was reached with the increase of the contact time from 2 to about 80 minutes and then with the excessive increase of the contact time, the efficiency decreased gradually. The increase in efficiency at early contact times may be due to the increase in the number of vacant sites on the adsorbent surface. After the period of time when the empty sites were occupied, the amount of removal of the adsorbent depends on the activity of the added substance, in this case, copper acetate has removed the nitrate particles more strongly.Therefore, in high concentrations of nitrate, zeolite modified with zinc chloride was the most suitable adsorbent, while in low concentrations of nitrate, zeolite modified with copper acetate showed the highest removal efficiency.

Keywords:Zeolite, clinoptilolite, nitrate removal, zinc chloride, copper acetate

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Optimization of nitrate removal process from aqueous solution by Clinoptilolite zeolite using surface response method

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Nitrate is one of the most important pollutants in nature, which is considered a serious threat to human health and the quality of water resources. One of the methods to remove this pollutant is the use of modified adsorbents such as oxide nanoparticles on clinoptilolite zeolite[1].In this study, the samples were prepared synthetically at a concentration of 100 mg/liter of nitrate. The independent variables included the amount of adsorbent in g/L, the percentage of copper oxide loaded, and pH. The performance of the process was evaluated based on the nitrate removal percentage. Determining the number of tests, statistical analysis of laboratory data and optimization of nitrate removal efficiency were done by using response surface method and central compound design.The results showed that pH, the percentage of copper oxide loaded, pH, the square of the percentage of copper oxide loaded were the most important parameters affecting nitrate removal by this method.

Keywords:Clinoptilolite zeolite, copper oxide nanoparticles, surface response method, central composite design, optimization

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Photocatalytic activity of alumina supported *meso*-tetra(3-pyridyl)porphyrin

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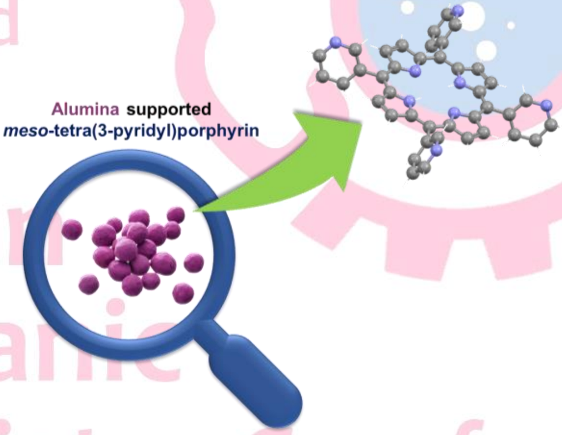
In order to design a new heterogenous porphyrin photosensitizer, in the present study, *meso*-tetrakis(3-pyridyl)porphyrin was immobilized on alumina and its photocatalytic activity for the aerobic photooxidation of organic substrates was studied. It is noteworthy that due to the advantagesof heterogeneous catalysts over the homogeneous counterparts [1,2] including higher stability and ease of catalyst separation, the former is of great interest in improving the performance of catalyst and photocatalysts [3,4]. Very rapid oxidation of 1,3-diphenylisobenzofuran as a specific quencher of singlet oxygen [5] in the presence of the hybrid compound showed the involvement of singlet oxygen as the main reactive oxygen species.



Keywords: *Meso*-Tetrakis(3-pyridyl)porphyrin, Singlet oxygen, Aerobic photooxidation, Alumina

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Fabricated a Novel and High Capacitance Symmetric Supercapsitor Electrode by Electrosynthesis NiCo LDH@Vertical Oriented Graphen Sheets on Graphite Sheet

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Supercapacitors are energy storage devices that have gained significant attention due to their high power density and long cycle life. The performance of supercapacitors is largely dependent on the properties of their electrodes[1]. NiCo LDH/VOGN/Graphite sheet electrode with very high surface area and excellent capacitive behavior was fabricated through the anodizing of the graphite followed by electrodeposition[2]. In this study, fabricated a novel electrode-based graphite sheet was anodized to increase its porosity and conductivity for the fabrication of Vertically Oriented Graphene Nanosheets (VOGN) that were covered by NiCo Layer double hydroxide (NiCo LDH) nanoparticles.[3] NiCo LDH was deposited onto the VOGN using an electrosynthesis method. The prepared electrodes were investigated by Fourier transform infrared (FT-IR), scanning electron microscopy (SEM), and BET (Brunauer–Emmett–Teller). The nanoarray structure can provide a large specific surface area and more channels, which facilitate rapid ion transfer and electron migration between electrolyte and electrode. The effect of anodizing graphite sheets and different ratios of Co and Ni on the electrochemical performance was investigated. It has been found that anodizing graphite sheets on the one hand increase the conductivity of the electrode, on the other hand, it provides more active sites for NiCo LDH attachment[4]. The resulting electrode exhibited excellent electrochemical performance, with high specific capacitance and good cycling stability. This approach provides a promising strategy for developing high-performance supercapacitor electrodes with enhanced porosity and surface area. The NiCo LDH/VOGN/Graphite sheet electrodes showed a very high capacitance of about 943 F g^{-1} at a current density of 1 A g^{-1}, an excellent energy density of 68.4 mWh g^{-1}, the power density of 1496.4 mW g^{-1}, and stable capacity of about 85.6% after 5,000 cycles in the charge/discharge process.

Keywords:Supercapacitor, NiCo LDH, Vertically Oriented Graphene Nanosheets, Graphite sheet Anodizing

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Design, preparation, and catalytic activity of the new nanocellulose-based catalyst

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With the development of global industrial and manufacturing activitiesreduction of aromatic and aliphatic nitro compounds has become a more serious and criticalissue. Synthetic procedures of the active nanocatalysts are toxic, expensive and harmful for envirenment. accordingly, many efforts have been devoted to achieve green methods for the synthesis of nanocatalysts, avoiding the disadvantages of currently used procedures.Therefore it is necessary to use environmental friendly catalysts.Cellulose as the most abundant natural polymer and, can be used as a renewable, biodegradable, and non-toxic support. Cellulose be used as a basic raw material for the preparation of various functional materials. Because of its strong inter- and intramolecular hydrogen bondings, cellulose is insoluble in water and most organic solvents. This restricts its chemical reactions to having to be carried out under heterogeneous conditions [i]. In this work, we utilize a Fe_3O_4-cellulose as support to immobilize copper cation as a catalytic active site [ii]. The prepared Fe_3O_4-cellulose support was functionalized through simple methods to obtain a copper-based catalyst for the reduction of nitroarenes [iii]. The formation of this catalyst was validated through Fourier transform infrared spectroscopy (TF-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), vibrating sample magnetometry (VSM), and thermogravimetry analysis TGA). Then, the catalytic activity of the prepared catalyst was evaluated in the reduction of various nitroarenes in the presence of sodium borohydride as a reducing agent at room temperature in aquous solution. The significant magnetic property of the nanocatalyst provides simple separation from the reaction solution by an external magnet [iv].

Keywords:Heterogeneous catalysis, Cellulose, Reduction, Nitroarenes

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The construction of electrochemiluminescence new sensor by Using of Si/C nanostructures for signal amplification in order to measurement of Cyanotoxins in water samples

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Accurate evaluation of trace organic pollutants such asCyanotoxinswith facile methods, is critical to prevention and controling of environmental pollutants [1,2]. Electrochemiluminescence (ECL) assay as an impressive analytical technique has attracted significant interest in recognition and sensing [3]. Herein, we proposed a moleculary imprinted polymer (MIP)-based ECL sensor platform for high sensitive detection of Cyanotoxins in real samples [4]. This proposed sensor with use of Si/C nanoparticles, were designed and made [6]. The established uniform MIP film on the surface of ITO electrode and nanocomposite embedded in MIP, showed an anodic ECL emission using TPrA. When the imprinted cavities were occupied by Cyanotoxin molecules, the ECL emission was efficiently increased. Under optimal conditions, the represented sensing platform illustrated accurate and high sensitive analytical performance toward Cyanotoxin detection with a linear range from 2 ng/ml to 3 fg/ml and detection limit of (S/N=3). In addition, this sensor demonstrated good recovery rates, high reproducibility and stability and excellent selectivity for Cyanotoxin determination. Furthermore, the application of the developed ECL sensor for measurement of Cyanotoxin in water samples was evaluated and the satisfactory results were founded.

Keywords: Electrochemiluminescence, MIP, Cyanotoxins, TprA, Si/C nanostructures.

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Aluminium -based ionic liquid grafted on Biochar as a heterogeneous catalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-one

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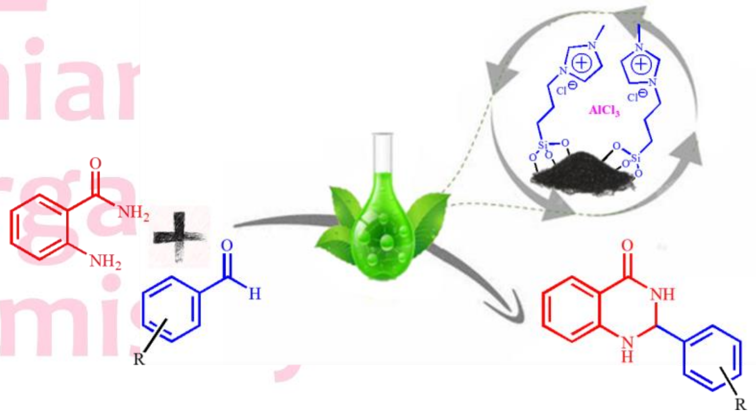
Biomass as the only carbon neutral alternative, has the unique chemical structure containing tailored surface functional groups and large surface area. Having these features has made it easy to prepare by activation and/or functionalization.The selection of biochar as a surface will be ideal for the preparation of heterogeneous catalysis [1, 2].Recently, ionic liquids are suitable substitute for old conventional catalyst and do not leave any toxicity in the reaction medium [3]. Aluminium -based ionic liquid grafted on biochar surface (BC\[TESPMI]$_2$AlCl$_3$) was synthesized as a catalyst for the synthesis of 2,3-dihydroquinazolin-4(1H)-one and characterized by FTIR, XRD, TGA, FESEM, and EDS. This results disclosed that the chemical grafting was successfully performed. The high activity in mild condition and the simple recoverable from the reaction are the suitable characteristics of this catalyst. Finally, the catalyst sustained activity for five cycles of reaction.

Keywords: Biochar, 2,3-dihydroquinazolin-4(1H)-one, Ionic liquid, Recoverable nanocatalyst



Scheme 1. Synthesis of 2,3-dihydroquinazolin-4(1H)-one in the attendance of BC\[TESPMI]$_2$AlCl$_3$

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Cu immobilized on Fe_3O_4@Biochar nanoparticles: a novel, inexpensive and highly efficient heterogeneous magnetic nanocatalyst for C-O coupling reactions in green media

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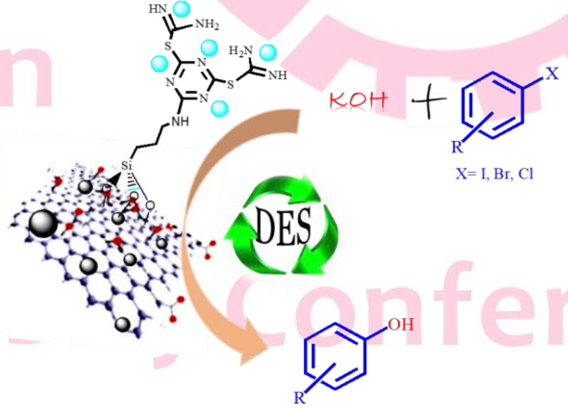
Carbon-heteroatom cross-coupling reactions based on transition metal catalyst systems have Transition metals include Pd, Cu, Co, Fe, Ag, Au, and Ni allow chemists to catalyze cross-coupling reactions, however, using affordable and friendly environment designed catalytic systems have more attentions among scientists, lastly [1, 2]. Biochar as the only carbon neutral alternative, has the unique chemical structure containing tailored surface functional groups and large surface area. The selection of biochar as a surface will be ideal for the preparation of heterogeneous catalysis [3]. magnetic modification can be more suitable technique to separate them by applying a magnet, make long centrifugation and filtration steps unnecessary [4]. Herein we report the synthesis of a magnetically separable core-shell-like Fe_3O_4@Biochar-Cu (MBC@BTT-Cu(II)) as an environmentally friendly heterogeneous catalyst. The as-prepared nanocatalyst was well characterized by various techniques such as FT-IR, XRD, BET, FE-SEM, EDX, TGA, VSM, ICP-OES and elemental analysis and evaluated for the C-O coupling reactions in DES as green solvent. Also, the separation of the nanocatalyst was easily performed by an external magnet and applied again for eight fresh runs with no considerable loss of catalytic activity.

***Keywords**:* Heterogeneous Catalysis, Magnetic Biochar Nanoparticles, C-O Coupling Reactions.



Scheme 1. C-O Coupling reactions catalyzed by MBC@BTT-Cu(II)

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Salting effect of tetraalkylammonium salts on the clouding thermodynamic functions of aqueous butanol system

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Biobutanol,the primary four-carbon alcoholproduced based on fermentation processes,has been considered a renewable energy source to reduce the emission of greenhouse gases and air pollutants[1].Moreover, 1-butanol, having complete miscibility with organic solvents and partial miscibility with H_2O, is widely used as a solvent (purely or in mixed solvent systems) in a variety of chemical and industrial processes[2].Investigatingthe salting effectsof different solutes on the clouding (liquid-liquid demixing) phase diagram of 1-butanol/water mixed solvent systems provides valuable information for extracting biobutanol from fermentation broth or optimum designing of separation processes involving alcohol-based aqueous biphasic systems[3]. This work focused onthe salting effect of a wide range of tetraalkylammonium salts, including tetramethylammonium bromide, tetraethylammonium bromide, tetrapropylammonium bromide, tetrabutylammonium bromide, tetrabutylammonium chloride, tetrabutylammonium hydrogen sulfate, dodecyltrimethylammonium bromide, and cetyltrimethylammonium bromide on the water-solubility of 1-butanol. The effects of anion type, cation alkyl chain length, and concentration of the salts on the thermodynamic quantities of the clouding process have been scrutinizedin a wide temperature range (283.1-353.1 K).The values obtained for the relative contribution of enthalpy and entropy to the clouding Gibbs free energy demonstrate that the clouding process of 1-butanol in aqueous solutions of tetraalkylammonium salts with smaller hydrocarbon portion is entropy-driven. However, the clouding process for 1-butanol in aqueous solutions of tetraalkylammonium salts with longer hydrocarbon chains, especially at higher temperatures and higher salt concentrations, is often enthalpy-driven.

Keywords:Clouding diagram; Butanol; Tetraalkylammonium salts; Salting effect

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Aerobic photooxidation of 1,3-diphenylisobenzofuran in the presence of manganese and iron porphyrins

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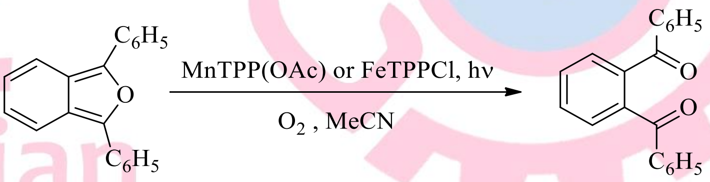
Due to the very short lifetime of the triplet state, paramagnetic metalloporphyrins were found to show no photocatalytic activity for the oxidation of organic compounds, with the intermediacy of singlet oxygen as the reactive oxygen species [1,2]. In the present study, two high spin manganese(III) and iron(III) were used as photosensitizers to investigate the singlet oxygen generation ability of the metalloporphyrins, using 1,3-diphenylisobenzofuran (DPBF) as a specific singlet oxygen quencher [3,4,5]. Although, the rate of degradation of DPBF in the presence of the iron porphyrin was much higher than that observed in the presence of the manganese counterpart, both metalloporphyrins showed photocatalytic activity for the oxidation of the organic substrate.



DPBF

DBB

Keywords:Paramagnetic manganese and iron porphyrins, Degradation of 1,3-diphenylisobenzofuran, Aerobic photooxidation

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Synthesis of a new potentially octadentate macroacyclic N_8 ligand containing two pyridine groups and its corresponding Cu (II) complex and investigation of its biological property

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In this work, A new potentially octadentate macroacyclic N_8 ligand containing two pyridine groups (L) was prepared from the direct reaction of a previously known dialdehyde (N’-bis(5-formylpyrrol-2-ylmethyl) (A) with 2-(aminomethyl)pyridine (Fig. 1). The reaction of this ligand with Cu(II) metal ion resulted in the formation of a macroacyclic Schiffbase complex. The compounds were characterized by FT-IR, elemental analysis, ^{1}H and ^{13}C-NMR. The IR results showed a considerable shift in C=N band of L from 1637 cm^{-1} to 1614 cm^{-1} upon complexation. Moreover, the splitting of the bands attributed to the ClO_4 counter ion confirmed the complex formation. Also, the antibacterial properties of this compound indicated that the Cu(II) complex have high antibacterial activity against Bacillus cereus bacteria in a way that its growth inhibition is much more than that of the reference antibiotics.

Keywords:Schiff base complex, macroacycle, piperazine, antibacterial property, pyridine

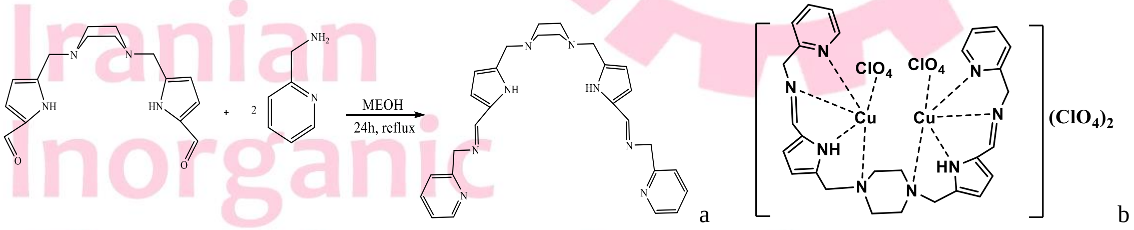

Fig.1. a) The synthesis process of L, b) The proposed structure for the Cu(II) complex.

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Oxidation of organic compounds with nanostructured iodosylbenzene catalyzed by manganese porphyrins

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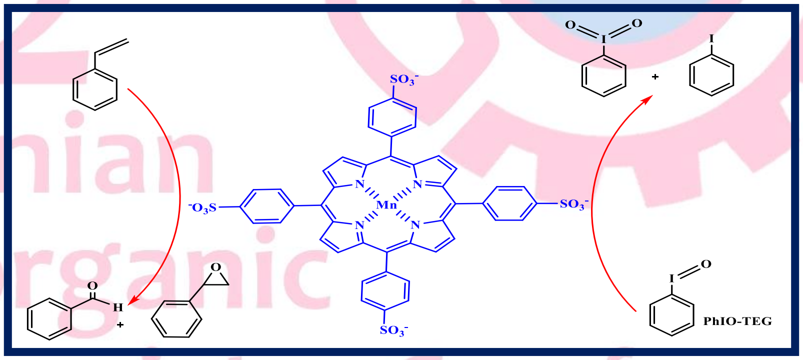
The manganese complex of the sulfonated derivatives of meso-tetrakis(4-methoxyphenyl)porphyrin, $H_2T(4\text{-}OCH_3)PP$, meso-tetrakis(2-chlorophenyl)porphyrin, $H_2T(2\text{-}Cl)PPS_4$ also a porpyrin with cationic substituents at the meso positions, meso-tetrakis(4-methylpyridyl)porphyrin, H_2TMPy, were used as catalysts in biomimetic oxidation of olefins with bulk and nano-structured iodosylbenzene under homogeneous conditions. The nanostructured oxidatnt, PhIO-TEG was synthesized by controled alkaline hydrolysis of iodobenzene diacetate in the presence of triethylene glycol monomethyl ether (TEG) [1]. The product distribution as well as the conversion yields were found to be significantly infuenced by changing the oxidant from bulk to nano-structured PhIO. It is noteworthy that due to the very low solubility of most hypervalent iodine compounds, many efforts were devoted to the synthesis of more soluble and reactive I(III) and I(V) derivatives [2-4].



Keywords: Iodylbenzene-triethylene glycol monomethyl ether nanocomposite, Oxidation of organic compounds, Manganese porphyrins, Hypervalent iodine compounds

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Title: Removal and determination of heavy metals in real samples and industrial wastewater with nanosorbent.

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In this research, the effect of adding modifire such as nanoparticles and lihands for improving the performance of nanofiltration membrane made of polyether sulfone was investigated in laboratory conditions. At first, the production of the primary membrane started with the phase inversion method with a home made instrument. Dimethylacetamide has been used as a solvent, polyvinylpyrrolidone has been used to increase porosity and create holes, and graphene oxide synthesized from graphite in the laboratory has been used to increase the hydrophilicity of the membrane. The membran was characterized with appripriate methids shch FTIR, XRD and SEM. The effective parametrs for improving the regection percentage such as amounts of modifire, pH and water flux was optimized. Composite membranes made of polyether sulfone, dimethylacetamide, polyvinylpyrrolidone and graphene oxide were investigated in terms of water flux and heavy metal absorption. The concentration of heavy metal ions was determined with diffrebtioal puls voltametry (DPV). It was observed the amounts of metal ions such as chromium, mercury, lead, copper and silver have been significantly adsorbed by the modified membran, but it also causes a decrease in the amount of passing water flux

Keywords:Polymeric membrane, Nanofiltration, Heavy metals, Voltametry

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Thermodynamic Study of TiO_2/SBA-16-NH_2 as Drug Delivery System

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In this work, thermodynamic parameters related to carbamazepine loading on TiO_2/SBA-16-NH2 nanocomposites were investigated. Thermodynamic factors were calculated to understand the loading process. ΔH^0 and ΔS^0 values were obtained from $\ln K_c$ versus 1/T data. Thermodynamic values for CBZ drug adsorption on TiO_2/SBA-16-NH_2 were calculated. The values of ΔH°, ΔS° and ΔG° have been determined for the five studied temperatures of 30, 40, 50, 60 and 70 ℃. The negative values of ΔG° indicate that the adsorption process on the nanocarrier is spontaneous. It can be seen that the values of ΔG° become very positive with increasing temperature, therefore, increasing temperature is not always favorable in the adsorption process. The negative values of ΔH° indicated that the adsorption of CBZ on the nanocarrier is an exothermic process. ΔS° values play a vital role in reflecting whether the order of absorption during the absorption process will become less random $\Delta S°<0$ or more random $\Delta S°>0$. In addition, the negative value of ΔS° includes the decrease in the degree of freedom of CBZ drug inside the solution. Furthermore, the sign of ΔS° indicates whether the adsorption reaction is an associative or dissociative process. Therefore, given that ΔS° has a negative charge, it could be an associative mechanism. According to the value of ΔH°, the adsorption between drug and nanocarrier can be classified as physical adsorption. Physical adsorption is based on weak interactions between the adsorbent and the surface sites of the adsorbent.

Keywords: TiO_2/SBA-16-NH_2; Carbamazepine; Drug loading; Drug delivery system; Thermodynamic parameters.

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NiFe Oxide-Based Electrodes Loaded on Indium Tin Oxide as Effective Electrocatalysts for Oxygen-Evolution Reaction

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The oxygen-evolution reaction (OER) is a vital process in energy storage applications such as metal-air batteries and water splitting[1,2].NiFe oxide-based electrodes have gained significant attention for OER due to their promising features[3]. In this study, we investigated the effectiveness of NiFe oxide loaded on indium tin oxide as an electrocatalyst for OER in the presence of $NaHCO_3$.The electrocatalyst was characterized using various techniques, including Raman spectroscopy, diffuse reflectance spectroscopy (DRS), X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectrometry (EDX). Our findings revealed that NiFe oxide loaded on indium tin oxide serves as an effective and durable electrocatalyst for OER in the presence of $NaHCO_3$.Furthermore, our results suggest that the electrolysis of $NaHCO_3$ solution offers a highly promising alternative for producing oxygen and hydrogen compared to corrosive acidic or alkaline solutions. These findings demonstrate the potential of NiFe oxide-based electrodes for OER and offer insights into developing sustainable and efficient energy storage systems.

Keywords:oxygen-evolution reaction, indium tin oxide, electrocatalyst

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Synthesis of nanosized ZSM-5 zeolites by differentamounts of sodium hydroxide and their catalytic performance in methanol to propylene reaction

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Four nanosized ZSM-5 zeolites were successfully prepared from gels with different Si/Na ratios and the same preparation procedures that included the use of tetrapropylammonium bromide as a template and a seeding method. The effect of the amount of sodium in gel on the physicochemical properties of the prepared samples was investigated by XRD, XRF, N_2 physisorption, FESEM, EDX, and NH_3-TPD. The catalytic performance of the nanosized ZSM-5 zeolites in the methanol-to-propylene process was compared. The prepared samples were phase-pure and highly crystalline ZSM-5 zeolites in Na_2O/SiO_2 ratio between 0.04 to 0.169. Theother components in the initial gel were similar. The XRF and EDX results illustrated different Si/Al ratios in bulk and surface of synthesized zeolites, respectively. In addition, the change in the amount of sodium hydroxide in the initial gel affected the acidic properties and morphology of zeolites. The study of the prepared catalysts in methanol to propylenereaction revealed that both the acid characteristics of the ZSM-5 and their textural properties such as surface area were responsible for their performance in the reaction. A difference in the lifetime of every catalyst was attributed to the ability of the catalyst to coke forming on acid sites located on the external surface of the zeolite crystals. The sample with Na_2O/SiO_2 ratio equal to 0.084 in gel showed moderate acid sites with minimum strength, and this catalyst illustrated maximum surface area. The presented results show that the amount of Na_2O used to synthesize ZSM-5 zeolites is an important factor that determines the physicochemical properties, catalytic performance, morphology, selectivity, and acidity of final crystals.

Keywords:ZSM-5, Methanol to propylene, Na_2O/SiO_2.

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Synthesis of hierarchical SAPO-34 crystals with different preparation procedures for the conversion of methanol to olefins

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A series of SAPO-34 molecular sieves with hierarchical porosity were prepared via four different preparation procedures with similar composition and hydrothermal conditions. The catalytic performance of these catalysts for methanol to light olefins reaction was investigated. The results indicated that the order of adding components in the synthesis gel has an effect on the selectivity and lifetime of the catalyst. The samples have a high proportion of framework Si (Si/(Si + Al + P) between 0.49 to 0.62) and framework charge density (0.21<(Al–P) /(Si + Al + P) <0.38). The results proved that the prepared samples with a high degree of crystallinity ,high specific surface area and more number of strong acid sites illustrated the high selectivity to light olefins in the reaction of methanol to olefin. The recently results indicated the order of increasing the ingredients affected the composition and crystalline phase of the product and the XRD results confirmed the presence of SAPO-56 phase next to the main SAPO-34 phase.

Keywords:SAPO-34, different preparation procedures, methanol to olefins.

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Investigating the effect of crystallization temperature in the synthesis of SAPO-34 catalyst in the process of converting methanol to light olefins

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The reaction of methanol to light olefins is a non-petroleum process to produce light olefins[1]. In hydrothermal synthesis, investigating the effect of temperature is of significant importance[2]. In this study, the crystallization temperature was investigated in the synthesis of the SAPO-34 catalyst. For this purpose, by changing the crystallization temperature with a molar ratio of $1Al_2O_3:P_2O_5:1TEAOH:1MOR:70H_2O$, 4 samples were synthesized in 27 hours. To accurately check the characteristics of the synthesized catalysts, XRD, BET, FESEM, and NH_3-TPD analyses were used. In the end, the performance of the synthesized catalysts in the MTO process at 425℃ and WHSV=2.8 h^{-1} temperature was checked. The results showed that the crystallization temperature affects the specific surface area, morphology, particle size, and acidic properties of the SAPO-34 catalyst. The sample prepared at a temperature of 175℃ with the highest crystallinity, small particle size, high specific surface area, and suitable acidity had the highest selectivity of 82% with a lifetime of 280 minutes in the MTO process.

***Keywords*: conversion of methanol to olefin, catalyst, SAPO-34, crystallization temperature**

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Synthesis, characterization, and catalytic performance of Pd/CNT-MOF nanocatalysts in C-C bond formation reactions

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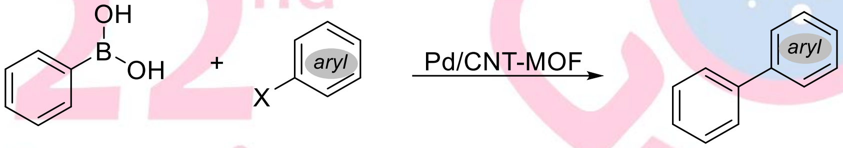
Nanocomposites generally have wide applications in various fields, including drug delivery and catalytic activity for organic synthesis. In this project, an attempt has been made to synthesize a heterogeneous catalyst based on metal-organicframeworks and magnetic carbon nanotubes. A porous multifunctional palladium-based metal-organic framework (MOF) was developed through combined covalent and dative by multi-wall carbon nanotube (MWCNT)[1]–[3]. A novel magnetic metal-organic framework (MMOF) consisting of supported Pd/CNT has been fabricated in this regard. As a result, the fabricated magnetic porous catalyst exhibited catalytic activity in Suzuki-Miyaura cross-coupling reactions. Some of the essential advantages of the synthesized catalyst are; high catalytic activity, short reaction times, mild conditions, high thermal stability, and reusability. Moreover, his porous magnetic nanomaterial can be used as a new support to immobilize other metals in different catalytic reactions.



Keywords:MWCNT, Palladium chloride, Suzuki Reaction, and nanocatalyst.

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Reaction between nickel hydroxide and cerium(IV) ammonium nitrate in aqueous solution

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Cerium(IV) ammonium nitrate (CAN) has been extensively used as a sacrificial oxidant tostudy water-oxidation catalysts (WOCs). Although nickel hydroxide has been extensively investigated as WOCs, water-oxidation reaction (WOR), and mechanistic studies in the presence of CAN and nickel hydroxide were rarely performed. Herein, using in situ Raman spectroscopy, in situ X-ray absorption spectroscopy, and in situ electron paramagnetic resonance, WOR in the presence of CAN and β-$Ni(OH)_2$ was investigated. As a WOR mechanism, it is proposed that β-$Ni(OH)_2$ in the presence of CAN is oxidized to α-NiO(OH). α-NiO(OH) in the presence of acidic conditions evolves oxygen and is reduced to Ni(II). In other words, the role of β-$Ni(OH)_2$ is the storage of four oxidizing equivalents by CAN, and then a four-electron reaction could result in WOR with low activation energy. In contrast to β-$Ni(OH)_2$, $Ni(OH_2)_6^{2+}$ (aq) could not be oxidized to α-NiO(OH).

Keywords: Cerium(IV) Ammonium Nitrate, Mechanism, Nickel Hydroxide, Oxygen, Water-oxidation Reaction

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Facile and Efficient Synthesis 2*H*-indazolo[2,1-b]phthalazine-triones Derivatives Using Fe_3O_4/eggshell/CS@HSO_4 NPs as a heterogeneous and recyclable nanocatalyst

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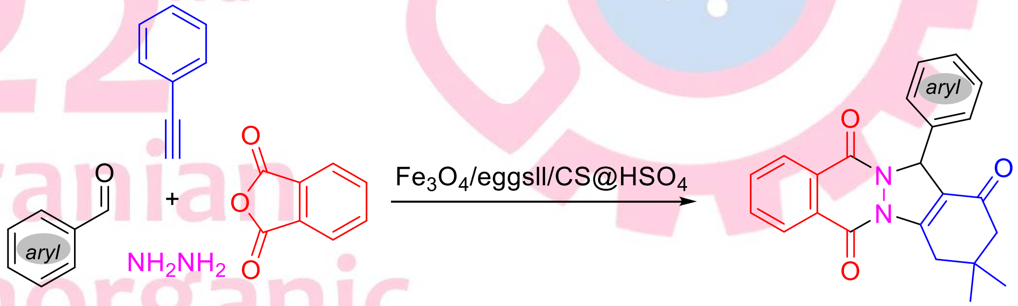
In this paper, a facile and efficient method for the synthesis of 2*H*-indazolo[2,1-b]phthalazine-triones based on the acid-catalyzed multicomponent reaction of dimedone, hydrazine, and phthalic anhydride with aldehydes reported in the presence of Fe_3O_4/eggshell/CS@HSO_4 in solvent-free. We have synthesized a new nanocomposite material in which eggshell membranes act as nucleation sites for the precipitation of Fe_3O_4/eggshell/CS@HSO_4 nanoparticles in the attendance of an external magnetic field. In the next step anchoring a chlorosulfonic acid on the surface of eggshell-coated magnetic nanoparticles as solid waste was transformed into a magnetic biomaterial, green, cheap, and environmentally friendly catalyst (Fe_3O_4/eggshell/CS@HSO_4). Techniques such as FT-IR, VSM, FESEM, TEM, EDX, XRD, and TGA characterized the as-synthesized catalyst. The catalytic property of the as-prepared catalyst was examined in synthesizing 2*H*-indazolo[2,1-b]phthalazine-triones [1-3].



Keywords: 2*H*-indazolo[2,1-b]phthalazine-triones, Eggshell, Multicomponent Reaction, and Nanocatalyst.

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Carbon dioxide (CO_2) adsorption by HKUST-1 (MOF-199)

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One approach to mitigating global warming is the capture and storage of CO_2as the major greenhouse gas[1]. Materials that are commonly used for CO_2 adsorption include activated carbon, zeolites[2], and metal-organic frameworks (MOFs)[3].HKUST-1 (also known as MOF-199) is a well-known metal-organic framework that has been extensively studied for its potential applications in gas storage and separation. In this work, HKUST-1 was investigated as an adsorbent for CO_2. HKUST-1was synthesized using the hydrothermal method and its chemical properties were investigated using various characterization techniques including XRD, FTIR, FESEM, BET, and TGA. It was shown that HKUST-1 has a crystalline structure with a surface area of over 1704 m^2/g, and a petal-shaped molecular structure. It also showed thermal stability up to a temperature of 366°C.The results of CO_2 adsorption showed that the amount of carbon dioxide adsorption by HKUST-1 at 20°C, 30°C and 40°C and 1bar was 3.788, 3.417, and 3.088mmol/g, respectively. However, in 10 bar and the same temperatures, its adsorbtion improvedto 9.090, 8.782, and 7.724mmol/g, respectively. Therefore, it can be concluded that the amount of carbon dioxide adsorption enhanced with increasing CO_2pressure and decreases when temperature increases. Therefore, HKUST-1 could be suggested as a promissing CO_2 adsorbent at moderate temperatures.

Keywords:CO_2 adsorption, metal organic frameworks, HKUST-1, CO_2 Capture, greenhouse gas

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Title: $TiO_2/H_3PMo_{12}O_{40}$ decprated SBA as Photocatalyst for Dye Removal from Wastewater

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The presence of dyes in wastewater is a major environmental concern due to their harmful effects on aquatic life and human health. Therefore, the development of efficient and sustainable methods for the removal of dyes from wastewater is of great importance. Photocatalysis has emerged as a promising technology for the removal of dyes from wastewater due to its high efficiency and low cost. In this study, we report the synthesis and characterization of a new photocatalyst for the removal of dyes from wastewater. The catalyst is composed of H3PMo12O40 immobilized on amine functionalized SBA and decorated with TiO2 nanoparticles. The catalyst was characterized using various techniques such as FTIR, XRD, SEM, and TEM. The photocatalytic activity of the catalyst was evaluated using methylene blue (MB) as a model dye. The results showed that the catalyst exhibited excellent photocatalytic activity for the removal of MB, with a degradation efficiency of 94% under UV light irradiation for 120 min. The catalyst was found to be stable and reusable for several cycles of MB degradation.

Keywords:photocatalyst, titanium oxide, water treatment, heteropolyacid

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Synthesis and study of zinc (II) and copper (II) complexes with mixed deferiprone and lamotrigine pharmaceutical ligands

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In this work, zinc (II) and copper (II) complexes with a mixture of lamotrigine (L) and deferiprone (D) as pharmaceutical ligands with chemical formulas $[Zn_2D_2L_2(OH_2)_2].(NO_3)_2$ and $CuDL_2.NO_3$ were synthesized. The characteristics of these complexes were identified by infrared and ultraviolet-visible absorption spectroscopy techniques and their structure was determined by single-crystal X-ray crystallography. The results of X-ray crystallography show that in these complexes, lamotrigine is coordinated to the central atom as a mono dentate ligand through nitrogen atom. In the di-nucleic zinc complex, the deferiprone ligand binds to the zinc centers through two oxygen atoms by losing the proton of the hydroxyl group. One oxygen atom is coordinated to a zinc center and the other oxygen atom is coordinated as a bridge to both zinc atoms. Deferiprone is coordinated to the copper atom through oxygen atoms by losing the hydrogen atom of hydroxyl groups. The metal centers have near square pyramidal coordination geometry according to the geometrical parameter τ_5 [1-3].

Keywords:Lamotrigine, Deferiprone, Zinc complex, Copper complex, X-ray diffraction

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Synthesis, Characterization and Anticancer Evaluation of Novel Macrocyclic Schiff Base Complexes of Cu(II), Ni(II), and Co(II).

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Schiff bases are chemicals that have been functionalized with azomethine or imine and have a wide range of therapeutic uses[1]. The Schiff base macrocyclic complexes are studied widely because of their easy synthesis, versatility and wide range of applications[2].Schiff base complexes have significantly contributed to the development of modern drug design due to their significance in a number of multi-discipline study fields[3]. In this work, from the reaction of novel polyamine N,N-bis(2-aminobenzyl)-2-methoxyaniline with 2-hydroxy-5-methylisophthalaldehyde by template method in the presence of metal ions Cu(II), Co(II), and Ni(II) with stoichiometric ratios of 1:1:1, mononuclear macrocyclic Schiff base complexes containing methoxyphenyl moiety as pendant arm were prepared. Proposed structures were presented based on the methods of elemental analysis, mass spectrometry, FT-IR, and determination of molar conductivity. The anticancer activity of these macrocyclic complexes was also assessed, using the MTT test, which found that the highest activity was observed for Cu (II) against breast cancer (MCF-7) cells.

Keywords:Schiff base, macrocyclic complexes, anticancer properties

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Assessment of the Anticancer Activity of Novel Macroacyclic Complexes of Cu(II), Ni(II), and Co(II) with a Newly Synthesized N^1,N^2-bis(2-aminobenzyl)-N^1,N^2-bis(pyridin-2-ylmethyl)propane-1,2-diamineLigand.

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Metal complexes exhibit promising potential in medicinal applications, such as cancer treatment[1].Metal complexes also play a crucial role in bioinorganic chemistry, particularly in understanding metalloprotein function[2]. In this work, three new metal complexes have been obtained from the reaction of a new N^1,N^2-bis(2-aminobenzyl)-N^1,N^2-bis(pyridin-2-ylmethyl)propane-1,2-diamineligand(L) with Ni(II), Cu(II), and Co(II) ions.To evaluate the biological potential of the ligand and the synthesized metal complexes, their binding behavior with DNA was studied by molecular modeling methods. The Molecular docking studies showed that the free ligand and its complexes were bound to the major groove of DNA. The synthesized compounds were tested for activity against lung carcinoma epithelial cells (A549) using the MTT cell viability assay. A comparative study of the IC50 values indicated that the Cu(II) complex exhibited the highest activity, while the Co(II) and Ni(II) complexes showed more potent antiproliferative activity than the ligand.

Keywords:metal complexes, biological activities, Molecular docking

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Synthesis and characterization of new copper-based metal-organic frameworks

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Metal-organic frameworks are structures that consist of metal ions or clusters coordinated with organic ligands. They have a high surface area, tunable pore size, and customizable properties that make them attractive for a wide range of applications. Some of the applications of MOFs include: the production of implants, drug delivery systems, medical imaging, Sensor, Energy storage systems, Gas storage, Building materials, Catalysis and Electrocatalysis [1-5]. In this study, the solvothermal synthesis of a new metal-organic framework based on copper is reported. The structure of the obtained product was identified by FT-IR, CHN, BET and PXRD analyses. The results confirmed the successful fabrication of Cu-MOF nanoparticles.

Keywords:Metal-Organic Frameworks (MOF), Synthesis, Characterization, Solvothermal

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Investigating the effect of copper(II) coordination compound with Carbonylbis(azanediyl)dibenzoic acid ligand on the phase-stabilization of ammonium nitrate

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In this work, a novel copper(II) coordination compound is synthesized using Carbonylbis(azanediyl)dibenzoic acid (CAD) as ligand (Cu(II)-CAD). The structural, and morphological property of the synthesized material are investigated using FT-IR, CHN, FE-SEM, BET and PXRD analyses. Evaluation of the obtained results indicates that CAD coordinated to copper ions. Ammonium nitrate (AN) is an affordable oxidant, which is widely used in gas generators. Since AN shows crystal structure transformation in ambience temperature accompanied by a change in volume, its application is limited without phase stabilization [1-5]. For phase stabilization of AN, AN/Cu(II)-CAD composite is prepared and its phase transitions is studied using differential scanning calorimetry (DSC). The results indicate that ANIV↔ANIII phase transition can be eliminated by hydrogen bonding between AN and Cu(II)-CAD.

Keywords: Ammonium nitrate (AN), Carbonylbis(azanediyl)dibenzoic acid (CAD), Phase stabilization, Cu(II)-CAD, AN/Cu(II)-CAD

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Efficient Removal of Heavy Metal Ions from Water Using Urea-Functionalized Metal-Organic Frameworks

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The pollution of surface and groundwater with heavy metals is a serious global concern, both environmentally, as well as with respect to human health. Recently, porous metal-organic frameworks (MOFs), with metallic clusters and organic linkers, have been developed as promising structures in capturing different toxic and hazardous substances, including heavy metal ions, because of their unique features[1-5]. This study synthesized two copper-based MOFs, using hydrothermal methods. These MOFs are densely decorated with urea functional groups, which enable them to selectively and efficiently remove various heavy-metal ions, such as Hg2+ and Pb2+, from water. The structures of these MOFs allow for the effective sorption of these metal ions. This research demonstrates urea-functionalized MOFs as a highly efficient adsorbent for removing heavy metals.

Keywords:Water pollution, Heavy metal ions, Metal-organic framework (MOF), Adsorption,Removal

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Synthesis of Fe-MOF nanostructure: A Study of Peroxidase-Like behavior for Sensing of H_2O_2

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In recent years, nanotechnology is widely used in sensing, biomedicine, food industry, agriculture and etc. as a newly developed science and technology, in which nanomaterials with enzyme-like catalytic activity, namely nanozyme, have been used in the development of new chemosensors [1]. Recently, nanozymes have drawn extensively studied for their applications in bioanalysis, disease diagnosis, and therapy. In addition to, compared with natural enzymes, nanozymes possess the advantages of low cost, easy-to-scale production, high tolerance to the environment, long-term storage, high stability, and controllability [2]. Studies in this field have shown that nanozymes are suitable substitutes for natural enzymes. Therefore, the development of stable materials exhibiting high substrate affinity and high activity as ideal artificial enzymes is a highly desirable research goal [3]. The nanozymes reported thus far are, for instance, noble metal-based, and carbon-based materials, metals/metal oxides, carbon materials, MOFs, and so on.Among these nanomaterials, MOF nanozymes due to their inherent porous structure, large specific surface area, low density, high porosity, structural diversity, and adjustable pore size open structure for the free transfer of substances and products in the catalytic reaction, have shown special enzyme-like activity[4].Due to availability effective active sites and enhancing the catalytic activity in MOFs, it has been reported that some of them can simulate natural enzyme activities such as POD-like (peroxidase) activity.Currently, Due to the same Fe metal centers as peroxidase for MIL-(Fe) peroxidase-like nanozymes (such as MIL-53, MIL-88, MIL-100 and MIL-101), the nanozymes based MIL-(Fe) have become a potential platform for exploring catalytic mechanisms and improving performances[5].Herein, we reported a Fe-MOF with excellent properties and peroxidase-like activity, which is synthesized with a simple method. The synthesized Fe-MOF under weakly acidic conditions, can catalyze the oxidation of TMB substrate to oxTMB by hydrogen peroxide. Therefore, asimple colorimetricassayforthedetectionofhydrogenperoxidebasedontheperoxidase-like activityof the Fe-MOF nanozyme hasbeenestablished.

Keywords:Nanozyme, Fe-MOF, Peroxidase.

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Less-lead $FAPbI_3$ (100) Surfaces, A theoretical Study

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Hybrid organic-inorganic perovskite solar cells (PSCs) have recently become one of the most efficient materials for photovoltaic applications [1]. Formamidinium lead triiodide ($FAPbI_3$)perovskites possess high light absorption and stability, making them strong candidates for efficient solar cells, yet they suffer from toxicity. The optoelectroniccharacteristics of environmentally friendly alkaline earth metals substituted $FAPbI_3$(100) surfaces,in various percentages, with PbI_6 and PbI_5 terminations has been investigated using density functional theory (DFT) as implemented in the Vienna ab initio simulation package [2], (VASP 5.4.4). We have created14 stable doped structuresaccording to the Goldsmith tolerance factor [3],in the form of $FAPb_{1-x}AE_xI_3$,(AE= Be, Mg, and Ca). Different terminations showed a negligible influence on the optical features, although their effect on the electronic properties is significant. Due to the conduction band (CB) shifting of the PbI_6 termination to the higher energies, an increase of about 0.3 eV in the bandgap of this termination was obtained compared to that of PbI_5, and suitable bandgaps of 1.623 and 1.309eVwere calculatedfor them, respectively. In doped systems, Mg and Ca substitutionmadebroader bandgaps, while two different decreasing and increasing trends on the bandgap of $FAPb_{0.95}Be_{0.05}I_3$ and $FAPb_{0.96}Be_{0.04}I_3$ structures were observed. Promising optical activitysuch as appropriate extinction coefficient and light harvesting efficiency for plain and doped (100) surfaces in the visible and UV windows and also the high capacity of all structuresto absorb more photons,especially in the near UV region for doped counterparts, altogether, indicate the capability of the (100) surfaces for optoelectronic applications.

Keywords: alkaline earth metals, $FAPbI_3$, perovskites,doping, density functional theory

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A first principles study of carbon monoxide hydrogenation on cobalt (001) surface.

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Carbon monoxide (CO) is a colorless, odorless, and non-irritable gas [1]. Fischer–Tropsch synthesis (FTS) is a process that has been used for many decades as it gives access to industrially important chemicals from CO [2]. As the products of FTS are a complex mixture of a wide range of organic compounds, selectivity toward desired products is the most important issue in this reaction. In recent years, there has been an increasing motivation to deploy FTS at commercial scales, which has fueled the search for high-performance catalysts [3]. Several catalysts have been examined for their potential to catalyze CO hydrogenation. Transition metal catalysis has long been recognized as a reliable and modular means of constructing complex molecules from simple, readily accessible starting materials[4]. Periodic plane-wave density functional theory (DFT) calculations were carried out to study the CO adsorption and its reactivity with adsorbed hydrogen on the Co (001) surface. All parts of this study employed the Vienna Ab initio Simulation Package (VASP) [5]. The results show that CH_4, CH_3OH, and C_2H_2 are the products, according to the calculations CH_4 is the main product. We found that the preferred mechanism for CO hydrogenation is through HCO and cis-HCOH, and the largest exothermic reaction energy in the CH_4 formation pathway is released during the hydrogenation of cis-HCOH (−0.773 eV). An investigation of the kinetics demonstrates that the CH production from cis-HCOH has the lowest energy barrier. On the other hand, the hydrogenation of CO to COH is the least favored reaction kinetically.

Keywords: Carbon monoxide; Fischer–Tropsch Synthesis; Cobalt catalyst; DFT

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DFT study on the hydrogenation of carbon monoxide on a SiO_2-based catalytic surface

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The increasing demand to obtain clean fuels and useful products has created an interest in finding active and selective catalysts for the conversion of carbon monoxide into desired products. The hydrogenation process of carbon monoxide is often polymerized into liquid hydrocarbon chains using catalysts. In this research, density functional theory (DFT) [1] calculations have been used to investigate the reaction mechanism of Fischer-Tropsch synthesis on silica-based catalytic surfaces. [2] Silicon dioxide is known as a catalytic substance that can be a suitable surface for hydrogenating the carbon monoxide molecule and thus reducing the amount of pollutants in the atmosphere. Periodic plane-wave density functional theory (DFT) calculations were carried out to study the CO adsorption and its reactivity with adsorbed hydrogen on the Co (001) surface. All parts of this study employed the Vienna Ab initio Simulation Package (VASP) [3]. After examining the paths of methanol and methane production, it was found that the exothermic methanol production and the COH production stage in it are the rate-determining steps, and in the case of the methane path, which is an endothermic process, the CH + H step is the rate-determining step. The results show that methane formation is more favorable compared to other products.

Keywords: Carbon monoxide, Fischer–Tropsch Synthesis, DFT, SiO_2

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Introduction of a new DABCO-based ionic liquid as an efficient catalyst for the synthesis of benzimidazoquinazolinone derivatives

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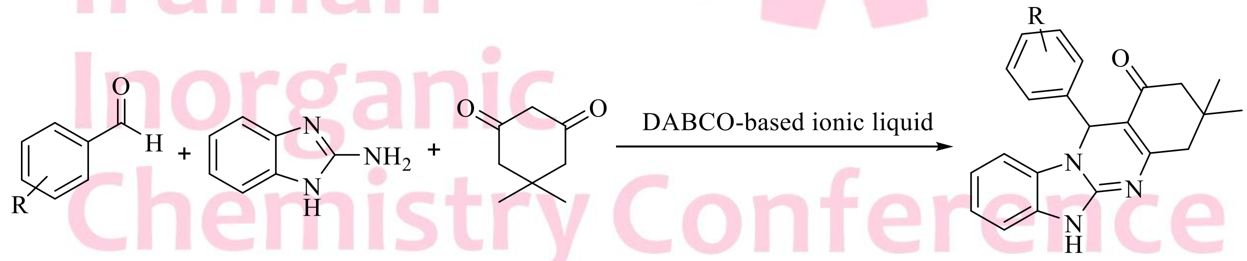
Benzimidazoquinazolinones are heterocyclic compounds that have been shown various pharamacological activities such as anti-cancer, anti-inflammatory, anti-oxidant, antimicrobial and neuroprotective activity. The diverse pharmacological activities exhibited by benzimidazoquinazoinone make it a promising lead compound for the development of novel therapeutic agents. These attempts resulted in the introduction of a variety of reagents for the promotion of the synthesis of these compounds. Although, each of these methods have their own advantages, some of them often suffer from one or more disadvantages such as use of stoichiometric amounts of reagents, expensive metal precursors, tedious work-up, long reaction times, unsatisfactory product yields, excess of organic solvent, high temperatures, harsh reaction conditions, and difficulty in preparation of the catalyst, which limit the use of these methods. Therefore, it is important to find more convenient methods for the synthesis of benzimidazoquinazolinone derivatives. In this research, we have reported the preparation of a new DABCO-based ionic liquid catalyst which can be used for the promotion of the synthesis of benzimidazoquinazolinone derivatives. It is expected that using the mentioned dicationic ionic liquid with its remarkable features be useful for the elimination of some of the disadvantages of the previously reported methods [1,2].



Keywords: DABCO, multi-component reactions, ionic liquid catalyst, benzimidazoquinazolines

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Mechanistic insights of the key role of methylammonium iodide in the stability of perovskite material

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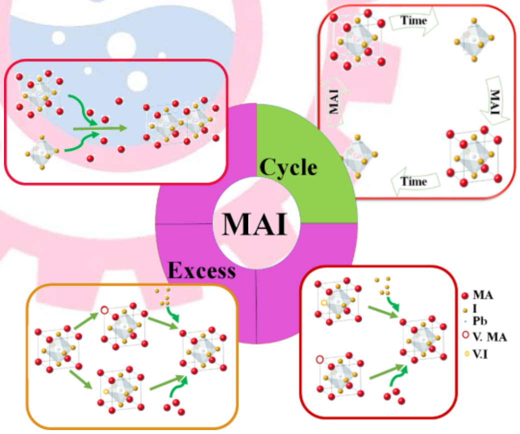
The possible mechanisms damaging perovskite solar cells have attracted considerable attention in the photovoltaic community[1-3]. This paper specifically answered some open problems regarding the critical role of methylammonium iodide (MAI) in informing and stabilizing perovskite cells. Surprisingly, by using Ultraviolet–visible (UV−vis) spectra, X-ray diffraction analysis (XRD), Field emission scanning electron microscope (FE-SEM) images, and X-ray photoelectron spectra) XPS, we found that when the molar ratio between PbI_2: MAI precursor solution increased from 1:5 to 1:25, the stability of perovskite cells dramatically increased over time. The stability of perovskite on air without any masking in the average stoichiometry was about five days, while when the value of MAI precursor solution increased to 5, the perovskite film was unchanged for about 13 days, eventually, when the value of MAI precursor solution enhanced to 25, the film of perovskite was stayed intact for 20 days. The outstanding XRD results indicated that the intensity of perovskite's Indices Miler was Increased significantly after 24 h, and the MAI's Indices Miler was decreased, which means that the amount of MAI was consumed to produce perovskite cells. This proposed mechanism is challenging because pieces of evidence claim that the charging of MAI continuously produces the perovskite cell, which significantly avoided damage to the perovskite material.



Keywords: Perovskite, Methylammonium iodide, Stability

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Shedding light on the environmental impact of the decomposition of perovskite solar cell

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Perovskite materials, as the heart of perovskite solar cells, attracted great interest in the photovoltaic community since the efficiency of perovskite solar cells (PSC) dramatically increased to over 25.8 %. However, the presence of Pb metal in the perovskite crystalline limits the progress of this new generation of solar cells from environmental aspects[1, 2]. Here, we have systematically investigated the impact of the decomposition of perovskite material on the plant. We found that the influence of the decomposition of a perovskite solar cell has lower destruction than commercial PbI_2. In particular, influenced the roots and leaves to be slower and smoother. Remarkably, the amount of water absorption with the plant's root is lower than, indicating that dramatically wasted water from roots shows the most harm. In the following, the atomic absorption spectroscopy measured the lead concentration of the plants ashe which conclude that the plant absorbed more Pb metal from commercial PbI_2 than perovskite, This paper opens new avenues and challenges about the actual scenario on the impact of perovskite materials in PSCs on the plant and live metabolisms. Therefore, we conclude that the plant absorbed more Pb metal from commercial PbI_2 than perovskite of a PSC, which is in contrast with recent report in Nature Communication′s paper[3]. This paper opens new avenues and challenges about the actual scenario on the impact of perovskite materials in PSCs on the plant and live metabolisms.

Keywords: Perovskite, Environmental, plant

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Biological Studies of upconversion nanoparticles

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Recently, researchers have focused to the synthesis of nanomaterials with extraordinary wonders to treat and diagnose diseases. These substances, which are called upconversion, have special characteristics that can have the least negative impact and the greatest depth of penetration on the tissues and cells of the body. In this research, we synthesized transforming materials, which had the ability to affect tumors with unique optical properties and due to the possibility of stimulation, in the infrared range, the condition of certain biological studies, with the least amount of damage to the tissues. In this wavelength provided [1]. In this research, various types of cubic, spindle like [2] and hexagonal structures of biocompatible upconversion were synthesized by hydrothermal method and identified by different detection methods such as XRD, TEM, PL, FTIR, UV-VIS. The identification results were in good agreement with the reference templates and their effects on MCF7 breast-derived cell lines were evaluated through Annexin PI and MTT assays. These $NaYF_4$ nanomaterials were combined with activator and sensitizer ions and their effects on breast cancer cells were investigated by flow cytometry and MTT analysis. This study will contribute to the development of new nanomaterials with promising biomedical applications[3] and provide new avenues for advanced diagnostic and therapeutic interventions. Synthetic nanoparticles were a good option for use in biological studies due to the appropriate intensity of emission radiation, optical stability under appropriate stimulation.

Keywords: Upconversion, Hexagonal, toxicity, Flow cytometry

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Modifying commercial sponges using magnetic nanoparticles and investigating the separation of organic pollutants from water

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As a source of life, water plays a decisive role in the existence and development of human society. However, global water pollution has become a much more pressing issue today [1]. The frequent occurrence of oil and chemical spills has caused severe environmental pollution and environmental problems, which has made the separation of oil from water a serious challenge [2]. In this research, a hydrophobic sponge structure with high absorption capacity of organic compounds was prepared. In all stages of the synthesis, we tried to use methods with less energy, water solvent, and low risk compounds to be based on green chemistry. First, iron oxide nanoparticles were synthesized by ultrasound waves and then coated with polyvinyl alcohol. FT-IR analysis was used to identify and investigate the synthesis and modification of nanoparticles. These modified nanoparticles were placed on the surface of polyurethane sponges. The modified sponges became hydrophobic after exposure to 300 °C due to the partial destruction of the structure and the loss of hydrophilic functional groups. The investigation of the interaction between water drop and hexane drop showed that hexane is immediately absorbed by the modified sponge, while the water drop is not allowed to enter and is placed spherically on the surface of the sponge. Examining the absorption properties of these sponges also showed that they have a high and fast ability to absorb organic pollutants from the water surface, so that when they come in contact with the organic pollutants on the water surface, they immediately absorb and remove the organic compound from the water surface.

Keywords: Iron oxide nanoparticles, hydrophobicity, separation of water from oil, environment

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Tuning the topology from (4,4)-connected to (6,3)-connected net in Cd (II) coordination polymers: synthesis, crystal structure and Hirshfeld surface analysis

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Coordination polymers (CPs) defined as coordination compounds with extended bonding in one, two, or three dimensions have become one of the main objects of study in crystal engeenering due to their potential applications in sensing [1], catalyst [2], gas storage and separation [3], drug delivery [4], and so on. The preparation of CPs in which the network topology is controlled by reaction condition is an important step in the design of new functional materials. In this regard, we report the synthesis of two CPs, namely $[Cd(L)(NO_3)_2(H_2O)]_n$ (**1**) and $\{[Cd(L)_{1.5}(NO_3)_2](MeCN)\}_n$ (**2**), by the self-assembly process using cadmium (II) ion as metal nodes and pyridine containing ligand as linker in MeCN and EtOH/MeCN, respectievly. These compounds were structurally characterized by single-crystal X-ray diffraction analysis and further characterized by powder X-ray diffraction (PXRD). As depicted in Fig. 1, topology of compound **1** can be considered as (4,4)-connected net, while the topology of compound **2** is (6,3)-connected network. Hirshfeld surface analysis of the structures **1** and **2** have been performed and find the percent of participation of intermolecular interactions in the crystal packing of compounds.

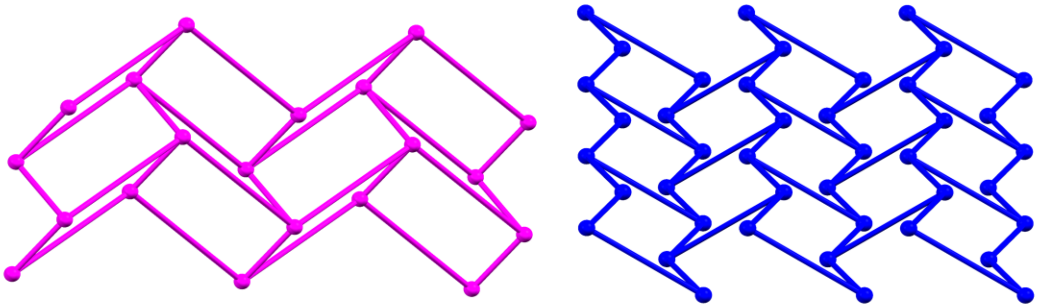

Fig. 1. Schematic view of the (4,4)-connected topology in **1** (left) and (3,6)-connected topology in **2** (right)

Keywords: coordination polymer, cadmium, topology, solvent effect.

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Concomitant crystallization of supramolecular isomers: 2-fold interpenetrated and non-intenterpenetrated coordination polymers

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Coordination polymers (CPs) have been undergoing rapid development due to their facile functionalization [1], diverse topologies [2] and varied potential applications [3,4]. Supramolecular isomerism is used to describe the existence of more than one type of supramolecular network for a given set of components. To the best of our knowledge, research on the concomitant formation of supramolecular isomers is still rare [5]. In this work, we report the one-pot synthesis of two CPs, namely $\{[Cd(L)_{1.5}(NO_3)_2](L)_{0.5}\}_n$ (**1**) and $[Cd(L)_{1.5}(NO_3)_2]_n$ (**2**), by the self-assembly process using cadmium (II) ion as metallic tectons and pyridine containing ligand (**L**) as organic tectons in EtOH. These compounds were structurally characterized by single-crystal X-ray diffraction analysis and further characterized by powder X-ray diffraction (PXRD). As illustrated in Fig. 1, compound **1** can be considered as 2-fold interpenetrated framework, while compound **2** is a non-intenterpenetrated coordination polymer. Hirshfeld surface analysis of the compounds **1** and **2** have been performed to investigate the relative contributions of each interaction in crystal packing.

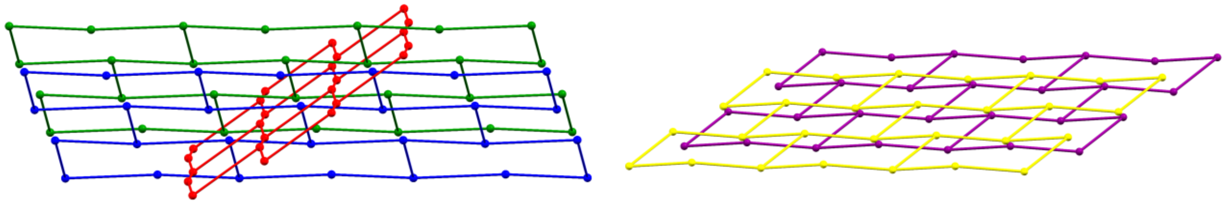

Fig. 2 Schematic view of 2- fold interpenetrated 2D CP in **1** (left) and non-interpenetrated 2D CP in **2** (right).

Keywords: coordination polymer, cadmium, concomitant.

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Synthesis, specteral characterization, structure, and application of tridentate ONO hydrazone Schiff base metal complexes

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An imine or Schiff base is a chemical compound in which the C=O has been changed to a C=N [1]. Schiff base works like a ligand and may coordinate with the metals by its iminic nitrogen and another donating moiety, generally OH [2]. Numerous Schiff bases prepared from diverse amines have been studied utilizing various techniques, and it has been demonstrated that these compounds have promising uses in materials chemistry, agriculture, and industry [3]. Schiff bases can also serve as catalysts in a variety of organic procedures as well as in the invention of biologically active substances, plant growth regulators, and organic dyes [4]. Hydrazones, a particular group of species in the family of Schiff bases, are recognized by the existence of $R_1C=N-NR_2$ group. The existence of two interconnected N atoms sets them apart from the rest of the members of this family (oximes and imines). The nitrogen atoms are nucleophilic, whereas the carbon atoms have electrophilic property. When hydrazones are combined with a variety of functional groups, new compounds with distinctive biological characteristics are created. We hope to offer a fresh perspective on this class of compounds by highlighting the significance of various types of tridentate ONO Schiff base ligands and their complexes, whose single crystals were reported in the recently years through the reactions of salicylaldehyde and its derivatives with various acylhydrazides such as nicotinohydrazide and isoniazid. This kind of Schiff bases exhibit amide-iminol tautomerism, in which the carbon-nitrogen double bond is a component of the iminol tautomer. The molecular structure, spectral characterization, and applications of ONO Schiff base complexes are covered in this paper.

Keywords: Tridentate, ONO Hydrazone, Schiff base, Metal complex

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Investigation of the catalytic activity of Mo and V complexes with tridentate pyridyl hydrazone Schiff base ligands in oxidation reactions

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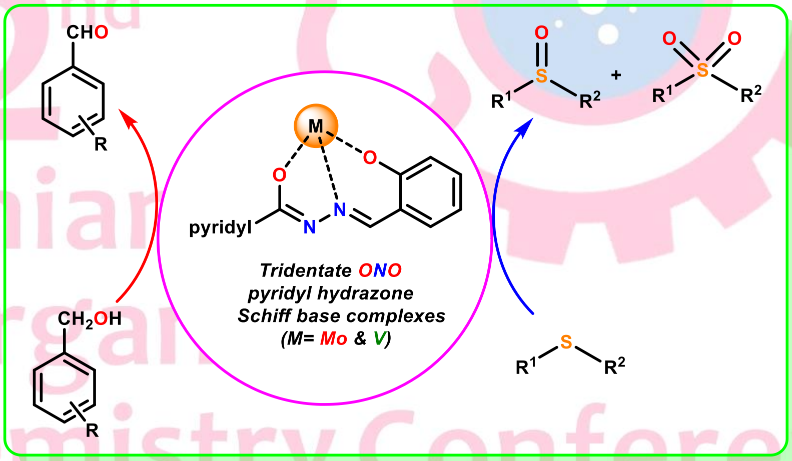
Most Schiff base metal complexes have an azomethine group as a coordination site, which makes them amenable to easy structural alterations. They may also be easily produced *via* one-step condensation processes, which promote coordination when three, four, or five bonds separate other donor sites. Mo and V complexes with several hydrazone-based Schiff bases have outstanding catalytic activities in various chemical processes [1-4]. Numerous studies on their use in homogeneous and heterogeneous catalysis have been documented during the past several years. Considering the features of both ligands and metals, they can support the production of extremely effective complexes because their properties are often boosted by complexation. Therefore, significant catalytic activity data for the Mo and V complexes prepared using ONO donor pyridyl hydrazone-based tridentate Schiff base ligands in oxidation reactions are summarised in this paper.



Keywords: Catalytic activity, Pyridyl hydrazone, Schiff base, Oxidation reaction

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Synthesis, characterization and crystal structure determination of Ni(II) complex with N_2O_2 symmetrical tetradentate Schiff base ligand

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The low-spin square-planar nickel(II) complexes and high-spin octahedral nickel(II) complexes with Schiff base ligands have been received much attention in optical materials [1]. Nickel is also recognized as a considerable important biological metal forming the active site of a variety of metalloproteins such as hygrogenase, carbon monoxide dehydrogenase, and urease [2, 3]. A symmetrical Schiff base ligand has been prepared and characterized by elemental analyses and spectroscopic methods. The corresponding nickel(II) complex was synthesized with tetradentate Schiff base ligand derived from 5-bromosalicylaldehyde and 2,2-dimethyl-1,3 diaminopropane. This complex was characterized by ^{1}H NMR, FT-IR and its solid state structure was determined using single crystal X-ray diffraction. The Ni(II) ion is coordinated by two N atoms and two O atoms from the tetradentate Schiff base ligand in a distorted square-planar geometry (Fig. 1).

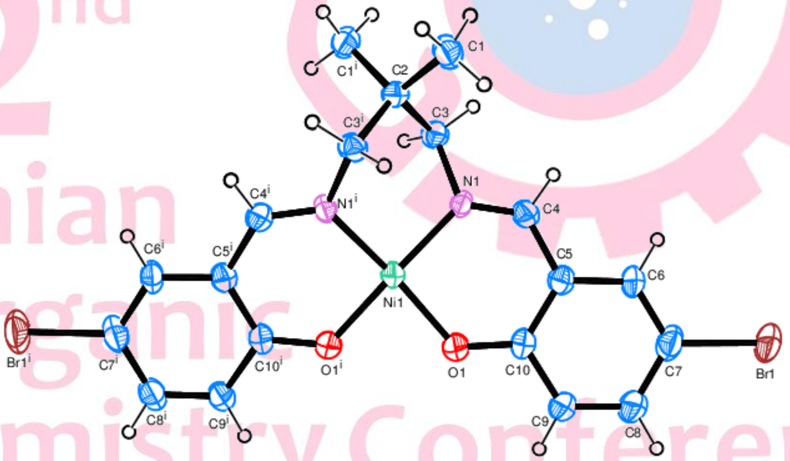

Fig. 1. The molecular structure of the title compound with 50% of ellipsoid probability.

Keywords: Schiff base, N_2O_2 donor, Nickel complex, Crystal structure

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Full protonation and also metal cation affinity of adenine in gas and solution phases; a theoretical study

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Adenine is a purine nucleobase. Purine is a heterocyclic aromatic organic compound that consists of two heterocylic rings (pyrimidine and imidazole) fused togther [1]. In this work, we report a theoretical study on protonation and metal cation affinity (Na^+, K^+ , Mg^{2+}, Ca^{2+}, Fe^{2+} and Zn^{2+}) of adenine molecule at M06-D3 level of theory, with def2-TZVPP basis set using GAUSSIAN 09 program. The possibility of the protonation of different nitrogen atoms of the above molecule in both gas phase and aqueous solution was studied.The microprotonation constants for all different nitrogen atoms of adenine in solution was also computed. The complete protonation of this molecule was also investigated threough our previously known methodology [2-4] and the most stable isomers for adenineH^+, adenineH_2^{2+}, adenineH_3^{3+}, and adenineH_4^{4+} were determined in the gas phase. The possibility of the binding of adenine and its protonated form to metal ions through its different nitrogen atoms has been also studied (see Figure 1).

Keywords: Adenine, Proton affinity, Metal cation affinity, Gibbs free energy

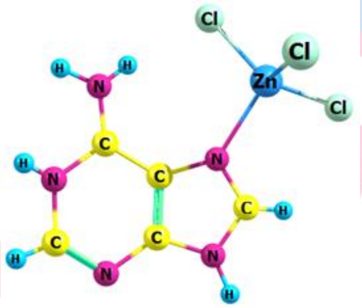

Figure 1. Optimized structure of a Zinc complex of the protonated adenine

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Phytosynthesis of silver nanoparticles on the woolen yarn with synthesized by sumac (Rhus coriaria L.) seed extract

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The development of green synthesis of silver nanoparticles instead of using toxic chemicals has attracted the attention of researchers. Most of the proposed methods are based on the use of natural compounds of plant origin [1], with a special focus on the principles of green chemistry. In this regard, the synthesis of silver nanoparticles using agricultural and industrial waste or food as a regenerating and capping agent can be a valuable and economic method. Examples of this approach are the production of silver nanoparticles using rice husk extract, blueberry and red berry waste, tamarind peel and tangerine peel [2, 3]. Although there are a limited number of reports about the green synthesis of silver nanoparticles by the sumac seed as a regenerating and stabilizing agent. The present study aims to use of the synthesized nanoparticles for dyeing of woolen yarns. For this purpose, different concentrations of sumac seed extract and silver nitrate solution were used on the wool fabric. The colorimetric data of the dyed samples was determined using a reflectance spectrophotometer. In addition, the size of silver nanoparticles in dyeing solution was determined by absorbance method and DLS device.

Keywords: Natural dye, Silver nanoparticles, Sumac seed extract, Color fastness, Dyeing

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Investigating the synthesis methods of alumina nanoparticles

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Alumina nanoparticles have attracted much attention due to their unique properties and potential applications in various fields such as electronics, catalysis, biomedical engineering, energy, etc. Alumina nanoparticles can be prepared and synthesized through various methods such as sol-gel, hydrothermal, deposition, combustion, etc. The properties of alumina nanoparticles include high surface area, high mechanical strength, high thermal and chemical stability, which makes them suitable for various applications [1-3]. In this article, various synthesis methods, properties and applications of alumina nanoparticles have been reviewed. The results of the investigations have shown that each synthesis method has advantages and disadvantages in terms of particle size, morphology, purity and efficiency, and the choice of synthesis method depends on the properties and applications of nanoparticles.

Keywords: Alumina nanoparticles, Synthesis methods, Applications Alumina nanoparticles, Properties Alumina nanoparticles

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Synthesis of quinoxalines accelerated by a new nanocatalyst based on ionic liquid stabilized on TiO_2 and Kaolin

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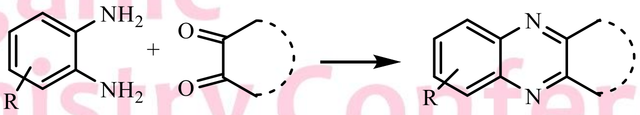
Ionic liquids (ILs) have been recognized as appropriate green catalysts/solvents in organic transformations. This is due to their remarkable properties such as negligible vapor pressure, thermal stability over a wide temperature range,non-flammability and ability to dissolve organic and inorganic compounds. Nevertheless, several drawbacks of ILs such as high cost, high viscosity, large consumption and separation difficulties restrict their large-scale applications. However, these issues can be solved efficiently by using supported ionic liquids (SILs) prepared by the immobilization of ILs on solid supports. SILs offer several advantages such as ease of handling, minimizing the amount of IL utilized in the reactions and simple separation, and reuse. In this regard, various supports have been used to immobilize ILs, including silica, clays and metal oxides. In the meantime, natural clays such as kaolin have received more attention due to their outstanding physical and chemical properties, abundance in nature around the world, low cost, and environmental advantages. Also, TiO_2 nanoparticles due to their low cost, easy synthesis and high thermal stability can efficiently be used for this purpose. In this project, we want to make a catalyst by the immobilization of an the ionic liquid on a solid substrate prpared from TiO_2 and Kaolin that can be easily separated from the reactions. The simple preparation of the catalyst, short reaction time, high efficiency, and the ability to recycle the catalyst are the main advantages of this method. Also, this catalyst is effective in increasing the speed of the synthesis of quinoxalines or benzopyrazines, as very important groups of nitrogen-containing compounds.



Keywords: TiO_2, Kaolin , Ionic liquid, Nano-catalyst, Quinoxalines

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Preparation and Characterization of Chitosan/Borax Nanocomposite Based on Copper Iodide: An Efficient Nanocatalyst for Synthesis of Imidazo [1,2-a] Pyridines

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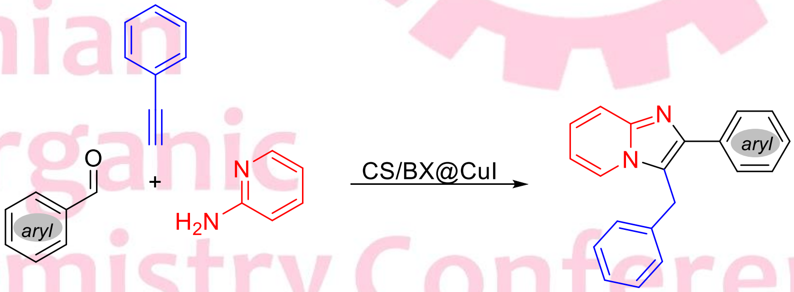
Organic synthesis is one of the most important areas where catalysts are used, especially on a commercial scale, because they allow for a more cost-effective preparation of various organic compounds than would otherwise be possible. In their natural state, organo-catalysts are homogenous, but when modified as nanocatalysts, they exhibit heterogeneous catalytic behavior. Although popular traditional catalysts such as pyridine and piperidine, as well as triethyl amine, have been utilized in organic synthesis transformations for many years, nanoparticles are currently being used for greener and novel organic reactions [1,2]. Chitosan (CS) and its derivatives can be used as efficient, recyclable, and environmentally friendly catalyst supports in various applications [3]. An efficient route was developed for the synthesis of a new polymer, porous cross-linked borax (BX), as an organic support for the immobilization of CuI nanoparticles (CS/BX@CuI). The resulting catalyst works as a recyclable heterogeneous catalyst for the synthesis of imidazo[1,2-a] pyridines from the reaction of 2-aminopyridine, aldehydes, and phenylacetylene. The method possesses significant advantages, including easy purification, functional group tolerance, recyclability of the catalyst, and synthesis of new derivatives in high to excellent yields and short reaction times.



Keywords: Chitosan, Copper Ioddide, Multicomponent Reaction, and nanocatalyst.

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Oxidative desulfurization of model diesel using natural kaolin clay modified with MoO_3/Ni/Fe

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This work focuses on the optimization of the experimental factors affecting oxidative desulfurization process. To achieve that, kaolin was modified using acid treatment. The encaging of metal oxide was performed by impregnation method to improve catalytic activity. Dibenzothiophene (DBT) was chosen as the model substrate and the effect of several parameters such as temperature, catalyst amount, sulfur contamination concentration, and reaction time in the removal process was studied using design experiment. In addition, the effect of interaction of parameters was investigated. The obtained results showed that the prepared catalyst has unique characteristics such as: cheapness, easy access, stability, ability to recover, easy separation. Catalyst shows excellent efficiency in the removal of DBT. This catalyst is recoverable and the catalytic activity remained after 6 run.

Keywords: Desulfurization, kaolin, H_2O_2, Reusability

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Removal of Abamectine from wastewater by Fe-kaolin modified

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The aim of this paper is to evaluate the effectiveness of photocatalytic treatment modified kaolin with $FeCl_2$ as fenton reagent in the degradation of abamectin pesticide**.** The results reveal that the photocatalyst performance depends on catalyst loading, pH effect, hydrogen peroxide amount, UV irradiation, abamectin concentration, and reaction time. However, removal of abamectin is studied in the soil sample. COD and BOD5 experiments were used to measure the mineralization of abamectin and the results shows 80% and 2.02 for COD and BOD5, respectively. Catalyst is recovarable and remained catalytic activity after 5 runs. It was found that the photodegradation kinetics follows pseudo-first-order kinetics. In addition, the activation energy Ea = 1512.1 $KJ.mol^{-1}$ was achieved based on the Arrhenius equation.

Keywords: Modified Kaolin, Photodegradation, Abamectin, BOD5.

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Synthesis and investigation of antibacterial behavior of Zn $_{1-x}$Cu$_x$O(Ag) hybrid nanocomposite

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According to the development of human life, control of the harmful effects of microorganisms is unavoidable. In the last decade, the development of nanotechnology has created opportunities to discover the antimicrobial effects of nanoparticles. In recent years, too much use of antibiotics causes many problems including poisonous effects and creating resistant types. Therefore, nanoparticle metal oxides have attracted deal attention. In this present work, the preparation of Zn$_{1-x}$Cu$_x$O hybrid nanocomposites Ag-doped has been reported. Polyethylene glycol was used as a stabilizer of nanoparticles to control the morphology and size of nanomaterials. FTIR, EDX, XRD, and SEM techniques investigate their structural, superficial, and morphological properties. The antibacterial behaviour of prepared nanoparticles was investigated against Gram-negative, Gram-positive Bacteria, and fungus showed excellent antibacterial activity. However, they were generally more sensitive to hybrid nanomaterials towards ZnO and CuO nanoparticles.

Keywords: Ag-doping, Polyethylene glycol, Co-precipitation, Antimicrobial agent, Hybrid nanocomposite.

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Evaluation of inhibitory potential of phosphoramide compound OP[NH-^{2}Py(4-CH$_3$)]$_3$ against acetylcholinesterase and urease enzymes by using molecular docking method

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Phosphoramide compounds with the main skeleton O═P─N have received much attention in various medical fields such as their application as acetylcholinesterase and urease inhibitors [1,2]. Therefore, in the present work, a compound of the phosphoramide family with the formula OP[NH-^{2}Py(4-CH$_3$)]$_3$ (tris(4-methylpyridin-2-yl)phosphoric triamide) was selected and its inhibitory effect against acetylcholinesterase (1EEA) and urease (4GY7) enzymes is investigated by using the molecular docking method. The results show that this compound with the binding energy of –7.4 kcal/mol can be suggested as a suitable candidate to inhibit acetylcholinesterase enzyme. Moreover, the appropriate inhibitory effect of this compound on urease enzyme is confirmed by the binding energy of –6.2 kcal/mol.

Keywords: Phosphoramide, Acetylcholinesterase, Urease, Molecular docking

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Nanomagnetic Schiff base complex of copper(II): Synthesis, characterizations, and its catalytic application in synthesis of 5-substituted-۱H-tetrazole derivatives

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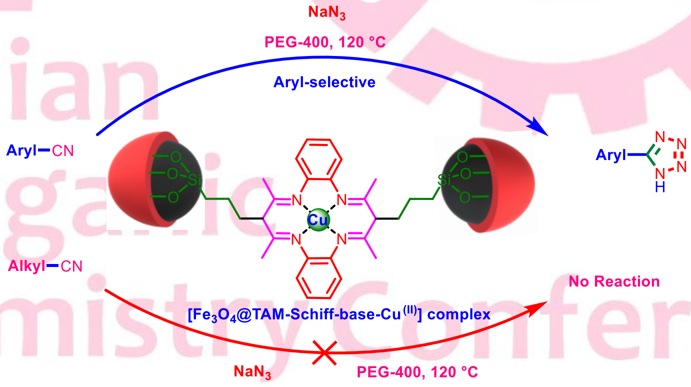
Homogeneous catalysts, which have been widely utilized to catalyze chemical processes, have low recoverability, reusability, and stability [1]. To circumvent these constraints, heterogeneous catalysts that are more efficient and environmentally benign are being investigated [2-3]. Several investigations have been carried out in which supported precious metals, such as palladium, gold and silver, were utilized as catalysts for the click functionalization of aryl nitriles to their corresponding 5-substituted-1H-tetrazoles (RCN_4H). Generally, the immobilization of transition metals on high-surface-area materials, such as nanomaterials, has been documented [4]. Herein, Fe_3O_4 is used as a support material for the ACAC functionalities. Afterwards, the corresponding Cu(II) Schiff base complex was synthesized using the template approach and, then, it was applied as a promoter to assist the sustainable synthesis of 5-substituted-1H-tetrazole derivatives in PEG-400 as a greener alternative for the traditional solvents (Scheme 1).

Keywords: Magnetic Nanoparticles, 5-substituted-1H-tetrazoles Immobilized Copper Complex.



Scheme 1. Synthesis of 5-substituted-1H-tetrazoles

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Synthesis and characterization of new nano organic-inorganic hybrid film $(TBA)_4PW_{11}Fe@TiO_2@PVA$ for oxidative desulphurization of gasoline

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Oil pollution is one of the causes of air pollution, which will have harmful effects on human health. Also, in addition to the presence of sulfur compounds, especially mercaptans, in oil cuts, it causes environmental pollution, but it also causes corrosion in transmission lines and storage tanks. Therefore, it is necessary to adopt appropriate methods to remove the amount of sulfur and mercaptans in oil cuttings up to international standards [1-4]. In this work, an efficient oxidative desulfurization (ODS) process of real gasoline was introduced using $(TBA)_4PW_{11}Fe@TiO_2@PVA$ as catalyst. The catalyst was successfully prepared by saturated and substituted Kegini structure such as $(TBA)_4PW_{11}Fe$) and stabilized on titanium dioxide (TiO_2) and polyvinyl alcohol (PVA), by sol-gel method. The composite was characterized using various analytical techniques including FT-IR, UV–vis, XRD, and SEM. The effects of various parameters such as: amount of catalyst, type of catalyst, type of oxidizer, temperature and time in desulfurization were investigated. The synthesized nanocomposites showed the ability to desulfurize real gasoline with high efficiency. The results showed that the desulfurization process with synthesized polyoxometalates has advantages such as low cost, simplicity and environmental friendliness.

Keywords: Oxidative desulfurization, Polyoxometalate, Gasoline, Catalyst

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Synthesis of chiral (*R*)- and (*S*)-Betti bases and investigation the copper complexes of them in asymmetric allylic oxidation of olefins

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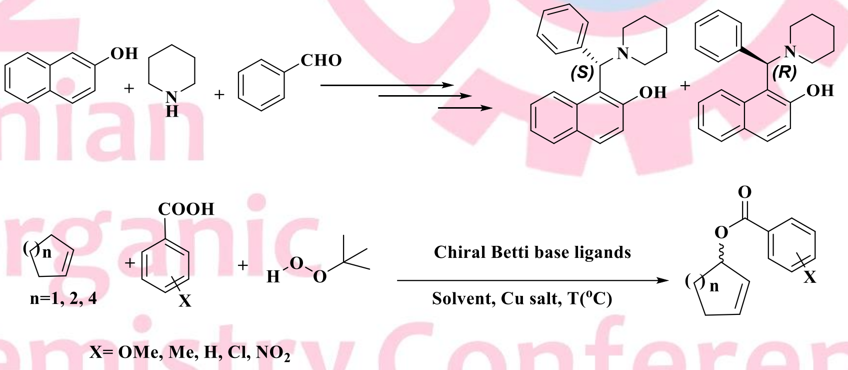
Betti bases are pharmaceutically and synthetically important scaffolds that are readily synthesized through a Mannich-type three-component condensation, known as the Betti reaction, from β-naphthol, aldehyde, and 1° or 2° amine [1]. The most important application of chiral betti bases is their application in asymmetric synthesis, either as chiral ligands or chiral auxiliaries [2]. The Kharasch-Sosnovsky reaction, which involves the copper-catalyzed allylic oxidation of olefins with peresters, is a highly effective method for performing direct C-H bond functionalization at the allylic position of olefins. The asymmetric Kharasch–Sosnovsky reaction of cyclic olefins has been developed with high enantioselectivities [1, 3]. Racemic aminonaphthol 1-(α-N-piperidylbenzyl)-2-naphthol is obtained from simple condensation of benzaldehyde, 2-naphthol and piperidine in ethanol under refluxing conditions. The racemic aminonaphthol has been resolved by diastereomeric recrystallization method using *R*-(+)-1,1′-bi-2-naphthol and boric acid. Subsequently, the copper complexes of these chiral ligands were investigated for asymmetric allylic C-H bond oxidation of olefins, resulting in high yields of chiral allylic esters with moderate enantioselectivity (Scheme 1).



Scheme 1: Asymmetric allylic oxidation of olefins in the presence of chiral betti base ligands

Keyword: Chiral Betti base, *R*-(+)-1,1′-bi-2-naphthol, Diastereomeric recrystallization, Chiral allylic ester

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Electrochemical Water Oxidation Catalyst: Iron/Nickel/Zinc mixed oxide

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Switching from fossil fuels to renewable energies is an inevitable task that should be performed in the near future to provide clean and sustainable energies for human beings. Water splitting toward hydrogen production is a promising approach to store such energies. In this regard, there are some bottlenecks for water splitting systems. Among different solutions, electrocatalytic water oxidation process is considered to be a breakthrough in water-splitting technology. Some research groups previously reported that Ni/Fe (oxy)hydroxides have the lowest overpotential toward water oxidation under the alkaline conditions. The purpose of this study is to describe a new procedure to synthesize an efficient Fe/Ni/Zn-based water-oxidizing catalyst by the thermal decomposition of a trimetallic organometallic compound. The catalyst were studied using scanning electron microscopy, transmission electron microscopy, electrochemical methods, X-ray diffraction, X-ray absorption spectroscopy, and X-ray photoelectron spectroscopy. In addition to Ni and Fe as important ions for water oxidation, the present organometallic compound includes Zn ion as an amphoteric ion which can be removed in the presence of KOH solution to obtain more active sites on the surface of the catalyst and thus a self-improvement is observed during reaction. On the basis of the obtained results, a structure similar to (Ni, Zn)Fe_2O_4 is proposed. Long-time amperometry also indicated an increase in the current density. Continued CVs showed that the water-oxidizing activity of the compound increased during the cyclic voltammetry process. Since Zn ions are amphoteric, they can be soluble in KOH solution and results in a self-improvement for the catalyst. Removing the Zn ions from the NiFeZnOx structure may be a promising method to increase the catalytic activity of the present oxide. Introducing a new procedure to synthesize an efficient Fe/Ni/Zn-based water-oxidizing catalyst by the thermal decomposition of a trimetallic organometallic compound. The catalyst showed a good long-term stability and performance. The composition of the compound was characterized by some common methods and found to be an efficient wateroxidizing catalyst.

Keywords: Water Splitting, Iron-nickel based catalyst, Nanostructure.

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Simultaneous dehydrogenation and allylic oxidation of cycloalkane in the presence of chiral heterogeneous oxazoline-based catalysts for the synthesis of chiral allylic esters

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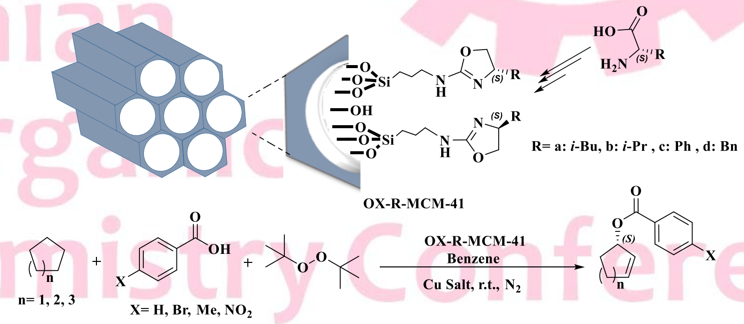
Dehydrogenation of alkanes and allylic oxidation of alkenes are both known reactions separately, but the combination of them in a single reaction is rare [1]. There is also no report about the use of chiral catalysts in this type of reaction in order to the synthesis of chiral allylic esters. There are many ways to access enantioenriched compounds which one of them is using chiral catalysts. Using heterogeneous chiral catalysts has drawn a lot of attention because of some advantages such as easy separation and reuse as well as the possibility of giving a product with high enantioselectivity [2]. Immobilization of an efficient chiral ligand on an inorganic substrate such as MCM-41 is a way to access these catalysts. Chiral oxazoline-based ligands are considered as selective and efficient catalysts in recent years [2, 3]. In this study, first, MCM-41 mesoporous silica was prepared and then functionalized with 3-chloropropyl trimethoxysilane. Next, the chiral amino oxazoline ligands, synthesized from chiral amino alcohols and cyanogen bromide, were immobilized on it. In continue and for the first time, the copper complexes of synthesized heterogeneous oxazoline ligands were used in simultaneous dehydrogenation reaction and allylic oxidation of cycloalkanes in the presence of *benzoic acid derivatives* and *di-tert-butyl peroxide* (DTBP) (Scheme 1). The resulting chiral allylic esters, were obtained in high yields and good to excellent enantioselectivities.



Scheme 1: Synthesis of chiral allylic esters from cycloalkane using chiral heterogeneous oxazoline-based catalysts

Keywords: Chiral heterogeneous oxazoline-based catalysts, Dehydrogenation, Allylic oxidation, Chiral allylic ester.

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Preparation and application of alginate-graphene oxide magnetic beads to remove Zn^{2+} cation in aqueous solutions

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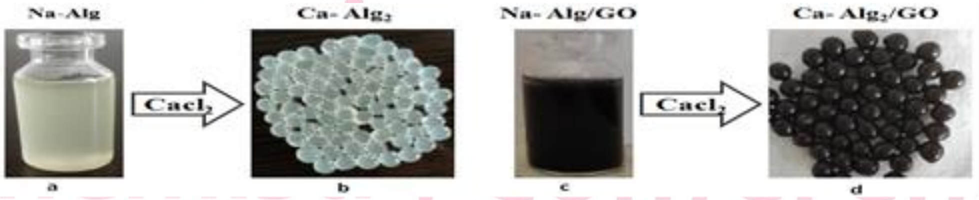
In this study, alginate has been used as a magnetic particle of graphene oxide absorbents to remove Zn^{2+} ions from aqueous solutions. The results demonstrated the following: At pH 6 in 180 min, zinc removal effectiveness was found to be optimal. [1]. The effectiveness of the removal process was also enhanced by increasing the initial concentration and adding more adsorbents. The Langmuir adsorption isotherm The model of zinc removal has been more closely matched to the test results. Conversely, the adsorption kinetics of zinc were in accordance with a model called Pseudonquadratic. Thermodynamic studies showed that the removal of zinc on the alginate-graphene oxide magnetic composite nanofibers is endothermic and the adsorption rate increases with increasing ambient temperature [2]. To identify the appearance and properties of absorbent nanocomposites, an analysis was performed on XDR, TEM, FESEM and VSM with a view to confirming the synthesis steps. TEM and FESEM analysis showed that the mGO/Alg Beads nanocomposite was a porous nanoabsorbent and a magnetite nanoparticle with an average diameter of 33.69 nm could be easily seen on the surface of the nanocomposite. Results from desorption tests show that, at the end of 5 absorption and desorption cycles, 90% of nanomaterials are able to be effectively used. Finally, these nanocomposites are very promising because of being easy, fast, healthy, cost-effective and highly efficient separation of pollutants[3].

Keywords: Magnetic beads, Alginate, Graphene oxide, Zinc, Removal, Aqueous solution



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Solid-liquid equilibrium measurements on aqueous ternary systems composed of amino acids and tetraalkylammonium bromides

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The solution behavior of amino acid + electrolyte aqueous systems provides valuable information about the complex behavior of proteins in biological systems [1]. Further, ternary solutions of {water + amino acid + solute 2} could undergo the soluting-out phenomenon as aqueous biphasic systems formation [2] or precipitation [3]. In this respect, the liquid-liquid and solid-liquid equilibria (LLE and SLE) studies are essential for designing, optimizing, and scaling up separation processes handling with amino acid-based systems. In this work, to obtain thermodynamic information about the soluting effect in aqueous ternary systems of amino acid + tetraalkylammonium bromide (TAAB) salt, solid-liquid equilibrium (SLE) behavior was studied by measuring the solubility of tetramethylammonium bromide (TMAB) and tetrabutylammonium bromide (TBAB) in aqueous solutions of S(-)-proline, as well as the solubility of S(+)-serine and S(-)-proline in aqueous solutions of TMAB. The SLE results revealed that the water-solubilities of TMAB and TBAB decrease in the presence of S(-)-proline, while the water-solubilities of the amino acids are not meaningfully affected by the addition of TMAB. The soluting-out coefficient obtained by correlating the solubility data with the Setschenow equation is positive and whose value for TBAB is more than TMAB. From the gathered results, the investigated amino acids (S(+)-serine and S(-)-proline) act as the soluting-out agent in amino acid + TAAB aqueous solutions, and the strength of the soluting-out effect increases with increasing the difference between the hydrophobic character of the solutes.

Keywords: Solid-liquid equilibrium, Soluting-out effect, Amino acids, Tetraalkylammonium salt

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Soluting-out effect of amino acids on aqueous solutions of tetraalkylammonium salts revealed by isopiestic measurements

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Tetraalkylammonium (TAA) salts are used in many environmental and biological processes because of possessing both ionic and hydrophobic properties [1]. The possibility of evaluating the effects of TAA salt's alkyl chain length and anion type on the interactions governing the solution behavior causes TAA salts to be a good choice for investigating the soluting effects occurring in aqueous solutions containing another solute [2,3]. In order to expand the knowledge of the soluting-out/in phenomena occurring in aqueous solutions, in this work, several ternary systems of {water + amino acid + quaternary ammonium salt} were subjected to isopiestic (vapor-liquid equilibrium (VLE)) measurements at 298.1 K. The amino acids used are glycine, DL-alanine, S(+)-serine, and S(-)-proline and the tetraalkylammonium salts are tetramethylammonium bromide (TMAB), tetrapropylammonium bromide (TPAB), tetra-n-butylammonium bromide (TBAB), tetra-n-butylammonium chloride (TBAC), and tetra-n-butylammonium hydrogen sulfate (TBAH). The deviations of water iso-activity curves from the semi-ideal behavior have been taken as a criterion to determine the soluting-out/in effect occurring in the investigated systems. The VLE results generally showed negative deviations from the semi-ideality, indicating that there are no favorable interactions between amino acids and quaternary ammonium salts in aqueous media, and aqueous solutions composed of these solutes undergo the soluting-out phenomenon (except for DL-alanine/S(-)-proline-TBAH aqueous ternary systems that show small positive deviation from the semi-ideality). For a given amino acid, the magnitude of negative deviations and the strength of the soluting-out effect increase with increasing the cation alkyl chain length (TBAB > TPAB > TMAB) and the hydrophobic character of the anion of the quaternary ammonium salts (TBAB > TBAC > TBAH). Amino acids act as the soluting-ou agent, and their soluting-out ability follows the order S(+)-serine > glycine > DL-alanine > S(-)-proline.

Keywords: Amino Acids, Tetraalkylammonium Salts, Isopiestic, Soluting-Out

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Enhanced decolorization of organic dyes using $CeCoO_3$/PbS heterojunction as an excelent photocatalyst

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Recently, there is a significant interest among researchers in the case of oxide perovskites characterized by the general formula ABO_3 [1]. Among them, $CeCoO_3$, known as cerium cobalt oxide perovskite, has shown great potential as a nanophotocatalyst in the conversion of organic dyes [2]. Moreover, PbS, or lead sulfide, has emerged as a high efficient semiconductor in light absorption due to its favorable band gap energy (0.41eV) [3,4]. The $CeCoO_3$/PbS photocatalyst was synthesized via the hydrothermal method and characterized by FT-IR, FE-SEM, EDS, PL, and DRS analyses. The obtained results revealed successful deposition of PbS on the surface of the $CeCoO_3$ perovskite, as demonstrated by the FE-SEM images. The influence of catalyst dosage, temperature, pH, and electron acceptor toward the decolorization of methylene blue (MB) under UV light irradiation was investigated. In the presence of $CeCoO_3$/PbS photocatalyst the conversion percentage achieved to 98% within 10 min. This enhanced photoactivity of $CeCoO_3$/PbS can be attributed to its lower charge recombination rate in comparison to the pure perovskite.

Keywords: Conversion of Dyes,Perovskite,Photocatalyst

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Photocatalytic heterojunction of $CeCoO_3$/CdS for conversion of organic dyes

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Recently, oxide perovskites with the general formula ABO3 have attracted the attention of many scientists [1]. Cerium cobalt oxide perovskite, represented by CeCoO3, exhibits promising capabilities as a nanophotocatalyst in the conversion of organic dyes [1]. Additionally, Cobalt(II) sulfide (CdS), a semiconductor, shows high performance in light absorption due to its suitable band gap energy [2,3]. The CeCoO3/CdS photocatalysis was synthesized using the hydrothermal method. The prepared heterojunction structure was characterized using various techniques and applied to the decolorization of methylene blue under visible light irradiation. FT-IR, FE-SEM, EDS, PL, and DRS analyses were employed to identify the properties of CeCoO3/CdS photocatalysis. The FE-SEM images demonstrated the successful deposition of CdS on the surface of CeCoO3 perovskite. The effect of catalyst amount, temperature, pH, and electron acceptor was investigated. In the presence of the CeCoO3/CdS photocatalyst, the decolorization rate of methylene blue reached 99% within 15 minutes, whereas no significant conversion of methylene blue was observed with the perovskite alone. The higher photoactivity of CeCoO3/CdS is attributed to its lower charge recombination compared to pure perovskite. Additionally, the photocatalytic mechanism and recycling tests of CeCoO3/CdS are discussed in detail.

Keywords: Conversion of Dyes,Perovskite,Photocatalyst

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Efficient photoactivity of Ag/$CeCoO_3$ toward the conversion of MB dye under the irradiation of light source

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Photocatalysts are potent substances that play a vital role in the conversion of organic dyes [1]. Through the process of photocatalysis, photocatalysts harness light energy to initiate chemical reactions that break down harmful organic substances into harmless byproducts. These catalysts find wide-ranging applications, including water and air purification [2], as they offer an efficient and environmental friendly solution for eliminating organic pollutants [3].With their ability to harness the power of light, photocatalysts have emerged as a promising tool in the pursuit of cleaner and safer environments [4]. Here in, silver nanoparticles (AgNPs) were doped on the surface of $CeCoO_3$ perovskite. Several measurement techniques including UV-Visible spectroscopy, XRD, TEM, FE-SEM, EDS, and FT-IR were utilized to characterize the catalyst.The synthesized photocatalyst was employed for the conversion of Methylene Blue (MB) dye under UV light. The results demonstrated complete conversion of the MB dye within 25 min.

Keywords: Conversion , Silver nanoparticles,Photocatalyst, $CeCoO_3$

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Supported Diamond-like carbon films on anodized titanium oxide as high-efficient electrocatalyst for electrochemical Ozone production

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Titania nanotubes are of interest in various fields such as electrocatalysis, sensing, and photoelectrolysis due to their high surface area ratio due to their high volume and size-dependent properties. TiO2 nanotube arrays were produced by various methods including titanium anodization in fluoride-based baths [1]. Recently, diamond-like carbon (DLC) films have attracted much attention as electrocatalysts. One of the new strategies for the synthesis of diamond-like carbon films (DLC) is liquid phase synthesis by electrochemical methods [2-3]. Ozone (O3) as one of the environmentally friendly oxidants, has found wide applications in disinfection and sterilization. Unfortunately, ozone cannot be produced during conventional water electrolysis because water is preferentially oxidized to O2 rather than O3. [4-5]. The efficiency of ozone generation through electrochemical ozone generation (EOP) is high (50%). Among all types of carbon-based materials, DLCs show the highest additional potential for OER due to tunable diamond and graphite, which is controlled by chemical deposition parameters during deposition [4-5]. A DLC film was prepared on the anodized titanium oxide surface by electrodeposition method in acetonitrile solution. The prepared electrodes were characterized by scanning electron microscopy (SEM) and X-ray diffraction (XRD), and the electrochemical performance of the electrodes was evaluated for ozone calculations by electrochemical methods.

Keywords: diamond-like carbon ,titania nanotubes ,ozone

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Synthesis, crystal structure, DNA/BSA interaction, Molecular Docking, and catecholase activity of a new phenoxo-bridged dicopper Schiff base complex

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There have been enormous efforts towards synthesizing new compounds for cancer treatment. Since the interaction with DNA determines drug activity, designing new complexes with different DNA-binding modes is essential. The Cu(II) complexes could find better applications as pharmacological agents among various metals. Besides, a drug's distribution, metabolism, and efficacy depend on its effective interaction with proteins. BSA is the most practical protein in biochemical studies due to its diverse physiological functions [1]. Also, mimicking metalloenzymes' active sites is crucial in coordination chemistry studies. Considering the dicopper(II) moiety of catecholase structure, many dicopper(II) complexes have been used for this purpose [2]. In this study, the DNA/BSA interaction and catecholase activity of a new binuclear water-soluble Cu(II) complex $[Cu^{II}_2L(\mu_{1,1}\text{-}NO_3)(\mu\text{-}OH)(NO_3)(H_2O)]$, where L=[2,6-bis{N-(2-pyridylethyl)formidoyl}-4-methylphenol] involving μ-phenoxo N_2O_4 Schiff base ligand, have been studied. The complex interaction with FS-DNA/BSA was investigated by absorption and fluorescence titration, cyclic voltammetry, circular dichroism, and viscosity measurements. The complex is characterized by CHN, UV-vis, and FT-IR spectroscopy. X-ray analysis revealed the dinuclear Cu(II) ions in a six-coordinated distorted environment. Docking simulation analysis and competitive binding experiments with ethidium bromide showed the complex interaction with DNA mainly via intercalation mode with the K_b value of $2.78 \times 10^4\ M^{-1}$. Furthermore, this binuclear system was employed to check the possibility of catecholase activity in acetonitrile and DMF, showing high activity in catalyzing the oxidation of 3,5-DTBC to 3,5-DTBQ in acetonitrile.

Keywords: Schiff base, Cu(II) complex; DNA/BSA interaction; Molecular docking; Catecholase activity.

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Some new cadmium halide Schiff base complexes: preparation, thermal stability and antibacterial/antifungal bioassay

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Metal Schiff base ligands introduce potential active sites for preparation of biochemical active compounds against various pathogen microorganisms [1]. Moreover, metal complexes of Schiff base ligands can present a variet of applications in biological, analytical, clinical and industrial fields [2]. Regarding the antimicrobial activity and highly qualified physicochemical, stereochemical, electrochemical, structural and catalytic properties of Schiff base metal complexes, these compounds have been considered to be of interest and this is attributed to their applications as pharmacological constituents [3]. Necessary biological reactions in life processes mostly involve transition metals; these metals usually coordinate with O- or N- terminals from protein in several modes and play a dominant role in the conformation and function of biological macromolecules [4]. Recently many papers have been reported on the cadmium Schiff base complexes and their properties such as antimicrobial and antioxidant activities. These complexes have shown powerful activity against bacteria and fungi[5]. In this work, a new bidentate Schiff base ligand entitle as Bis(3-(2-methoxyphenyl-2-propenaldehydene)-1,2- diaminobenzene and its four coordinated cadmium halide complexes(inwhich halide is chloride, bromide and iodide) have been synthesized and investigated by analytical and spectral data(FT/IR, UV-Visible and ^{1}H and ^{13}C NMR) and thermal analyses. Moreover antibacterial and antifungal properties of the ligand and its complexes were evaluated by well diffusion method.

Keywords: Cadmium complex, Schiff base, Antimicrobial.

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Investigation of the performance of carbon quantum dots as pseudo-enzymatic catalase in inhibiting hydrogen peroxide in the body.

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Rerecently,The enzyme catalase is the main regulator of hydrogen peroxide metabolism. Hydrogen peroxide in high concentrations is a toxic agent, while in low concentrations it performs some physiological processes such as signalling in cell proliferation, apoptosis, carbohydrate metabolism and platelet activationI [1]. Synthetic enzymes with high stability and performance have attracted the attention of many scientists [2]. In this project, we prepared carbon quantum dots (CQDs) by the hydrothermal method and their activity as catalase enzyme in the decomposition of hydrogen peroxide into water and oxygen was investigated. The activity of the CQDs was measured by UV-visible spectroscopy. The prepared Catalase were identified using EDS, FT-IR, PL, TGA, CHN and UV-vis spectroscopy.As a result, the CQDs could be used as synthetic catalase enzyme to inhibit the action of hydrogen peroxide in body cells.

Keywords: Carbon Quantum Dots, Catalase Pseudo-Enzyme, Hydrogen Peroxide,

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Ce/SiQDs as pseudo-enzymatic catalase to inhibit H_2O_2 inside the cells of the body

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Catalases, in biological systems, serve as protectors against oxidative damages resulting from hydrogen peroxide [1]. This enzyme transforms millions of hydrogen peroxide molecules into water and oxygen every second [2]. It exhibits the highest concentration in the liver, kidneys, pancreas, and red blood cells [3]. The active site of this enzyme comprises an iron porphyrin.In this study, we utilized the hydrothermal method to synthesize Ce/SiQDs. We investigated the catalytic activity of these Ce/SiQDs in decomposing hydrogen peroxide into water and oxygen. The activity of the Ce/SiQDs was evaluated using UV-visible spectroscopy. Additionally, we employed FE-SEM, DRS, EDS, FT-IR, PL, TGA, CHN, and UV-vis spectroscopy for the identification of the prepared catalase. The results demonstrated that Ce/SiQDs possess the potential to act as synthetic catalase enzymes capable of inhibiting the action of hydrogen peroxide in body cells.

Keywords: Quantum Dots, Catalase Pseudo-Enzyme, Hydrogen Peroxide, Silicon quantum dot

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The performance of , CQD/Sb_2Wo_6 catalase-like enzyme in inhibiting hydrogen peroxide

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Nanoparticles' catalytic activity and intrinsic ability in generating or scavenging reactive oxygen species in general can be used to show the catalytic activity of natural enzymes. Many nanoparticles with enzyme-like activities have been found, potentially capable of being applied for commercial applications, such as in biosensors, pharmaceutical processes, and the food industry [1] . Compared with natural catalase or artificial CAT enzymes, CAT-like nanozymes have unique properties of low cost, size-dependent properties, high catalytic activity, stability, and easy surface modification[2] . One of the key oxidative threats to oxygen-tolerant organisms is hydrogen peroxide (H_2O_2) [3] . Virtually all organisms employ catalases and peroxidases to keep the steady-state level of endogenous H_2O_2 below the threshold of toxicity. Herein, , CQD/Sb_2Wo_6 were used as a catalase, catalyzing the decomposition of hydrogen peroxide to oxygen. , CQD/Sb_2Wo_6 had better stability than natural catalase when they were exposed to solutions with different pH values and temperatures. The activity of the , CQD/Sb_2Wo_6 was measured by UV-visible spectroscopy. The prepared Catalase were identified using FE-SEM, DRS, EDS, FT-IR, and PL.

Keywords: Intrinsic, Hydrogen Peroxide, Enzyme-like, Catalase

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Green Synthesis of **Zinc Oxide with** Polyvinyl alcohol by **lavandulifolia** Extract and development of hydrogen storage capacity

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The United Nations General Assembly, in its declaration of the right to development (1986), declared energy in different forms an essential need to achieve the specified targets [1]. Today, most energy needs are met through non-renewable sources [2]. The use of non-renewable resources in addition to the environmental issues due to long-term use has reached a saturation level [3]. Therefore, renewable sources for energy production at different levels are in demand. Among the renewable sources, hydrogen is one of the most attractive [4]. At the same time, this energy carrier needs efficient and secure storage to have a bright future [5].Polyvinyl alcohol (PVA) with high active sites is used as natural layered mineral supports. ZnO as a conductive additive was decorated on a PVA support to design an effective and environmentally friendly active material. Herein, an eco-friendly PVA/ZnO nanocomposite is fabricated via a green method to equip developed hydrogen storage sites and to allow for quick charge transportation for hydrogen storage utilization. The hydrogen storage capacity of PVA/ZnO was 300 mAhg^{-1} at a current density of 1 mA after 5 cycles. It was also conceivable to increase the hydrogen sorption ability through ZnO in the nanocomposite.

Keywords: ZnO,Hydrogen storage, PVA/ZnO

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Green synthesis of zinc oxide with hydrocharby lavandulifolia extract and development of hydrogen storage capacity

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In recent years, the environment has become seriously polluted as a result of the growth of industries. Polluted water sources have become a critical concern as a result of human activities, and different industrial operations have discharged organic contaminants that can cause carcinogenicity and toxicity in aquatic ecosystems [1]. In light of this, water purification has been regarded as an effective method of reducing pollution and water shortages. A number of traditional water treatments, including adsorption [2], ion exchange [3], biological processes [2], and membrane [4], have been developed in recent years.The goal of this study is to produce environmentally friendly nanomaterials that have a high hydrogen storage capacity(1). The researchers in this study used inexpensive material to produce hyrochar and a green solution synthesis combustion method to produce ZnO nanoparticles and nanocomposite using a Stachys lavandulifolia extract as the source material. Metal oxides such as ZnO are used to increase hydrogen storage capacity. Hydrochar and Hydrochar/ZnO nanocomposites have been confirmed via XRD (X-ray diffraction), SEM(scanning electron microscopy, FT-IR (fourier transform infrared. In terms of discharge capacity, ZnO, Hydrochar/ZnO display respective capacities of 220, 500 mAh/g after 4 cycles, respectively. .

Keywords:Hydrochar/ZnO, nsnocomposite, Hydrogen storage

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Reduction of aldehydes and ketones using $NaBH_4$ catalyzed by DABCO-based ionic liquid

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Ionic liquids (ILs) are a class of non-molecular compounds that are composed solely of ions. Researches on ionic liquids have moved toward the consciously selection and design of these materials due to their increased rate, property, and performance. The design of ionic liquids focuses on the development of new cations and anions to create the essential specific physical properties for each application.[1]Reduction is one of the most momentous and essential chemical transformations in organic synthesis and industrial chemistry.Sodium borohydride as a hydride transferring agents and versatile reagent can be mention, which is used for creating easy and favorable ways for the reduction of many organic functional groups.Reduction of aldehydes and ketones is very important due to incomparable role of alcohols in the pharmaceutical and food industries.[2,3]In this project we wish to introduce a new DABCO-based ionic liquid for the promotion of the reduction of ketones and aldehydes, which can be easily separated from the reaction. Easy work up, simple prodecure of the preparation of the catalyst, high yields, short reaction times and recoverability of the catalyst are the main advantages of this method.

***Keywords*:**DABCO, Ionic liquids, DABCO-based ionic liquid, Reduction, Sodium borohydride

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Some new zinc pseudohalidebis-imine complexes: Synthesis, characterization, thermokinetic decomposition study and antimicrobial properties

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Nowadays synthesis of new ligands suitable and then preparation of their complexes are in the frontier in pure and applied inorganic chemistry. Accordingly, the iminic ligands are important, which can be coordinated to metal ions via thier iminic nitrogen atoms to form the related imine complexes. These complexes are applicable in catalytic, industrial and medicinal(as antibacterial, anti fungal and antioxidant agents) fields in recent years[1-4].Imine complexes have also cytotoxicity effects aginst varios cancerious cell lines. Recently also these complexes are appliedas precursor to prepare nano-structured metal oxides. Among various metal oxides that were studied, zinc oxide nanoparticlesare of great interestdue to various applications in optic and biological properties.

In this work, a new bidentate bis-imine ligand obtained from 2-methoxyphenyl-2-propenal and phenylenediamineand its four coordinated Zn(II) pseudohalidecomplexes(inwhich pseudohalide is SCN^-, N_3^- and NO_3^-) have been synthesized and investigated by analytical and spectral data(FT/IR, UV-Visible and ^1H and ^{13}C NMR) and thermal analyses. Moreover antibacterial and antifungal properties of the ligand and its complexes were evaluated by well diffusion method. Finally the zinc complexes were used as precursor for preparation of nanostructured ZnO..

Keywords:Zinc complex, Bis-imine, Antibacterial, Nanostructure.

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Preparation, spectral characterization and thermal study of somebiological active mercury(II) complexes

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Mercury ionis of importance in biological and chemical point of view. This metal ion also forms useful amalgams with many metals, which has various applications in a variety of industrial and medicinal research fields. Because of the diverse applications and the toxic character of mercury compounds, there is a need to develop the cheistry and especilly coordination chemistry of this metal ion.. The toxicity of mercury depends on its occurring forms; organomercurials such as methylmercury are more toxic than elemental mercury and other inorganic mercury compounds. Mercury containing Schiff base ligands are known to form stable complexes with various biological and industrial chemistry.Recently some reports on mercury Schiff base complexes show that these stable compounds can act as antimicrobial and antioxidant matterial [1-5]. In this research, a new bidentate ligand entitled as *N,N'*-Bis-(3-(2methoxyphenyl-2- allylidene)-benzene-1,2-diamine and its Hg(II) complexes were synthesized and identified by analytical and spectral data(FT-IR, UV-Visible and ^{1}H and ^{13}C-NMR). Moreover, thermal analysis of ligand and its complexes were studied in the range of room temperature to 1000 °C with a heating rate of 20 °C min^{-1} and then some thermokinetic data were estimated for all thermal decomposition steps. Moreover antibacterial and antifungal properties of the ligand and its mercury complexes were evaluated *in vitro*by well diffusion method.

Keywords:Mercury(II) complex, Schiff base, Thermal, Antimicrobial.

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Computational Calculations of pK_a Values of Metal Ligands in Proteins

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Metalloenzymes are enzymes that use a metal cation as a cofactor in their active site. They catalyze various reactions, such as hydrolysis, oxidation, and reduction. Some examples of metalloenzymes are hydrogenases, which facilitate the uptake of molecular hydrogen; superoxide dismutase, which inhibits the oxidative damage to cells; nitrogenase, which enables the fixation of atmospheric nitrogen; proteases, which break down peptide bonds; and phosphodiesterases, which cleave phosphate ester bonds [1-4]. Many metalloenzymes are involved in acid-base reactions and have experimentally determined p*K*a values. In this study, we calculate the p*K*a values of 18 acid-base reactions in nine different metalloenzymes with varying metal ligands, metal centers (Zn, Mn, or Fe), protein cofactors, enzyme variants (wild type or mutated), or redox states of the metal centers. We compare our calculated values with the experimental ones. The metalloenzymes we study are alcohol dehydrogenase, superoxide dismutase, Rieske protein, thioredoxin-like ferredoxins, carbonic anhydrase, heme nitric oxide/oxygen binding protein, cytochrome P450, and myoglobin. We use quantum mechanics/molecular mechanics (QM/MM) calculations and the QM-cluster method in a continuum solvent to perform the calculations. We explore different variations of the approach, such as the QM method, the basis set, the size of the QM system, and the inclusion of the environment either implicitly as a continuum dielectric or explicitly as point charges. We also use the QM/MM thermodynamic cycle perturbation (QTCP) method to examine the effect of environmental dynamics on the calculations. Additionally, we use the Big-QM method, which employs a large QM system to do single-point QM/MM calculations on the structure that has been optimized using the original QM/MM technique. This study aims to determine which of the methods we test are the most accurate and whether they can be used for predictive analyses. We have obtained a set of data for p*K*a using various methods, but we have not yet reached a conclusion on which method is the best.

Keywords:Metalloenzyme, pK_a, QM/MM, BigQM, QTCP

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Synthesis and Characterization of Co_2SiO_4as Ceramic Pigment

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There is an increasing research interest of pigments. One of the important of this pigments is nanoparticles of Cobalt(II)silicate (Co_2SiO_4). The Cobalt(II) silicate has olivine structure, pink color and that applied for preparation ceramic pigments, catalysts, electronic devices and biomedical systems [1,2].Various methods have been taken to prepare the Co_2SiO_4 at low temperature, such as the precipitation method, the hydrothermal-reaction methodand sol-gel method [3].Olivine-type Co_2SiO_4 is stable at high temperature and has a high Co content and consists of hexagonal closed-packed oxygen atoms with halfof octahedral sites occupied by Co atoms and one-eighth of tetragonal sites occupied by Si atoms [1].

In this work, nanoparticles of $Co_2SiO_4$was prepared by two methods including the co-precipitation method and the method of mixing metal oxides and were characterized by XRF, XRD, SEM analyses. The results show that particles of Co_2SiO_4 were synthesized by two methods, have particle size about 20-65 nm anda mixture of the rod-shape and spherical structures.Also, the nanoparticles of Co_2SiO_4 have high thermal stability and its can use as a pigment in glazing of ceramic and tile.

Keywords: Co_2SiO_4,ceramic pigments, Olivine structure

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Synthesis and Characterization of praseodymium zircon as Yellow Pigment

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There is an increasing research interest of yellow pigment for coloring ceramics that must show thermal and chemical stability at high temperature [1]. Throughout history various yellow ceramic pigments have been used: yellow of vanadium-zirconia, tin-vanadium yellow, cadmium yellows, lead antimoniate , etc. The praseodymium zircon (Pr-$ZrSiO_4$) yellow ceramic pigment is believed to be a solid solution of Pr^{4+} with the zirconlattice, but studies are poor and scarce [2].

The aim of this work, is the synthesis of Pr-$ZrSiO_4$yellow pigment in the presence of NaF and NaCl by the method of mixing metal oxides and toinvestigate the nature of the pigment. The Pr-$ZrSiO_4$particles are characterized by XRD, SEM and XRF to analyze their structure and morphology. The results show that particles of Pr-$ZrSiO_4$was synthesized, has particle size about 60-1000 nmby olivine-baddeleyite structure.

Keywords: Pr-$ZrSiO_4$,Zircon lattice, Yellow Pigment

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Pereparation and Characterization of(Co-Si-Mg)Al_2O_4Spinel:New Blue pigment

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Oxide spinels comprise a large group of structurally related compounds, many of which are of considerable technological significance. Aluminate spinels are of interest due to their technological applications as catalysts, refractories and pigments. Ceramic pigments are widely used in the ceramics industry as coloring agents in glazes for floor or wall whitewares and for the bulk coloration of polished, unglazed and porcelainized stoneware[1].The synthesis of cobalt-based ceramic pigments must be optimized in order to minimize the production costs and environmental impact of the manufacturing process of thesepigments.

In this work, nanoparticles of (Co-Si-Mg)$Al_2O_4$was prepared by the method of mixing metal oxides and was characterized by XRF, XRD, SEM and thermal analyses. The results show that the (Co-Si-Mg)Al_2O_4 system, has spilnel structure and a blue color with particles sizes about90-680 nm.The color properties and the high thermal stability of this nanostructure suggest that it has the potential to be applied as satisfactory ceramic pigments.

Keywords: Oxide spinels, Ceramic pigments, (Co-Si-Mg)Al_2O_4,Blue color

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Nature of metal-ligand bond in some metal complexes of a number of tetradentate(N_2O_2) asymmetric Schiff baseligands

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Schiff-base ligands and their coordination compounds have attracted the esearchers'attention and taken an important area in chemistry as compounds having azomethine inkage(C═N)[1].This interest is still growing due to their attractive properties, simple synthesis,stability, low toxicity, good biocompatibility [2] and diverse fields of applications inindustry, medicine, analytic and catalysis [3].To the best of our knowledge the nature of bond in metal complexes of salentype ligands have never been studied. Herein, we want to report a theoretical study on the strength and nature of metal–ligand bondin tetradentate(N_2O_2) asymmetric Schiff base ligands (Salpyr). The goemetry of all complexes wereoptimzed at BP86-D3/TZ2P level of theory using ADF program.Then, thenature of bond in the mentioned complexes was studied with an Energy Decomposion Analysis of metal–ligand bond.

Keywords:Theoretical Study, Schiff basecomplexes, Interaction and stabilization energies,Nature of bond

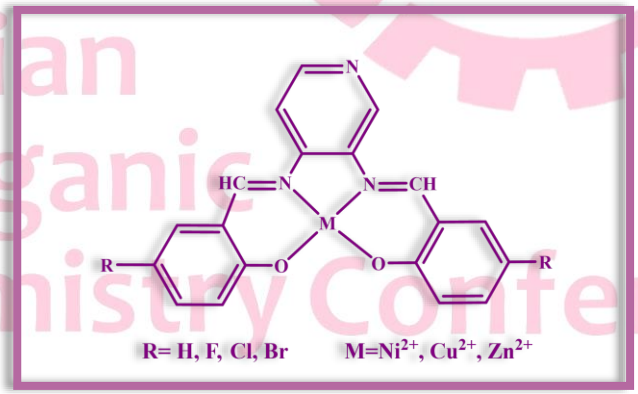

Figure 1.Chemical structure of metal complexes studied here

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DNA interaction studies on the drug sotlol and its Cu(II) complex using viscosity measurements, UV-Vis spectroscopy and molecular docking simulation methods

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Recent years have seen a rejuvenation of interest in studies on the interaction mechanism of deoxyribonucleic acid (DNA) with small molecules, especially in interaction with drugs [1, 2].In this project, the interaction of the drug sotalol (SOT)and its Cu(II) complex (CuSOT) with calf thymus DNA(ct-DNA) was investigated using viscosity measurements, UV-Vis spectroscopy and molecular docking simulation methods. Viscosity measurement studies indicated that the SOT interacts with ct-DNA via a groove mode of binding. The molecular docking simulation visualized that both the SOTand CuSOT arelocated in the minor groove ofthe DNA helix.The binding constant measured from the UV–Vis absorption studies showed that the binding strength of SOT to ct-DNA,compared to the drug cytarabine as a known anticancer agent,is significant [3]. Also, the calculated binding constants (K_b) by AutoDock Vina showed that the affinity of CuSOT for DNA is higher than that of the drug SOT.

Keywords:Sotalol, Copper complex, DNA interaction, Molcular docking.

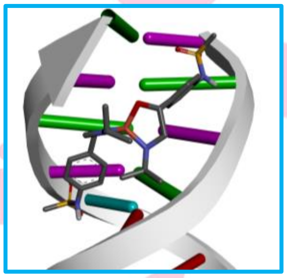

Figure 1. Molecular docking 3D visualization of DNA–CuSOT systemwhich shows the location of CuSOT in DNA (PDB ID: 1BNA).

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Study on the mode and strength of DNA interaction with Thiamine and some of its metal complexes

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DNA binding mechanism of molecules, especially metal complexes, has been studied in order to develop anticancer drugs for several decades. In order to reduce side effects and improve the effectiveness of treatments, researchers are trying to design and synthesize newbiometal complexes [1-3]. In this project, three complexes of the thiamine chloride (ThmCl) with the proposed formula [M(Thm)Cl_3] (M= Zn(II), Cd(II), Co(II)) and also a new salt of thiamine chloride hydrochloride, with the chemical formula of [ThiamineClH][$CuCl_2$], were synthesized and characterized with elemental analysis (CHNS), FT-IR, and UV-Vis spectroscopies in all cases, and also with ^{1}H NMR, except in the case of Co(II) complex. In addition, the structure of the synthesized new thiamine chloride hydrochloride salt was characterized using X-Ray crystallography (Figure1). The comparison of binding constants (K_b) measured from the UV–Vis absorption studies showed that the binding strength of the above compounds to ct-DNA is as follows: ThmCl·HCl >[Zn(Thm)Cl_3] >[Cd(Thm)Cl_3] >[Co(Thm)Cl_3]. The results of viscosity measurements indicated that the thiamine chloride hydrochloride and its complexes bind to ct-DNA via an intercalation binding mode. Moreover, the molecular docking simulation visualized that the thiamine and its complexes bind to DNA via an intercalation binding mode which is in agreement with the results of viscosity measurements studies.

Keywords:DNA interaction, Thiamine, Crystal structure, Intercalation.

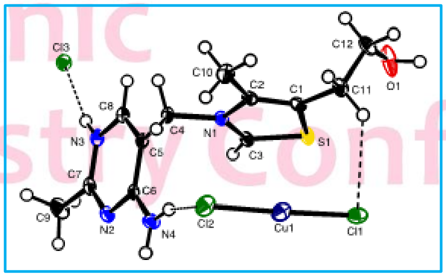

Figure 1. ORTEP diagram of [ThiamineClH][$CuCl_2$]. Ellipsoids are drawn at the 50% probability level.

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A fluorinated cyclometalated Pt(II) complex bearing a phosphine ligand: photophysical and theoretical investigations

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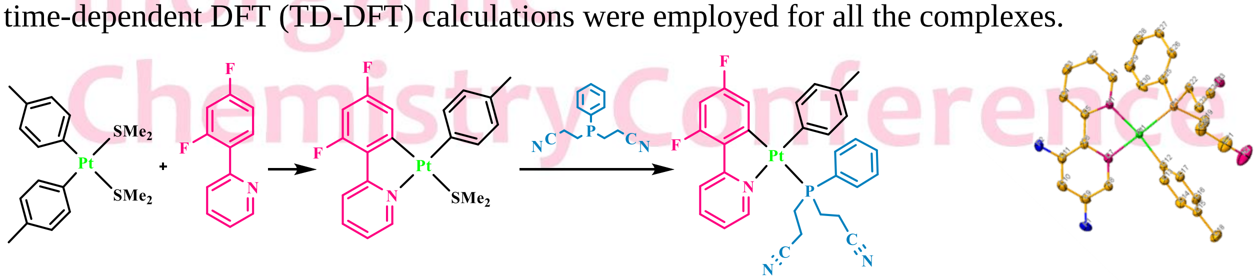
In recent decades, numerous researchers have extensively explored luminescent cyclometalated platinum(II) complexes, and the number of publications in this area of study is growing. Various uses for the luminous cycloplatinated complexes include light-emitting devices, dye-sensitized solar cells, photoswitches, photocatalysts, and chemical or biological sensors[1]. The principal chromophore involved in producing room-temperature phosphorescence is the cyclometalated ligand. In addition, heavy metals like Pt induce high spin-orbit coupling and allow singlet-triplet intersystem crossing. The photophysical characteristics of such complexes are greatly influenced by the auxiliary ligands, in addition to the previously listed parameters. These ligands control the electron density at the metal center and, consequently, the degree of metal to ligand charge transfer (MLCT) in the lowest energy transition [2].

Herein, a heteroleptic cycloplatinated(II) complex [Pt(p-MeC$_6$H$_4$)(dfppy)(PPh(EtCN)$_2$)], dfppy=2-(2,4-difluorophenyl)pyridinate; and PPh(EtCN)$_2$ = bis(2-cyanoethyl)phenylphosphine, was synthesized and characterized. The complex exhibits greenish-blue phosphorescence under UV light at room temperature in the solid state, with mostly well-structured emission bands in the range of 450–490 nm (solid and CH$_2$Cl$_2$ fluid solution states, 298 and 77 K). Their emissions appear as structured bands, which indicates that the emissions mainly originate from the electronic transitions in the ligand with a small contribution of metal to ligand and/or ligand to ligand charge transfers. To rationalize the experimental photophysical data, density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations were employed for all the complexes.



Scheme 1: Synthetic route for the preparation of the Pt(II) complex(left) and its crystal structure (right).

***Keywords*:** Phosphine; Cycloplatinated(II); Photophysics; Theoretical elucidation.

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Green synthesis of Nickel oxide nanoparticles by extract of Nigella sativa.

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Nanomaterials are the materials that have sizes on the order of a billionth of a meter. Since the mechanical, thermal, electrical, optical, electrochemical, catalytic properties of the nanomaterials are different from the bulk materials, nanomaterials can be used in a wide variety of application fields. [1].One of the most innovative methods consists of replacing polluting chemical reagents with living organisms like bacteria, fungi , plants , yeasts and etc, during inorganic and organic synthesis, to reduce the quantity of reagents and also save energy[2].The advantages of using plant extracts during the green synthesis of nanostructures prompted researchers to examine the reduction mechanisms of metal salts, trying to understand the formation mechanisms of nanoparticles in the presence of plant extracts[3].Among various nanoparticles, nickel oxide nanoparticles (NNPs) are important because of their physical, chemical, and biological properties. In the past two decades, significant research has been done on the synthesis of NNPs. Their applications range from energy storage to catalysis to antifungal and antibacterial activity[4].In this research, nickel oxide nanoparticles synthesized by green synthesis method and using nigella sativa extract. Then the structural properties of nanoparticles characterized by XRD, SEM and FT-IR techniques.

Keywords:Nanoparticles, Green synthesis, Nickeloxide

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Evaluation of inhibitory potential of phosphoramide compound [2,6-F_2-$C_6H_3C(O)NH]P(O)[N(CH_2CH_3)_2]_2$against coronavirous and monkeypox by using molecular docking method

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In recent years, two *infectious viral diseases*, coronavirus and monkeypox,and the preparation of compounds with suitable biological properties as drug to inhibit these diseases have attracted attention of the world health organization and medical association[1]. Phosphoramide compounds with the main skeleton O═P—N are among the chemical compounds that show appropriate biological and medicinal activities against various illnesses such as cancer[2], hepatitis[3] and coronavirous[4]. Therefore, in the present work, a compound of the phosphoramide family with thename *N*-(2,6-difluorobenzoyl)-*N'*,*N'*,*N''*,*N''*-(tetraethyl) phosphoric triamide has been selected and its inhibitory effect against coronavirous and monkeypox are investigated by using the molecular docking method. Survay of the protein-ligand interactions by docking simulation on the studied compound shows that this compound with the binding energy of –5.4 kcal/mol can be proposed as a suitable candidate to inhibit thecoronavirus (7ACS). Moreover, suitable inhibitory effect of this compound against monkeypox virus (4QWO) is confirmed by the binding energy of –6.4 kcal/mol.

Keywords:Phosphoramide, Molecular docking,Coronavirous,Monkeypox

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Electronic Tuning of the Cycloplatinated(II)-Thiolate Complex through Borane Interaction in the Secondary Coordination Sphere

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Cycloplatinated(II) complexes are one of the noteworthy classes of organoplatinum(II) compounds with impressive photophysical properties that are structurally and electronically tunable through supporting ligands[1]. For example, thiolates play important roles in the capacity of tuning both steric and electronic properties of transition metal complexes as supporting ligands by coupling strong σ-donating, which would make the metal center more electron-rich (based on the electron-donating ability of the aromatic ring coordinated to the S atom) and hence promote the luminescence properties of the complexes by increasing the energy of the *dd** states[2].Commonly, the usual modification of a complex is brought on by one or more covalent modifications to the supporting ligand environment, requiring ground-up synthesis of the modified ligand and complex. But beyond that, postsynthetic addition in order to modify Lewis acid-base interactions is a synthetic strategy that complements covalent modification and tunes the optical and electrochemical properties of cycloplatinated(II) complexes. This technique of tuning is more rapid and methodical than that offered by the usual covalent substituent modification[3].

In this work, we're up to demonstrate the concept that borane-pyridine thiolate Lewis acid-base interactions in the secondary coordination sphere can bring about significant and systematic changes in the photophysical properties of cycloplatinated(II) complexes bearing the ppy (2-phenylpyridine) as a cyclometalated ligand with the general formula [Pt(ppy)(κ^1-S-Spy)(PPh$_3$)], where Spy = 4-pyridine thiolate and PPh$_3$ = triphenylphosphine.The complex was titrated with BPh$_3$as a Lewis acid at room temperature and was finallyprimarily identified by NMR, HR ESI-MS, and X-ray crystallography.UV-Vis and photoluminescence spectroscopies were applied in order toconduct photophysical investigations (Figure 1), and the obtained results were rationalized with the help of DFT (densityfunctional theory) calculations.

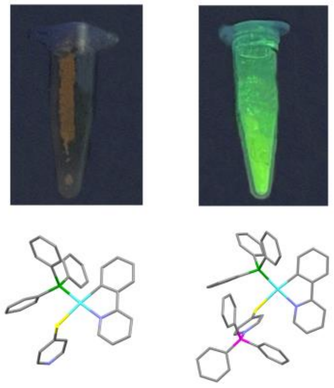

Figure 1. The chemical structures of Pt(II) complexes (down) and their emission under a UV lamp (up).

Keywords:Cycloplatinated complex, Photophysical properties, Thiolate ligand, Borane.

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Fenton degradation of methylene blue (MB) using Nanosized ZSM-5 type ferrisilicate

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Water pollution caused by synthetic dyes, such as methylene blue (MB), is a significant environmental concern. Advanced oxidation processes (AOPs) have gained attention as effective methods for dye removal due to their high efficiency and ability to degrade complex organic compounds. The Fenton reaction, involving the generation of hydroxyl radicals ($OH^{\cdot}$) through the reaction between hydrogen peroxide (H_2O_2) and ferrous ions (Fe^{2+}), is a widely used AOP [1]. In recent years, zeolites have emerged as promising catalysts for enhancing the Fenton reaction's efficiency and reducing its drawbacks [2 , 3]. This paper provides an overview of the role of using nanosized ZSM-5 type ferrisilicate in the Fenton reaction for the removal of methylene blue, highlighting their catalytic properties, adsorption capabilities, and potential mechanisms. Our research indicates that synthesized ferrisilicate samples exhibit remarkable catalytic, adsorptive, and stability properties, which make them excellent candidates for enhancing the efficiency of the Fenton process.

This paper discusses the utilization of zeolite as a catalyst in the Fenton reaction to enhance the removal of methylene blue, addressing challenges like: use of zeolites in wastewater treatment, zeolite modifications for enhanced performance and limitations and challenges faced in zeolite-assisted fenton reactions.

Keywords:Ferrisilicatezeolites, Fenton reaction, Methylene blue, Advanced oxidation processes, Catalysis, Water treatment

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A Novel Procedure for Green Synthesis of Silver Nanoparticles on Activated Carbon

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Activated carbon (AC) is the most efficient adsorbent used for pollutant removal due to its large surface area, well-developed pore structure, high-speed adsorption and thermal and chemical stability [1]. Silver nanoparticles (AgNPs) have attracted significant attention due to their remarkable properties and diverse applications. They are important antibacterial materials as an effect of their larger surface areas in comparison to the bulk material. Researches have shown that silver nanoparticles, silver ions, and nano silver-containing complexes have antimicrobial behavior with a high ability to inactivate bacteria and viruses [2, 3]. However, conventional synthesis methods often involve the use of toxic chemicals and generate environmental concerns. This work investigates the preparation and characterization of activated carbon from semecarpus anacardium nutshell by KOH activation. In this study also, we present a green synthesis approach for fabricating Ag Nano particles on ACs using starch and glucose as novel materials for stabilizing and reducing agents, respectively.Transmission Electron Microscopes (TEMs) images confirm the particle size distribution of the silver nanoparticles mainly in the range of 1–5 nm.

The synthesized AgNPs were characterized for their physicochemical properties, including morphology, particle size distribution, and surface chemistry. The environmentally friendly synthesis method demonstrated the potential for large-scale production of silver nanoparticles with enhanced stability and reduced environmental impact. The study also highlights the diverse applications of green-synthesized AgNPs in various fields.

Keywords:Green synthesis, Silver nanoparticles, Activated carbon, Physicochemical characterization, Environmental impact, Applications.

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Asymmetric Henry reaction catalyzed by chiral heterogeneous Betti base ligands

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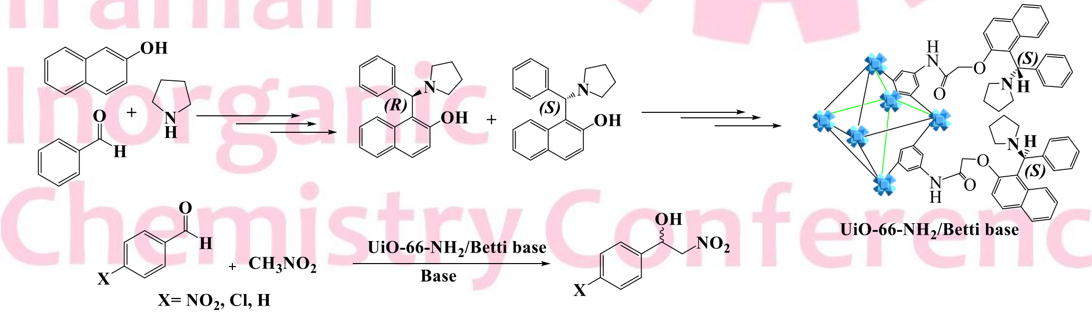
Henry reaction is one of the most famous methods for the formation of carbon-carbon bonds, which is carried out through the addition of nitroalkane compounds to carbonyl-containing compounds such as aldehyde or ketone in the presence of a base and finally produces β-Nitroalcohol compounds, which are valuable raw materialsare in organic synthesis [1,2]. The immobilization of chiral ligands on an inorganic substrate such as UiO-66-NH_2, in order to prepare a heterogeneous chiral catalyst, has attracted much attention due to different advantages of heterogeneous catalysts [3]. Chiral Betti bases can be used as ligands in various reactions to induce chirality [4].In this work, racemic Betti bases were first synthesized by a multicomponent reaction between 2-naphthol, benzaldehyde and pyrrolidine, and then the resulting enantiomers were separated by diastereomeric crystallization method using L-tartaric acid in acetone. Next, the UiO-66-NH_2 metal-organic framework was synthesized by solvothermal method and after functionalization of it using 2-chloroacetyl chloride, the synthesized chiral Betti ligand was immobilized on it. Finally, this heterogeneous chiral ligand was used in theasymmetricHenry reaction in order to chirality induction, which resulted in the synthesis of chiral β-Nitroalcohol products with good enantioselectivities and high yields (Scheme 1).



Scheme 1: Synthesis of chiral heterogeneous Betti base ligands andusing in enantioselective Henry reaction

Keywords: Chiral Betti base, Heterogeneous catalyst, Henry reaction, Chiral β-nitroalcohol

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Green Synthesis of CuO@PVAby lavandulifolia s Extract and development of hydrogen storage capacity

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Today, due to the depletion of fossil fuel resources and the high importance of energy in developed and developing countries, scientists are looking for environmentally friendly, cheap, safe, and high energy density alternatives. Hydrogen, as a clean and environmentally friendly energy, has a high energy density, which promises to reduce or eliminate fossil fuels that pollute the environment [1]. Hydrogen, as a clean and environmentally friendly energy, has a high energy density, which promises to reduce or eliminate fossil fuels that pollute the environment. Using hydrogen energy is really the most effective strategy to deal with the problems of energy exhaustion and the environmental pollution. Many new method and new topic for hydrogen-energy process chain and hydrogen economics, such as one-step approach towards hydrogen production, storage and transportations have been investigated [2-5]. In this work, PVA/CuO nanostructures organized with Stachys lavandulifolia extract have been used in hydrogen storage due to the importance of hydrogen storage and green synthesis of nanoparticles. The synthesized PVA/CuO nanostructures have been characterized by using XRD, FT-IR and their morphology, Morphology are investigated with SEM. The use of polymeric surfactants (PVA) increased the hydrogen storage capacity from 1100mAh/g (for synthesized without surfactant)to 3000 mAh/g and also improved the Columbic efficiency from 55 to 75%.

Keywords:CuO, Hydrogen storage, CuO@PVA

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Green Synthesis of CuO@Hydrochar by lavandulifolias Extract and Evaluation of Extract effects on the Nanoparticles Morphology and Size

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The use of plant extracts in the synthesis of nanoparticles can be an eco-friendly[1], cost-effective and easy-to-synthesize method as well as an alternative to conventional methods such as physical and chemical ones; this has made the green synthesis of nanoparticles of interest to many researchers[2,3]. As part of this work, CuO nanoparticles and nanocomposites with hydrogen storage capability were synthesized. The extract of Stachys lavandulifolia is used as the reducing agent for $Cu+^2$ in the biosynthesis of CuO NPs in the presence of 1 Mm $CuCl_2$ solution, then the nanocomposite was synthesized based on hydrochar. The physical and chemical properties of the CuO nanoparticles and nanocomposite have been analyzed in the facility of X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier transform infrared (FT-IR). X-ray diffraction (XRD) patterns have been investigated for the detection of phase and size and crystal structure as well as the proof of the formation of CuO nanoparticles and nanocomposite, scanning electron microscopy (SEM) for morphology and Fourier Transform Infrared (FT-IR) analysis is for difference bonds checked.

Keywords:lavandulifolia, CuO, Hydrochar, green synthesis

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Immobilization of L-proline on functionalized MCM-41 and its application in the synthesis of chiral allylic esters

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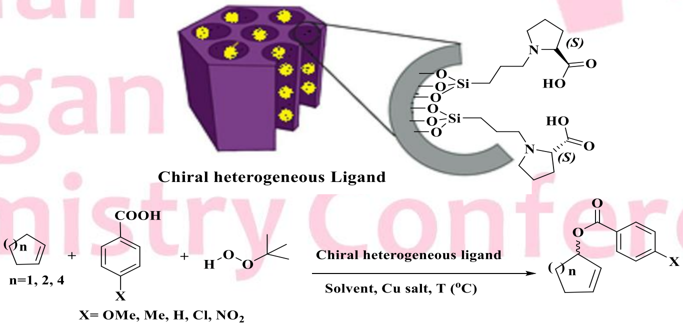
Recently, metal-catalyzed organic reactions through C-H bond activation have attracted a lot of attention from the point of view of atom economy, and also various types of catalytic processes have been developed using different modes to activate the existing bond [1]. Allylic esters which can be prepared through allylic oxidation, play an important role as effective intermediates in the preparation of organic and pharmaceutical compounds[2]. Using chiral catalysts is an available, low-cost and effective method for the preparation of chiral products. Most of organic catalysts are homogeneous and require high molar concentrations; As a result, they increase the cost of separation. One of the ways to recover homogeneous catalysts is the immobilization of them on different substrates, including inorganic substrates [3]. In the meantime, mesoporous MCM-41 has attracted countless attention due to its different advantages such as higher and better efficiency compared to other similar compounds [4].For this purpose, MCM-41 was prepared and functionalized by 3-chloropropyl trimethoxy silane. Afterwards, the chiral L- proline ((2*S*)-pyrrolidine-2-carboxylic acid), was immobilized on it. Finally, the copper complex of synthesized chiral heterogeneous ligandwas used for the preparation of chiral allylic esters and the resulting chiral products were obtained in relatively good yields and enantioselectivities (Scheme 1).



Scheme1: Asymmetric allylic oxidation of olefins in the presence of chiral hetreogeneous ligand

Keywords: L- proline, MCM-41, Chiral heterogeneous catalyst, Chiral allylic ester

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Oxygen-evolution Reaction by Silicate Stabilized Manganese Oxide.

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Oxygen-evolution reaction (OER) through water oxidation under acidic conditions mediated by efficient and stable first-row transition metal compounds remains a challenge in artificial photosynthesis [1,2]. A critical issue in the field is the solubility of first-row transition metal compounds during OER and under acidic conditions. In this study, the silicate-stabilized Mn oxide was investigated for OER under acidic conditions ($pH < 1$). Compared to Mn oxide, the silicate-stabilized Mn oxide is significantly more stable than Mn oxide under acidic conditions ($pH < 1$), with the overpotential of 457 mV for the onset of OER. The Mn oxides forming in the absence and presence of silicate groups are α-Mn_2O_3 and α-MnO_2, respectively. For the Mn oxides forming in the presence of silicate groups, the corresponding current densities of 1 and 10 mA/cm^2 are recorded at 527 and 640 mV, respectively. Silicate-stabilized Mn oxide was characterized by a number of methods before and after OER. The 29Si NMR spectrum for silicate-stabilized Mn oxide shows that the Si-O groups chemically bonded to Mn ions. The scanning transmission electron microscopy shows small 2 – 10 nm particles of Si-O compound in silicate-stabilized Mn oxide. Especially, Si-O to stabilize the higher indices facets of the Mn oxide crystallites. X-ray absorption spectroscopy confirms that the predominant structure for silicate-stabilized manganese oxide is α-MnO_2, with di- and mono-μ-oxo-bridged Mn atoms. After prolonged oxygen evolution, a certain fraction of the mono-μ-oxo bridges disappear for silicate-stabilized manganese oxide. Adding silicate to Mn oxide is a low-cost and environmentally friendly procedure to increase the stability of Mn oxide toward OER under acidic conditions, thus our procedure is a clear improvement on current methods to stabilize Mn oxide for OER under acidic conditions.

Keywords:Acidic conditions, catalyst, oxygen-evolution reaction, silicate stabilized manganese oxide, stability

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A novel coordination complex based on amidine-functionalized polyacrylonitrile fiber/copper (I) : A recyclable solid acid catalyst for click reaction

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In this research, a novel modified polyacrylonitrile fiber with an amidine functional group as an effective platform for stabilization of homogeneous active catalytic species of copper (I) iodide was prepared and its utilization as a recyclable heterogeneous catalyst for Click reactions for the first time. During this study, a new heterogeneous catalyst of copper (I) fixed on polyacrylonitrile fiber was designed by two-step rooting of amine ligands and two-toothed amidine ligands in the surface layer of existing commercial polyacrylonitrile fiber (PANFEA/CuI). Amidine groups in functionalized fibers were used to stabilize copper (I) ions bybonding these ions with amidine two-binding electron donor ligands then evaluate the catalyticactivity of the resulting two catalysts respectively in Click multi-componentreaction were studied. Fibers from different stages are identified and by X-raydiffraction (XRD), infrared spectroscopy (FT-IR), solid ultraviolet spectroscopy, CHN elementalanalysis, scanning electron microscopy (SEM) and optical microscopy (OM) techniques. The capacity of heterogeneous catalyst (mmol/g of catalytic species using EDX and ICP techniques. The PANFEA/CuI system effectively catalyzes the one-pot three-component Click reactions of halides, azides, and alkynes and selectively produces the 1,4-isomer 1,2,3-triazole with high yield in water under mild conditions for 2-4 min. The PANFEA/CuI system was successfully recycled up to five times without reducing its catalytic efficiency and selectivity. The XRD pattern of the recycled catalyst after five times used in the model reaction shows that the fibrous structure of the catalyst is preserved. Cheapness, ease of separation and purification process, recyclability and reuse, and low leaching of catalytically active particles are prominent features of this new green environmentally friendly catalysts.

Keywords:Coordination Complex, Heterogeneous Polymeric Catalyst, Click Reaction, PolyacrylonitrileFiber

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Adsorptive removal of tetracycline from water using MOF-808nanoadsorbent

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Environmental pollution by antibiotics has severely affected human health and development[1]. This paper presents synthesis of MOF-808 and its adsorptive performance for tetracycline (TC) removal. MOF-808 were synthesized by the solvothermal method. We designed MOF-808, BTC (0.056 g), and ZrOCl2·8H2O (0.257g,) in a solventmixture of DMF/formic acid (12mL/12 mL) were placed in a screw-cap jar, which was subsequently heated at 120 ◦C for 48 h [2] and The centrifugation activation methodwere employed.The featured powder X-ray diffraction (PXRD) peaksat 2θ values of 4.3, 8.3, and 8.69 can be easily identified in the obtained powders, indicating(111), (311), and (222) crystalplanes,respectively[3].The FTIR spectrum of the synthesized MOF-808 sample indicatespeaks at 710 and 758 cm^{-1} were assigned to the C–C bond of the benzene ring. Furthermore, the peaks at 1570 and 1400 cm^{-1} are assigned to asymmetric and symmetric stretches of coordinating carboxylates (C=O), respectively, indicating Zr^{4+} and BTC coordination[4]. Specifc surface areaof the materials was measured at − 196 °C and the calculated BET surface area of the sample is around 589 m^{2}g^{-1}. A SEM image of MOF-808 showed that the MOF-808 has a regular ochtahedral structure with particle size of about 500 nm. To obtain the adsorptive performance of MOF-808 adsorption, kinetic adsorption and isotherm experiments were employed.To quantify the adsorption equilibrium time, kinetic experiment was done and the high correlation coefficient) $R^2 = 0.99887$ (indicates that besides physisorption, chemisorption also plays a crucial role in terms of theinteractions that occur between TCand MOF-808. To find the maximum adsorption capacity of TC in MOF-808, adsorption experiments were performed for 4 h (equilibrium time) and showed that the uptake of TC by MOF-808 followed a Langmuir adsorptionmodel ($R^2 = 0.89368$). The maximum adsorption capacity of TC in MOF-808 is about 254.94 mg.g^{-1}, which indicates a great adsorption performance of MOF-808.

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Synthesis, characterization, and electrochemical properties study of a novel polyoxotungstate/metal-organic framework/MWCNTs-COOH nano-hybrid material

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Polyoxometalates (POMs) are a large group of metal-oxygen cluster anions that have unique structural and electronic characteristics[1,2]. Therefore they have many applications in various fields[1].One of the essential applications of POMs, specially Keggin-type POMs, is in the electrochemistryfield[2].The stability of these compounds in aqueous environment and with increasing pH decreases[3].These characteristics limit the analytical application of these compounds. Therefore, in this research, in order to overcome this limitation, a hybrid composition based on polyoxometalate stabilized on the surface of multi-walled carbon nanotubes ($SiW_{11}Co$@Cu-BTC/MWCNTs-COOH) was designed and prepared. Then $SiW_{11}Co$@Cu-BTC/MWCNTs-COOHnano-hybrid material was characterized by various methods such as Fourier transform infrared spectroscopy (FTIR), X-ray Diffraction (XRD), and transmission electron microscopy (TEM). Then the surface of the glassy carbon electrode was modified by this nano-hybrid compound during two stages of drop-casting and then electrochemical reduction method. The surface morphology, and electrochemical properties of the $SiW_{11}Co$@Cu-BTC/MWCNTs-COOH/GCE were evaluated by field emission scanning electron microscope/EDS (FE-SEM/EDS), and voltammetry techniques.

Keywords:Polyoxometalate (POM), Metal-Organic Framework (MOF), MWCNTs-COOH, Nano-hybrid materials, Electrochemical Properties.

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Comparison of structure, nature of bond, fluorescence response and biological activity of Cu(I) and Ag(I) complexes of a known tetradentate Schiff base ligand derived from tren and its reduced form

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The interaction of metal complexes with deoxyribonucleic acid (DNA) has been a subject of interest in bioinorganic chemistry, especially since the discovery of cisplatin and their analogues [1-3]. In this project, the Ag(I) and Cu(I) complexes of a known tetradentate Schiff base ligand derived from tris(2-aminoethyl)amine (L^1_{sb}) and its reduced form (L^1_r) were synthesized and characterized by CHN elemental analysis, UV-Vis, IR, ^1H NMR and ^{13}C NMR spectroscopies. In addition, the structure, nature of the bond, fluorescence intensity and biological activity of them were investigated and compared. DNA interaction studies through the UV-Vis method confirmed that L^1_r and $[AgL^1_r]NO_3$both have effective interaction with DNA, and the calculated binding constant (K_b) indicated that L^1_r has higher affinity compared to $[AgL^1_r]NO_3$.Density functional theory studies on the above Cu(I) and Ag(I) complexes and several similar complexes showed that the metal–ligand bond dissociation energies (BDEs) in copper complexes are larger than those in Ag(I) complexes.

Keywords:Schiff base, Tris(2-aminoethyl)amine, DNA interaction, Bond dissociation energy.

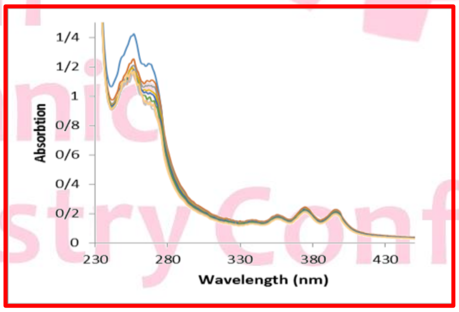

Figure 1. The changes of UV-Vis spectra of L^1_r in the DNA→L^1_rsystem at room temperature and pH 7.4 ($[L^1_r]$= 5.0×10^{-5} M and [DNA]= 0.0 to 9.7×10^{-5} M).

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Synthesis of chiral homogeneous and heterogeneous Betti bases and investigation of their catalytic activity in the Kharasch-Sosnosky reaction

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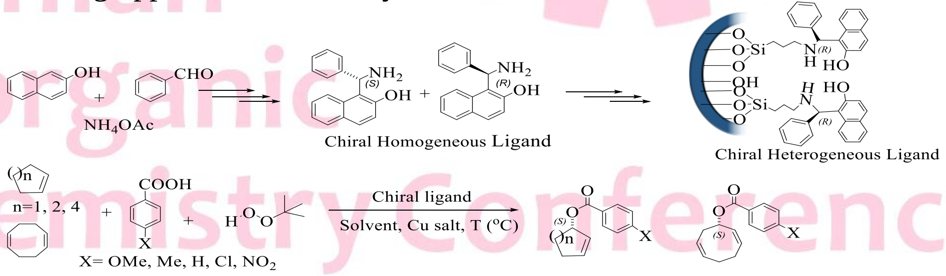
The enantioselective formation of C-H, C-C, C-O, and C-N bonds is an attractive method for producing single enantiomers, and chiral catalysts are the most effective means of achieving this goal[1].Chiral Betti bases are one of the important classes of compounds that possess beneficial biological properties and have been extensively studied for their catalytic applications in asymmetric organic reactions. These compounds can be used as chiral ligands in asymmetric allylic C-H bond oxidation, also known as enantioselective Kharasch-Sosnovsky reaction to prepare functional alkenes such as chiral allylic esters[2, 3].In this study, nanoporous silica SBA-15 was prepared using a hydrothermal method and functionalized with 3-chloropropyltrimethoxysilane.Chiral Betti base ligands were then synthesized via a multicomponent reaction of 2-naphthol, benzaldehyde, and ammonium acetate, and the resulting enantiomers were separated by diastereomeric crystallization [3]. The obtained chiral Betti bases were immobilized on functionalized SBA-15. The prepared chiral homogeneous and heterogeneous ligands were investigated in the Kharasch-Sosnovsky reaction by varying parameters such as temperature, solvent, and the amount of homogeneous and heterogeneous chiral ligands and copper salts (Scheme 1). The resulting chiral allylic esters were obtained in high yields and moderate enantioselectivities. These findings suggest that the mentioned ligands have promising applications as catalysts in the enantioselective Kharasch-Sosnovsky reaction.



Scheme 1: Enantioselective Kharasch–Sosnovsky reaction using chiral ligands

***Keywords*:**Betti base, Chiral homogeneous and heterogeneous catalyst, Chiral allylic esters, Kharasch-Sosnovsky reaction

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Investigation on effect of nanoclay particles on curing of unsaturated polyester resin and evaluation synthesized nanocomposite properties

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In this work, Unsaturated-clay nanocomposite (UP-Clay) prepared by a new method of in situ synthesis. The Cloisite 15A was used as nanofiller and isophtalic resin as matrix. In this new method, the nanocomposite prepared during synthesis of UP oligomers. UP monomers diffuse into the interlayer spacing of Cloisite 15A easily. Occurring condensation reaction between UP monomers leads to delamination of layered Cloisite 15A. In conventional methods for the preparation of nanocomposites, such as direct mixing, high viscosity and oligomers with high volume is the biggest barrier to dispersion of nanoclay in matrix that this causes local aggregation of nanoclay. In this new way was tried to overcome these problem. Condensation reaction in the presence of Cloisite 15A causes the functional group of surfactants of Cloisite 15A reacts with UP monomers, In order to achieve a strong interaction between the two components [1,2].

In this work, according to the results of XRD and SEM, dispersion of Cloisite 15A in matrix was increased for UP-nanocomposite prepared by in situ method. Iso- thermal curing of UP-Clay nanocomposite prepared by in situ method and pure UP resin system was performed in 55, 65 and 75. The results revealed decrease in the final conversion of curing with Cloisite 15A loading. Tensile teste was performed on UP-Clay nanocomposites prepared by both methods and pure UP resin. The result revealed increase in modulus and strength with Cloisite 15A loading. This increase was higher UP-clay nanocomposite prepared by in situ method. Optical image obtained from uncured UP-Clay nanocomposite prepared by both method revealed good stability of Cloisite 15A in matrix after nanocomposite storage for a long time, this relate strong interaction between two component.

Keywords: Nanocomposite, Unsaturated Polyester, Cloisite 15A, Mechanical properties

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Optimization of preparation and process conditions for production of light olefins via FTS on the Fe-Co catalysts

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Catalysts have many applications in various industries, so their production is very important. Among catalysts, various types of iron and cobalt base catalysts with different catalyst support are widely used in Fischer–Tropsch synthesis. The Fischer–Tropsch process is designed and implemented based on the two main methods of fixed bed and slurry [1, 2]. In this project, the basis of the work is based on the fixed bed method of Fischer–Tropsch synthesis, during which iron-cobalt catalysts have been prepared by three methods of solid phase, hydrothermal and wetness impregnation synthesis. Catalyst synthesis was performed in all three methods with 5 different ratios of iron to cobalt. The syntheses have been done by observing all the relevant points and details. A total of 15 catalysts were synthesized and evaluated under the reaction condition in order to produce light olefins by the Fischer–Tropsch method. The physical and chemical properties of the catalysts were investigated by SEM, BET, XRD and ICP/MS. Reactor test conditions were performed at a pressure of 1 atmosphere and temperatures of 270, 300, 330, 360 and 390°C with a GHSV of 3300 hr-1 and a ratio of H2 to CO equal to 2. Catalysts synthesized by wetness impregnation method with the iron to cobalt ratio of 0.25 to 0.75 had the best performance. For the production of these catalysts, gamma alumina was used as the catalyst support and iron and cobalt nitrate salts were used as iron and cobalt precursor respectively. The best CO conversion is about 46% and the best selectivity is about 28% based on ethylene selectivity. It is noteworthy that other olefins, including propylene, have been produced with ethylene.

***Keywords**:* Fischer-Tropsch Synthesis, Light Olefin, Solid Phase Synthesis

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Synthesis of mesoporous MCM-41 silica nanoparticles and surface modified by chitosan functionalized with folic acid for targeted drug delivery and controlled release

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So far, various materials have been used for the design of drug delivery systems. Among these materials, meso-porous silica nanoparticles have attracted many attentions due to their special characteristics such as high surface area, uniform pore size, large pore volume, and most importantly the selective functionalization of their internal and/or external surfaces.

In this project, the meso-porous MCM-41 silica nanoparticles have been made using conventional sol-gel method. At the next step, the anti-cancer drug (Capecitabine) molecules are loaded in the pores of nanoparticles that are immersed in the drug's solution. After that, the chitosan with folic acid was used as the ligand-targeted agents and also as a coating on the drug carrier nanoparticles. Finally, the drug release from nanoparticles are examined in PBS environment (at 37oC , pH = 7. 4).

In order to determine the absorption and the release of the drug, the UV-Vi method has been used. The morphology and surface properties of MCM-41 nanoparticles have been studied using the SEM and BET techniques. The FTIR spectroscopy has been used to study the folic acid's binding to chitosan, and the TGA analysis is also used to determine the amount of covered polymer on the nanoparticles.

The comparison between the obtained release charts indicates the controllability of the drug release from the modified nanoparticles. Overall, in this thesis we modified the nano-carriers in both aspects of controllable release and being as targeted agents. These aspects not only improve the performance of drug's molecules, but also reduce the harmful side effects of these drugs. This procedure could be very useful, especially for those drug molecules which require organic solvents with potential side effects, e.g. in chemotherapy for cancer treatment.

***Keywords**:* Drug delivery systems, Mesoporous silica nanoparticles, MCM-41, Surface modification, Capecitabine, Controlled release

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The effect of potassium promoter on the activity of wustite-based ammonia synthesis catalyst

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Ammonia synthesis reaction from N_2 and H_2 is composed of several steps. The main role of ammonia synthesis catalyst is to dissociate the N_2 bond, because of its high bond energy. It is the heart of the ammonia plant and has a direct effect on the economic benefits of the whole plant, and is thus called an economic catalyst[1]. Wustite-based ammonia synthesis catalyst (WASC) is the new generation ammonia synthesis catalyst that is more highly active than magnetite-based catalyst[2]. It was typically produced by a high-temperature fusion method in which a high-grade magnetite and iron/graphite and promoters are melted followed by cooling, crushing, and sieving. An electrical furnace will be used for melting material above 1800 °C. The usual promoters such as Al, Ca, K, Mg, and Si were used for improving activity, heat resistance, and antitoxic performances[3]. The most important promoter that is effective in the activity (NH_3 %) of wustite catalyst is potassium (K) which is named an electronic promoter. It is donated an electron to the anti-bonding N_2 bond that is facilitated the dissociation of N_2 in the rate-determining step. In this research, some samples of WASC were prepared with various content of K (0.5-2 %), and their activity of them was measured. It was shown that about 1 % K is enough for activity. It was concluded that the high amount of K promoter does not result in high activity.

Keywords: wustite, ammonia synthesis, potassium, promoter

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Theoretical study of the thermodynamic stability of the alkali metal complexes with ammonia as a ligand

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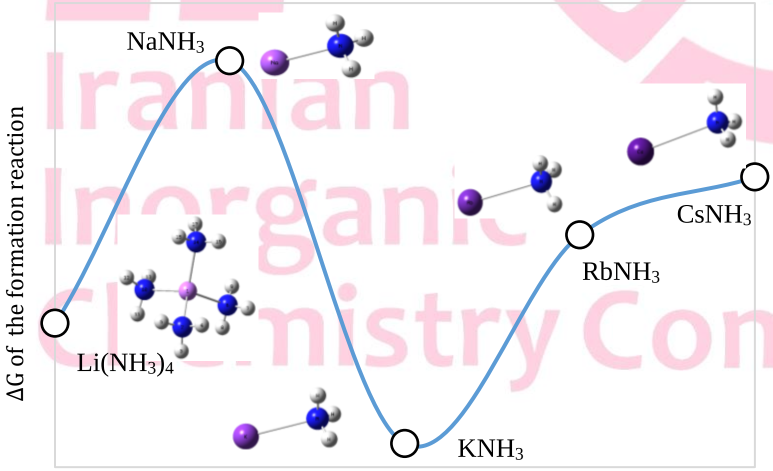
The thermodynamic stability of the alkali metals complexes was investigated using theoretical studies, based on DFT by the lanl2DZ/B3LYP level of theory [1,2]. In this research, the Gibbs free energy caused by the interaction of the ligand with the metal has been considered as a component of the theoretical stability of the complex, even in cases where the complex did not exist.Optimization and frequency calculations of metals, ligands and complexes were separately performed. To find the most stable of the $M(NH_3)_n$ complexes the ΔG_f/coordination number diagram has been drawn. After finding the most stable structure of each metal, the metal/energy diagram of the complexes was drawn to investigate the thermodynamic stability of the $M(NH_3)_{1-6}$complexes (Fig.1-a) [3-4]. The results showed that the most stable form of these metals according to the coordination number will be $Li(NH_3)_4$, $NaNH_3$, KNH_3, $RbNH_3$ and $CsNH_3$ complexes (Fig.1-b). Also, the comparison of the stability of thsese complexes showed the following order:KNH_3>>$Li(NH_3)_4$>$RbNH_3$>$CsNH_3$>$NaNH_3$

Keyword: Alkali Metal, Theoretical study, Thermodynamic stability, Gibbs free energy



(a)

$M(NH_3)_n$	ΔG (Kcal/mol)
$Li(NH_3)_4$	-104.55
$NaNH_3$	17024.49
KNH_3	-519.40
$RbNH_3$	2159.09
$CsNH_3$	4655.63

(b)

Fig.1. (a) Comparison of relativethermodynamic stability of alkali metal complexes. (b) The value of thetheoretical Gibbs free energy of the formation reaction

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Synthesis of *β*-nitroalcohols in the presence of amino acid-based chiral metal-organic framework.

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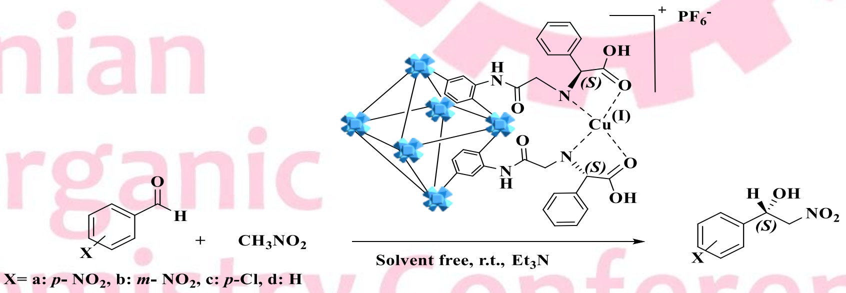
UiO-66-NH_2 is a type of metal-organic framework based on zirconium which hashigher thermal and chemical stability than other metal-organic frameworks. furthermore, the NH_2 groupin Metal-organic framework UiO-66-NH_2 can befunctionalized with chiral ligands[1].The formation of C–C bonds in the manufacture of valuable molecules using MOFs as heterogeneous catalysts is an important research field with applications in the chemical and pharmaceutical industries[2,3].In this work, the UiO-66-$NH_2$was prepared by solvothermal methodand functionalized with 2-chloroacetyl chloride, thenthe chiral aminoacid, L-phenylglycine, was immobilized onit.The structure of synthesizedheterogeneous chiral ligand was characterized by XRD, FE-SEM, BET, FT-IR and TGA techniques.Subsequently, copper salt was incorporated in the chiral metal-organic framework and it was used in theasymmetricHenry reaction for the preparation of chiral β-nitroalcohols under nitrogen atmosphere and different conditions (solvent, base, temperature, catalyst, etc).The resultingproducts were obtained with high efficiency and suitable optical purity in a short period of time (Scheme 1).



Scheme 1: Synthesis of β-nitroalcohols in the presence of amino acid-based chiral metal-organic framework

Keywords: Chiral metal-organic frameworks, Chiral catalyst, Henry reaction, β-nitroalcohols

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Preparation and characterization of a metal-containing ionic liquid DABCO based*Lewis* acid catalyst for the synthesis of quinoxalines

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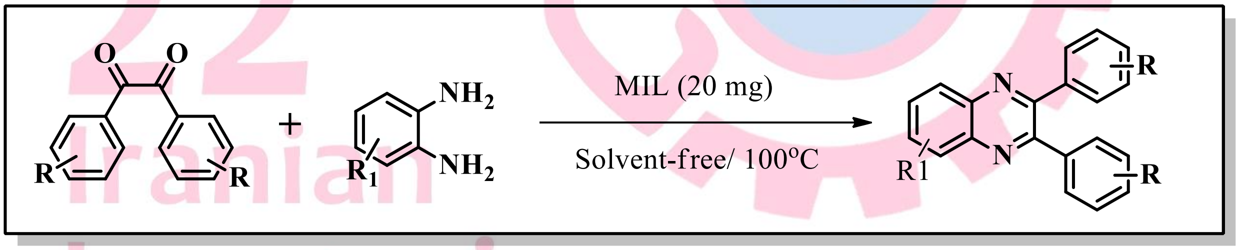
Quinoxalines are importan nitrogen containing heterocyclic compounds.this compounds can show biological activities, medicinal and therapeutic properties, and also are used in various fields such as paint industry, optoelectronics and agricultural chemistry.There are many methods for the synthesis of quinoxalines, but these methods have disadvantages, including environmental hazards, which cannot be the optimal method for the synthesis of them. Thereforehere in we wish to report the use of a new DABCO based metal-containing ionic liquid as a *Lewis* acidic catalyst to achieve the desired compounds [1,2].

This catalyst has unique properties such as high efficiency,short reaction time, easy workup, and the ability to bear a variety of functional groups wich brings economic as well as environmental rewords. (Scheme 1).



Scheme 1: Synthesis of quinoxalines in the presence of DABCO-based metal-containing ionic liquid.

Keywords:Quinoxalines, heterocyclic compounds, ionic liquids containing metal and DABCO

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Theoretical studies on the effect of substituents of the N-heterocyclic carbene ligand present in the Pd-PEPPSI complex on the formation mechanism of the Negishi cross-coupling reaction

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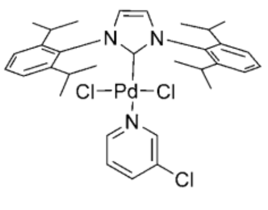
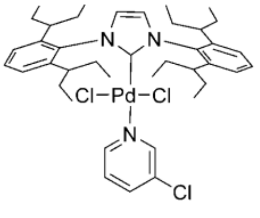
Transition metal complexes bearing *N*-heterocyclic carbene ligands (NHCs) have gained a place of crucial importance in numerous areas of research such as medicinal chemistry, material sciences, and homogeneous/heterogeneous catalysis.[1].Recently, several monoligated Pd–N-heterocyclic carbene (Pd–NHC) complexes have been prepared and have demonstrated high levels of activity in various Pd-catalyzed cross-coupling reactions, as reported [2].The increased catalytic activity is attributed to the enhanced steric bulk of the NHC ligand. While oxidative addition does not seem to be significantly influenced by the sterics, both metal–metal exchange and reductive elimination appear to be affected[3]. The main focus of this project is to investigate the effect of NHC ligand side chains in Pd-PEPPSI complexes. Mechanistic studies on biaryl compounds using Pd-PEPPSI complexes as catalysts in Negishi cross-coupling reactions are being examined. The theoretical results obtained in this project demonstrate that the Pd-PEPPSI-iPent catalyst outperforms Pd-PEPPSI-iPr, which is consistent with experimental findings. Calculations were conducted using the Gaussian09 program with the CAM-B3LYP/DEF2-SVP method.

Keywords:Negishi, Cross-coupling, Mechanisim



Pd-PEPPSI-IPr



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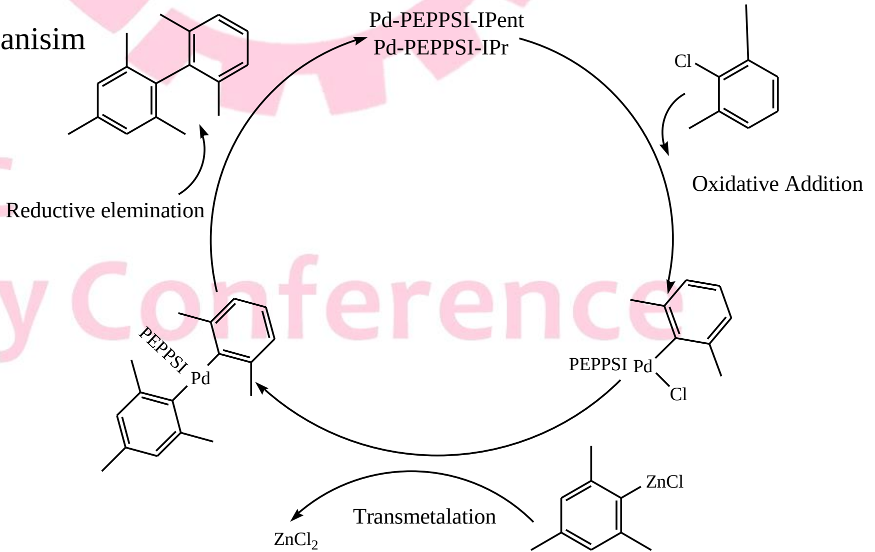

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Synthesis, characterization, molecular dockingand DFT calculation of a copper(II) mixed-ligand complex

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A mixed-ligand complex ([1]) consisting of [Cu(NO_3)$_2$].3H_2O, [2,4,6-trihydrazineyl-1,3,5-triazine] (THT), and Pyridine-2,6-dicarboxylic acid (PDCA) was synthesized and characterized using FT-IR spectroscopy and CHN analysis. The complex [Cu(THT)(PDC)] possesses a unique combination of ligands and has potential applications in coordination chemistry. The complex has a distorted squarepyramidalgeometry ($\tau = 0.22$) with a CuN_3O_2 environment, where THT acts as a bidentate ligand and PDC acts as a tridentate ligand, binding to the metal atom through one nitrogen atom and two oxygen atoms as shown in Fig(1). The thermodynamic stability of the complex was investigated using DFT([2]). Based on the obtained reaction values, the calculations demonstrate that the reaction products have achieved a higher level of stability, with a difference of (-0.003054) Hartree, compared to the initial substances. This result is presented in Table (1).The biological activity of the complex and its ability to interact with biomacromolecules were investigated through docking calculations ([3]). The results indicate that the complex has a similar activity to doxorubicin in the interaction with B-DNA (Major) and CatB protein, as presented in Table (2).

***Keywords*: Triazine,Mixed-ligand, Molecular docking, DFT, Coordination chemistry**

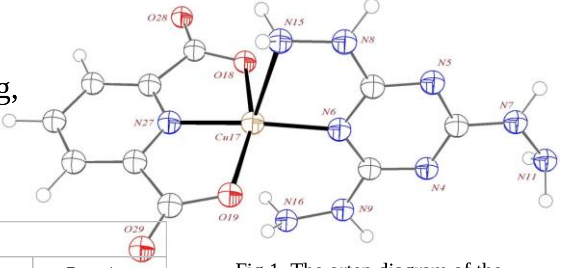

Fig 1. The ortep diagram of the molecular structure of the complex

Table 1.Reaction equation and ΔG calculation

	Reaction: THT + PDCA + Cu(NO_3)$_2$ → [Cu(THT)(PDC)]+ 2HNO_3					
	THT	PDCA	Cu(NO_3)$_2$	Complex	HNO_3	Reaction
ΔG	-612.328308	-625.358664	-756.576616	-1432.500836	-561.765806	-0.003054

Table 2.The calculated fitness values for the ligands and their complexes along with the doxorubicin.values

	B-DNA (Maj)	B-DNA (Min)	BRAF-Kinase	CatB	DNA-Gyrase	HDAC7	rHA	RNR	TrxR	TS	Top II
Complex	26.96	47.68	42.71	21.00	28.45	34.50	33.98	33.20	45.30	37.96	36.29
Doxorubicin	33.47	83.10	54.21	25.95	52.97	50.73	50.10	49.18	66.70	53.34	59.05

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Energy Decomposition Analysis of Metal-Ligand Bonding in Transition Metal Complexess with Carbenes and Ylides Ligands: Significance of Electrostatic Interactions in Bond Analysis ‡

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This work describes a pedagogical approach to understanding chemical bonding by emphasizing the significance of electrostatic interactions in Metal-Ligand Bonding, particularly in Transition Metal Complexes with Carbenes and Ylides Ligands. Energy Decomposition Analysis (EDA) is a powerful method for quantitatively interpreting chemical bonds in terms of three major components. The instantaneous interaction energy ΔEint between two fragments M and L in a molecule M←L is partitioned into three terms: (1) the electrostatic interaction ΔE_{elstat} between the fragments, (2) the repulsive exchange, Pauli interaction ΔE_{Pauli} between electrons of the two fragments with the same spin, and (3) the orbital (covalent) interaction ΔE_{orb}, which arises from orbital relaxation and orbital mixing between the fragments. The latter term can be further decomposed into contributions from orbitals with different symmetries, enabling the distinction between σ, π, and δ bonding The results demonstrate that the EDA terms can be interpreted in a chemically meaningful way, thus establishing a connection between quantum chemical calculations and heuristic bonding models of traditional chemistry. The nature of the L→M bond in the complexes was analyzed using NBO, AIM, EDA, and ETS-NOCV methods.The findings confirm that the electrostatic interaction term, ΔEelstat, becomes notably higher and contributes significantly to the orbital interactions in the studied complexes.

Keywords: EDA, Transition Metal Complexes, Ylide, Carbene

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Investigating the effect of mullite on the permeability of distilled water through geopolymeric membrane based on blast furnace slag

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geopolymerization technique has been used for membrane synthesis to replace conventional ceramic membrane synthesis. For the past decade, researchers have been working on geopolymerization reactions by mixing fly ash and minerals as raw materials to replace expensive raw materials and high-temperature sintering steps to make mineral membranes[1][2].In this research, 3 types of geopolymeric membranes (Z_1, Z_2, Z_3) have been used to check the permeability of distilled water at 3 different pressures of 1, 2 and 3 bar that in Z_1 and Z_2 membrane, with constant mullite percentage (4% W.t) withdifferent ratio of Sodium silicate to Sodium hydroxide(1 and 2)at 3 bar pressure, the permeability of distilled water through membrane Z_1 with ratio (W.G)/NaOH=1 is equal to 9.4× $10^{-7}\, m^3/m^2s$ and membrane Z_2 with ratio (W.G)/NaOH=2 is equal to 4.5× $10^{-7}\, m^3/m^2s$. In the comparison of Z_1 and Z_3 membranes, this time by keeping the ratio (W.G)/NaOH = 1 and increasing the amount of mullite by (12% W.t) at a pressure of 3 bar, the permeability increased to 42× $10^{-7}\, m^3/m^2s$.In the manufacturing of the mentioned membranes, the amount of micro silica in all membranes was determined to be (3% W.t) . Alkaline activators were used in the construction ofZ_3 membrane to activate furnace slag, with 5.84 (g) of sodium hydroxide, 5.86 (g) of Sodium silicate(W.G) and 28.50 (g) of distilled water.The duration of the experiments for each pressure was 30 minutes, and for testing each membrane, the synthesized membrane was compacted for 25 minutes with pure water under a pressure of 4 bar. The results of FT-IR analysis show a broad main absorption band and strong in the range of 1024.13cm^{-1}, which is the main band related to the asymmetric stretching vibrations of Si-O(Al) in the SiO4 tetrahedron and the asymmetric stretching of Al also in the peaks around 457.10 cm^{-1},[3]

Keywords:Membrane, blast furnace slag, mullite,geopolymerization

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Application of Zinc oxide nanostructures as a promising nanocarriers for 5-ALA in drug delivery system based on DFT-MD simulations

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We have examined the interactions between 5–aminolevulinic acid (ALA) drug and ZnO nanostructures using DFT method. In the context of the dispersion corrected PBE technic, the energetics, charge transfer, electronic structure and equilibrium geometries have been estimated.The ZnO nanostructures showed promising performance in the ALA drug functionalization, taking into account the interaction energy values. The band gap is almost remained unchanged for both of the substrates under consideration after ALA adsorption, and the semiconductor properties of the substrates are preserved, according to the analyzed DOSs spectra. The interaction nature of ALA–ZnO nanostructures according to the QTAIM analysis was found as polar attraction with partial covalent bonding between O and Zn.Our DFT based MD simulation results reveal that, in the aqueous solution, ALA moves toward the interior sidewall of ZnO nanostructures and binds to the Zn atom through its O and N atoms and the hydroxyl H atom was dissociated and bind to the O atom of ZnO surface.

Keywords:Drug delivery; Zinc oxide nanostructure; Adsorption; DFT; Molecular dynamic simulation.

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Synthesis and characterization of bentonite/Co_3O_4(Be/CO) nanocomposite

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Bentonite comprises a group of layered silicates.A comprehensive review of the literature reveals that the chemical composition of calcium-containing bentonite is not uniform and varies depending on its origin. In general, clay minerals consist of Si, Al, Fe, H_2O, and alkaline/alkaline earth metals[1]. The primary structure of bentonite consists of two atomic lattice units, namely tetrahedral and octahedral layers. The tetrahedral layer contains Si^{4+} ions at its center, surrounded by O^{2-} ions, while the octahedral layeris formed by Al^{3+} ions in the middle, surrounded by six OH^- ions at the corners[2].The ion exchange process of Si^{4+} and Al^{3+} is accomplished with cations of lower valence such as $Fe3^+/Mg^{2+}/Ca^{2+}$ and Na^+.The current study investigates the surface absorption capacity of natural bentonite soil, which has been modified with sulfuric acid, to enhance its absorption capacity. To achieve this, bentonite soil has been impregnated with cobalt oxide nanoparticles using the in-situ synthesis method[3].X-ray diffraction (XRD) analysis, Field emission scanning electron microscopy (FE-SEM), and X-ray scattering analysis energy (EDX) were carried out to identify natural bentonite soil and to modify it with cobalt oxide nanoparticles.The results indicated that the cobalt oxide nanoparticles were dispersed on the surface ofbentonite soil.

Keywords:Bentonite, Co_3O_4,characterization

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Tuning the performance of a novel functionality Zn-based MOF by incorporating a secondary linker in heavy metal ions absorption

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The rapid agricultural and industrial development is producing pollution of heavy metal ions because of their toxicity for humans and detrimental effects on the environment and ecology [1].Accordingly, removing heavy metal ions from water is a particularly significant issue before they are released into the environment. in recent years Metal-Organic Frameworks have been regarded as remarkable candidates for the adsorptive removal of heavy metal ions because of their amazing attributes such as high surface areas, and designable chemical functionalization of pore surfaces [2].In this work, a mixed-linker MOF strategy was chosen to show proof of this concept in accessing more active sites and preparing some defects in MOF structures to improve the adsorption efficiency of MOF-5 for heavy metal ion removal from water. a novel nitro functionalized pyrazole dicarboxylic linker (4-nitro-3,5-pyrazoledicarboxylic acid,PZDC-NO_2) as a second ligand and benzene-1,4-dicarboxylate (H_2BDC) was added to form a new mixed-ligand MOF material (MOF-5 (PZDC-NO_2)), under facile solvothermal synthesis, which was characterized by SEM, EDX, XRD, BET, and FTIR[3].The new porous MOF was tested for the adsorption of heavy metal ions and showed an improved adsorption capacity compared to MOF-5 and many other standard adsorbents.

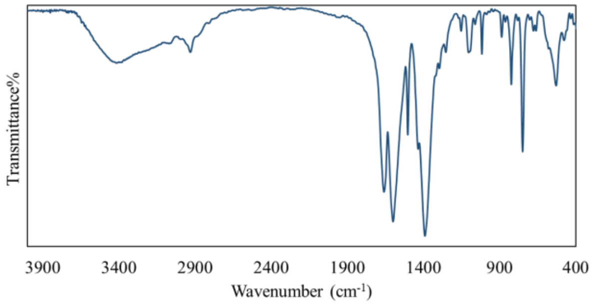

Figure1.The FTIRspectrum ofMOF-5 (PZDC-NO_2)

Keywords:Metal-organic framework, Metal ions absorption, Mixed linker.

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Competition between hydrogen bond , halogen bond and chalcogen bond in complexes of N-methylidenemethanamine(C_2H_5N)with HYX(Y=O, S and X=F, Cl, Br and I).

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An ab initio study of the complexes formed by N-methylidenemethanamine(C_2H_5N)with HYX(Y=O, S and X=F, Cl, Br and I) has been carried out at the MP2/aug-cc-PVDZ computational level. Interaction of HOX with N-methylidenemethanamine (C_2H_5N) lead to both hydrogen bond (C_2H_5N -HB) as well as halogen bond (C_2H_5N -XB) complexesMeanwhile Interaction of HSX with N-methylidenemethanamine (C_2H_5N) lead tohydrogen bond (C_2H_5N -HB) , halogen bond (C_2H_5N -XB) andchalcogenbond(C_2H_5N -YB) complexes The interaction strength and properties in all complexes are analysed with atoms in molecules (AIM) and natural bond orbital (NBO) theories.

Calculations were performed using the Gaussian 09 system of codes. The geometries of the isolated HYX(Y=O, S and X=F, Cl, Br and I) and C_2H_5N molecules as well as HYX-C_2H_5N complexes were fully optimized at the MP2 level of theory [1] with the aug-cc-pVDZ basis set for all atoms, except iodine, for which the DGDZVP[2] was used. Harmonic vibrational frequency calculations certified the structures as minima and provide the evaluation of the zero point energy (ZPE). The counterpoise procedure was used to correct the interaction energy for the basis set superposition error[3]. The AIM2000 package and AIMAll[4] were used to obtain bond properties; and to plot molecular graphs. The natural bond orbital (NBO) method has been used to evaluate the interaction of occupied and empty orbitals with the NBO package supplied with Gaussian 09.

Keywords:Hydrogen bond, halogen bond, chalcogen bond, blue shift, N-methylidene methanamine.

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Intercalation of Mefenamic Acid in Inorganic Nanomatrices with Layered Structure

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In this study, Mefenamic acid was intercalated into Mg-Al layered double hydroxides (LDHs) by ion exchange or coprecipitation methods to obtain mefenamic -LDHs nanohybrids. Mefenamic acid is one of the non-steroidal anti-inflammatory drugs that is used to treat some types of acute and chronic diseases. But its low dissolution rate is a limiting factor for its absorption, so in order to increase the solubility of this material, it can be used to intercalate it between LDH layers. Powder x-ray diffraction (XRD), Fourier transform infrared spectra (FT-IR), and elemental analyses indicate a successful intercalation of Mefenamate anions with a vertical orientation. Intercalation of Mefenamate anions into Mg-Al LDH caused the interlayer spacing of LDH to increase from 0.76 to2.1 nm as determined by x-ray diffraction studies. TG analyses propose that the thermal stability of the intercalated organic anion of mefenamate is largely improved compared to the pure form before intercalation.Furthermore, *in vitro* drug release experiments in pH 7.4 phosphate buffer solution have been investigated. The drug molecules during dissolution were exchanged with anions in the medium, this leading to a slow release, much slower than when the same matrix was used simply mixed with the drug[1-5].

Keywords: Mefenamic acid, Layered Double Hydroxides, co-precipitation, ion exchange, Intercalation

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Facile preparation of layered double hydroxide materials for high efficiency oxygen evaluation

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Today, applying of fossil fuels is considered as a challenge and the use of renewable.Clean energy can be as a suitable way for decrease this problem. Energy transport such as hydrogen evaluation reaction (HER) was considered as alternative energy technology in the recent years [1, 2]. The hydrogen can be product using water splitting reaction [3]. Although, the rate of the oxygen evolution process at the water splitting reaction is sluggish [4]. So, a way for obtain high efficiency at water splitting is applying the electrocatalysts which improve the oxygen evaluation reaction (OER). Therefore, OER contains conversion energy and store energy. The present study reported that the NiCr-LDH/SWCNT nanocomposite is as a superior active for oxygen evaluation reaction (OER). The NiCr-LDH/SWCNT composite was synthesized using the ultrasonic sound waves. Based on the characterization analyses such as X-ray diffraction (XRD) patterns, and field emission scanning electron microscopy (FE-SEM) images, the synthesis of NiCr-LDH/SWCNT using the ultrasonic method, was confirmed. Next, the NiCr-LDH/SWCNT composites were used as an effective nanomaterials for OER at near neutral media. The obtained data from the linear sweep voltammetry (LSV) process confirm that NiCr-LDH/SWCNT decreases the overpotential to about 70 mV in comparison with only NiCr-LDH, and RuO_2. The high activity oxygen generation can be attributed to the presence of NiCr-LDH and SWCNT at prepared nanocomposite.

Keywords: Layered double hydroxide, Oxygen evaluation reaction, Water splitting

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Effect of microwave-assistant intercalation on photoluminescence emissions and photo-stability

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The layered double hydroxides (LDHs) have several advantages such as unique structure, large intercalated anions within interlayer spaces, and uniform distribution of metals in the layered structure which make the LDHs significant layered materials[1].Recently, intercalation using microwave- assistant method has received more attention[2]. The advantage of this process is decreasing the time of reaction [3]. Intercalation using microwave- assistant method can be used as a method to control the dye molecules inside the LDH layers and improve the fluorescence properties of the nanohybrid but at the photoluminescence devices, photo-stability of prepared nanohybrids is as a key point for increased efficiency of the device [4]. On the other hands, the photo-stability of azoic dyes such as mordant orange 1 is very poor under UV light. The purpose of this study was the preparation of layered double hydroxide (LDH) based nanohybrids with improved photoluminescence emission with high photo-stability. The anion exchange based microwave method was applied for the intercalation of mordant orange 1 into MgAl-LDH. In the MgAl-LDH interlayer space, a tilted orientation and bilayer arrangement were predicted for the mordant orange 1 anions. Compared with the pure mordant orange 1, the MgAl–LDH/ mordant orange 1-MA (prepared using the microwave-based anion exchange method) has improved photoluminescence emission with high photo-stability. These findings supply a new approach for designing photoluminescence materials that potentially apply to optical devices with high photo-stability

Keywords:MgAl–layered double hydroxide, Mordant orange 1, photoluminescence emission

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Uncertainty quantification and sensitivity analysis of the efficiency of a biofilm reactor with a moving bed using a combination of Monte Carlo simulation and artificial neural network.

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In this study, the uncertainty and sensitivity analysis of the efficiency of a biofilm reactor with a moving bed were conducted using a combination of Monte Carlo simulation and artificial neural network. The qualitative prediction of the quality of petroleum source was estimated using artificial neural networks, and the removal efficiency of COD and TPH pollutants was predicted using a set of laboratory data.

This dataset included parameters such as TPH_{in}, COD_{in}, F/M, Filing Ratio, MLVSS/MLSS, DO, COD_{out}, and TPH_{out}, which are considered influential in the quality of petroleum sources. A 4-layer neural network with 7 neurons and an error rate of 4.06% was designed for COD removal efficiency prediction, and a 3-layer neural network with 8 neurons and an error rate of 3.95% was designed for TPH removal efficiency prediction. By incorporating the mathematical model as an activation function in the Monte Carlo method, the uncertainty and reliability of the estimated COD and TPH removal efficiencies were determined.In the Monte Carlo method, using the Latin Hypercubes algorithm, the removal efficiencies were obtained as intervals with a 95% confidence level, yielding satisfactory results. This is important as it reduces the risk of pollutant removal during managerial decision-making and covers sudden changes in the quality of petroleum sources that affect the removal efficiency.In previous random sampling methods, a random number was extracted from the probability distribution space of a data. However, this method divides the input's normal distribution into rows and columns, and then selects a random sample from among the created sections so that the realization of values with low probability is also practical. One of the advantages of using this method is obtaining confidence levels for risks with high effects but low probabilities [1].

Keywords:MBBR, Artificial Neural Network, Monte Carlo

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A theoretical study of two local minima for the structures of [4Fe–4S] clusters

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The accuracy of geometries is important for predicting the electronic properties of molecular systems using computational methods. A previous investigation has indicated that there exist two local minima for [4Fe–4S] clusters in proteins when optimized with a density functional theory (DFT) method [1]. In this work, we performed a detailed study of two distinct local minima for [4Fe–4S] clusters in five proteins and two oxidation states, using combined quantum mechanical and molecular mechanical (QM/MM) methods.The MM part of the QM/MM calculations was performed with the Amber software [2], using the Amber ff14SB force fields. In the QM part, we employed nine different DFT methods, PBE, BP86, BLYP, B97D, TPSS, r^2SCAN, TPSSh, B3LYP, and B3LYP*. All the functionals were combined withdef2-SV(P) or def2-TZVPDbasis sets.The QM system consisted of the Fe and S ions and the directly coordinated Cys groups modeled by $CH_3CH_2S^-$, for the whole cluster (cf. Figure 1).Weindicated that one local minimum (L state) has longer Fe–Fe distances than the other (S state) and that the L state is more stable for all cases studied. Also, our results showed that some DFT methods may only obtain the L state, while others may obtain both states. We recommend r^2SCAN for optimizing [4Fe-4S] clusters in proteins, which gives the most accurate structures.

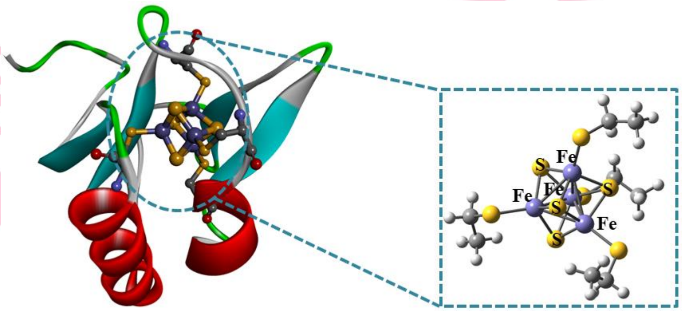

Figure 1.The close-up of the QM system we used in the calculations.

Keywords:Iron-Sulfur Cluster, Protein, DFT, Geometry, QM/MM

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The reaction mechanism of aphid myrosinase, a theoretical study

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The aphid *Brevicoryne brassicae* is a specialist feeding on *Brassicaceae* plants. The insect has an intricate defense system involving the myrosinase enzyme that hydrolysis glucosinolates sequestered from the host plant into volatile isothiocyanates [1].In this study, we investigated the reaction mechanism of aphid myrosinase usinga quantum mechanics/molecular mechanics (QM/MM) method [2]. A model of the active site of this enzyme was constructed based on the crystal structure of aphid myrosinase from *Brevicoryne brassicae* (1WCG PDB ID) [1]. The active site can be divided into two parts, the glucose and aglyconbinding sites (cf. Figure 1).Our result showed that in the first step of the mechanism (glycosylation), the catalytic residue (Glu-374) performs a nucleophilic attack on the anomeric carbon of the substrate, and then the other carboxyl residue (Glu-167), acting as a general acid, protonates the glycosidic sulfur. This leads to forming of a glycosyl–enzyme intermediate and the aglycon moiety leaves the reaction medium. In the next step (deglycosylation), Glu-167, acting as a general base, activates a water molecule to attack the anomeric center of the intermediate, and the covalent bond between the enzyme and the glycosyl is broken, and the β-glucose molecule is released.

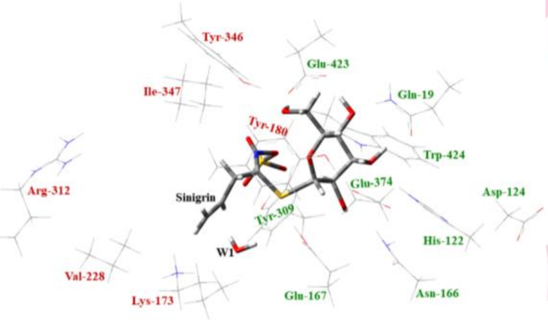

Figure 1.The QM system we used in the calculations.Residues of the glucose binding site are labeled in green and those of the aglycon binding site in red. Sinigrin is the substrate.

Keywords:Aphid myrosinase, Reaction mechanism, QM/MM

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Catalytic applications of metal-organic framework modified by yttrium containing sandwich polyoxometalate

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Polyoxometalates, including heteropolyoxometalates and isopolyoxometalates, can be used as excellent catalysts for both acid-catalyzed reactions and oxidation reactions [1]. The synthesis and characterization of new transition-metal-substituted (d-and f-block) polyoxometalates continues to be a focus of considerable ongoing research. Highly tunable nature of these compounds, coupled with their chemically robust nature, has led to applications in catalysis, medicine and molecular magnetism [2]. As homogeneous catalysts, polyoxometalates have a low specific surface area, and on the other hand, they are easily dissolved in polar environments, for this reason, it is difficult to recovery the catalyst [3]. Attempts to recover catalysts are of great interest [4]. In order to reach this goal, homogeneous catalysts must be converted into heterogeneous catalysts by different methods. One of these methods is to place the homogeneous catalyst on a solid support [5]. The A-type sandwich polyoxometalates of $[(PW_9O_{34})_2(H_2OYO)_3]^{15-}$ was immobilized for the first time into the porous metal-organic framework MIL-101(Cr). The new $P_2W_{18}Y_3$@MIL-101 nanocomposite characterized by means of FT-IR, XRD, TGA, SEM, EDX, BET analysis. The catalytic activity of heterogeneous catalyst was examined in the oxidation of sulfides to sulfones with H_2O_2 oxidant at room temperature.The effects of different dosages of polyoxometalates, type of solvent, reaction time, amount of catalysts and oxidant in this catalytic system were investigated. The effect of temperature on stability and catalytic activity of the new $P_2W_{18}Y_3$@MIL-101 was investigated. The new new $P_2W_{18}Y_3$@MIL-101 nanocomposite exhibited well recyclability and reusability in at least five consecutive reaction cycles without significant loss of activity or selectivity.

Keywords:yttrium sandwich type polyoxometalate, MIL-101(Cr), composite, sulfides, sulfones

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Application of metal-organic framework containing hydroxyapatite(MOF/HAp) in tissue engineering to improve bone function

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Today, tissue engineering has been given much attention in order to restore damaged tissues, especially bone tissue, and improve its function. For the regeneration of bone tissue, a scaffold with biological and biochemical properties is needed that can have high biocompatibility and porosity that can simulate the natural bone tissue[1].Hydroxyapatite has a chemical composition similar to the mineral part of teeth and bones, which gives them properties such as hardness and strength. On the other hand, it is possible to use the metal-organic framework (MOF), which is a three-dimensional network of metal ions connected by multidentate organic molecules, along with hydroxyapatite, which creates features such as increased surface area, flexibility, and structural diversity. One of the metal-organic frameworks is zinc-based zeolite-imidazolate framework (ZIF-8), which has small-sized particles, high specific surface area, and stable release performance, and also has antibacterial properties due to the release of zinc ions, which is useful for tissue repair. Bone is used along with hydroxyapatite [2,3]. In order to prepare the desired composite zinc nitrate hexahydrate, 2-methyl imidazole(2-MIM) and hydroxyapatite powder were dissolved separately in methanol and after complete dissolution, they were added to each other. Finally, after the dissolution of the sediment was complete formed was used as the desired composite.considering this issue, in this study, a metal-organic framework composite containing hydroxyapatite was successfully synthesized and characterized for potential applications. Structural and crystalline characteristics of synthesized composite were evaluated using Fourier transform infrared spectroscopy (FTIR)and X-ray diffraction (XRD). The peaks in the FTIR spectrum proved the presence of Hap on MOF. Morphological investigation usingscanning electron microscope (SEM) showed that the average particle size is~20.3nm, and the elemental composition of synthesized product by EDS analysis exhibits the presence of Zn,N,P,Ca,O and H atoms, confirming the successful synthesized. The results showed that the use of composite containing MOF/Hap has a potential application in improving bone tissue.

Keywords:Bone tissue engineering, Hydroxyapatite, Nanofibrous composite, Metal-organic framework

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Theoretical Study on the cooperativity/anticooperativity of metal–carbonyl and metal–dihydrogen bonds in some complexes of group 6 transition metals

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The aim of this project is to study the structure, interaction energy, stabilization energy, cooperative/anticooperative energy and the nature of the metal-ligand bond in some group 6 transition metal complexes containing dihydrogen and carbonyl ligands. For this project, some complexes with the general formula $[M(\eta^2\text{-}H_2)(CO)_4L]$ (M=Cr, Mo or W; L= SiO, PH_3, NO^+,N_2,NC^-, CS,CO, and CN^-) were selected [1-3]. It should be noted that, ligand L is in the cis or trans position to the dihydrogen ligand. To carry out this project, the initial structures of the above complexes were optimized by Gaussian09 computing software at the BP86 and B3LYP levels and using the def2-TZVPP basis set. Then, the values of total interaction and stabilization energies, cooperative energy and the length of $M–(\eta^2\text{-}H_2)$, M−CO and M–L bonds in the optimized complexes were calculated and compared. Then, using NBO calculations, the amount of the natural charges of atoms, hybrid orbitals and bond orders were checked in each complex. Good correlations were observed, only in trans isomers, between the values of positive cooperative energies with the length and Wiberg bond order of the $M–(\eta^2\text{-}H_2)$ bond. The lowest bond order and the longest $M–(\eta^2\text{-}H_2)$bond length were observed for the complexes that have the highest values of anticooperative energies between $(\eta^2\text{-}H_2)–M(CO)_4$ and $M(CO)_4–L$ bonds. Also, in all the trans complexes, the nature of bondswas investigated by the Energy Decomposition Analysis (EDA) method.

Keywords:Theoretical Study, Dihydrogen complexes, Interaction and stabilization energies, NBO calculation, EDA analysis

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Zinc/Cobalt-based metal-organic framework (Zn/Co-MOF) compositeassuperhydrophobic and superoleophilic materialfor potential oil-water separation application

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Recently, porous crystalline materials consisting of organic ligands and metal ions, called metal-organic frameworks (MOFs), have been attended by a wide range of researchers and industries. These nanostructures have attracted a lot of interest in a wide range of applications, due to their superior unique structural features including high porosity, tunable pore size, specific surface area, and versatile performance[1], [2]. Zeolitic imidazolate frameworks (ZIFs) are a category of MOFs with the same structures as zeolites. They have been built upon 4-connected nets of tetrahedral units, wherein metal ions, such as Zn^{2+} or Co^{2+}, are linked through N atoms in diatopic imidazolate anions. In this study, the Zn/Co-MOF nanocomposite was synthesized and applied to the polyurethane (PU) foam for potential oil-water separation application.Crystalline and structural characteristics of the synthesized nanocomposite were evaluated by X-ray diffraction (XRD)and fourier transform infrared spectroscopy (FTIR). The obtained results show that nanocomposite has been well synthesized. The morphology of the fabricated nanocomposite was studied by field-emission scanning electron microscopy (FESEM). According to the obtained results, ZIF-8 nanocrystals with an average particle size of about 100 nm have well covered the surface of ZIF-67 rods. The elemental composition of the synthesized product by EDS analysis exhibits the presence of Co, N, Zn, O, and C atoms, confirming the successful synthesis of Zn/Co-MOF nanocomposite. The MOF/PU foam exhibits superoleophilic and superhydrophobic properties. The water and oil contact angle were measured and found to be 119° and 0°, respectively.Moreover, the MOF/PU foam showed the capacity to absorb oil or organic solvents in about 20 times its weight.

Keywords:Metal-organic frameworks, superhydrophobic, superoleophilic

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Synthesis and characterization of MXene/metal-organic frameworks (MXOF) nanocomposite for dye removal application

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Organic dyes are the most important organic pollutants released from wastewater by different industries such as textile, printing, paper, and cosmetic industries[1].Their non-biodegradable nature, toxicity, and potential adverse effects on human health have made them a big serious environmental concern[2]. Among various wastewater treatment approaches, adsorption-based processes, due to their simplicity, high efficiency, and reliability, have gained immense attention. Recently, a new class of two-dimensional transition metal carbides, nitrides, and carbonitrides, named MXenes were discovered by researchers at Drexel University. MXene NSs have a general formula of $M_{n+1}X_nT_x$(n=1–3)[1]. On the other hand, metal-organic frameworks (MOFs), as relatively new emerging nanoporous crystalline materials, possess a large specific surface area, tunable pore size, and high porosity. Zeolitic imidazolate frameworks (ZIFs) are a class of MOFs. ZIF-8 is a typical representative of ZIF materials, which is a kind of albite zeolite with a nanoporous structure [3].In this study, a zinc-based metal-organic framework (MOF) decorated MXene (MXOF) nanocomposite was successfully synthesized [4] and utilized for the adsorptive removal of organic dyes from wastewater. Acid Red 88 (AR88) was selected as the model organic contaminant owing to its stable molecular structure and various application in the textile industry. Investigating the morphology of MXOF by field-emission scanning electron microscopy (FESEM)revealed the formation of crystalline spherical particles of ZIF-8 with an average particle size of ~450 nm over MXene NSs. Fourier transform infrared spectroscopy (FTIR)and X-ray diffraction (XRD)were also carried out to study, the structural and crystalline characteristics of MXOF. According to the results of the Brunner-Emmet-Teller (BET) analysis, the specific surface area and average pore size of the MXOF nanocomposite were found to be 1232.5 m^2/g and 0.5564 cm^3/g, respectively. Then, thedye absorption was studiedshowing a high adsorption capacity of 191.44 mg/g. The absorption isotherm and kinetics followed Temkepinisotherm model and pseudo-second-order kinetic model, respectively.

Keywords:Adsorption, Dye removal, Metal-organic frameworks; MXene nanosheets

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Facile synthesis of muscovite-supported metal-organic framework (MUS@MOF) composite forpotential antibacterial activity

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Uncontrollable bleeding has been considered one of the leading causes of death around the world. Thus, the development of new wound dressing materials with enhanced hemostatic properties is quite necessary. Meanwhile, bacterial infection is a crucial issue that can impair wound healing, as the blood clot can become a hotbed of bacterial growth and cause wound inflammation. So, today researchers focus on new materials and composites that enhanced the antibacterial properties of wound dressing.Metal-organic frameworks (MOFs), as relatively emerging crystalline nanoporous materials, have been gaining many interests thanks to their large specific surface area, high porosity, adjustable pore size, versatile functionality, and enriched host-guest chemistry. Among the MOFs, Cu-based MOF with antibacterial properties has been developed, recently [1].On the other hand, Muscovite (also known as common mica, isinglass, or potash mica) is a hydrated phyllosilicate mineral of aluminum and potassium. According to the good properties of Muscovite and MOFs, we intend to synthesize and characterize this composite for potential application in wound dressing.Crystalline structure, chemical structure and bounds, morphological, and elemental analysis of MUS@MOF nanocomposite were carried out by X-Ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), field-emission scanning electron microscopy (FE-SEM) and Energy Dispersive X-ray Spectroscopy (EDS), respectively. The analysis of the XRD and FTIR results confirmed the successful synthesis of MUS@MOF nanocomposite. The FTIR revealed that the MOF interacted with the muscovite surface.TheEDS analysis also exhibited the presence of Cu, Si, Al, O, and C atoms, confirming the successful synthesis of MUS@MOF nanocomposite.FE-SEM images showed that MOFs with nanometer particle size (minimum 18.38 nm, maximum 39.63 nm) have been well synthesized on two-dimensional (2D) muscovite sheets.

Keywords:Metal-organic framework, muscovite,antibacterial.

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Application of tropine as a suitable base for the preparation of an active catalyst in acceleration of synthesis of 1,2,4-triazolo[4,3-*a*]pyrimidines

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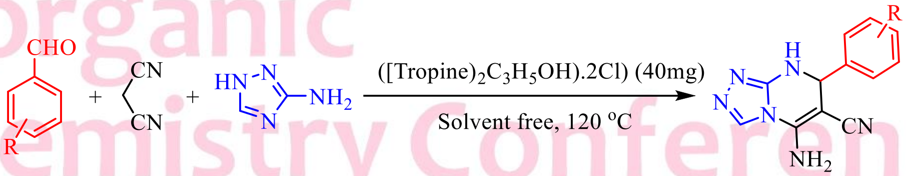
In recent years, dicationic ionic liquids (DILs) have attracted increasing interest, finding unique applications as electrolytes, stationary phases in gas chromatography, lubricants, catalysts, fuel cells, solar cells, solvents in high temperature organic reactions [1].DIL's cationic heads, the linker and the outer chains caused structural variability, high tunability, low volatility, high thermal stability and lower ecotoxicity to compare with parental monocationic ionic liquids. Tropine or 3-tropanol is an important member of azabicyclo compounds which contain a tropane ring.Pyrimidine and its derivatives are important heterocyclic compounds and the diversity of their chemical and biological importance have made them more vital in pharmaceutical chemistry [2]. On the other hand, triazole is a five-membered heterocycle with three nitrogen atoms which one of its isomers is 1,2,4-triazole. Among these compounds 3-amino[1,2,4]triazole derivatives which are composed of two rings, one pentamerous and the other senary, connected by a nitrogen bridge, have the ability to induce the growth of the cancer cells in the thyroid gland of rats [3].In this work, a green and efficient procedure is reported for the synthesis of 1,2,4-triazolo[4,3-*a*]pyrimidine derivatives using a suitable dicationic molten salt based on tropine ([(Tropine)$_2$C$_3$H$_5$OH].2Cl). The simple catalyst preparation, straightforward separation and recovery of the catalyst from the reaction mixture, simple work-up method requiring no special separation procedure, solvent-free conditions, short reaction timesand high yields of the products are the significant points of interest of this study.



Keywords: Dicationic molten salt, pyrimidines, Tropine, [(Tropine)$_2$C$_3$H$_5$OH].2Cl.

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Preparation, characterization and investigation of thermal and antimicrobial behavior activity of some new bis-imine Zinc(II) complexes

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Schiff bases or imines are one class of important ligands in the Inorganic chemistry. The easily coordination of these ligands to various metal ions causes the researchers to synthesized and characterized them that strongly develpoe the coordination chemistry in many aspects.. Schiff bases and their metal complexes have various applications especially in medicinal fields. These compounds have been proved to affect on a variety of bacteria and fungi. These compounds have also antioxidant properties and well show anticancer activity[1-3].

In this research, a new double Schiff base ligand (1E,1'E,2E,2'E)-N,N'-(butane-1-4 diyl)bis(3-(2-methoxyphenyl)prop-2- en -1- imine) and its zinc(II) complexes with the general formula $ZnLX_2$, ($X = Cl^-$, Br^-, SCN^-) were synthesized in ethanol solvent. Physical and spectroscopic methods and techniques such as IR, UV-Visible, H and C NMR, molar conductivity and melting point were used to identify and investigate the synthesized compounds.Thermokinetic study of thermal decomposition of the compound was performed to evaluate some kinetic activation parameters during the decomposition processes. In addition, the antifungal and antibacterial activity of the ligand and complexes *in vitro* against two gram-positive bacteria Staphylococcus aureus, Bacillus subtilis and two gram-negative bacteria Escherichia coli, Pseudomonas aeruginosa and two strains of fungi (Aspergillusaurinosa and Candidaalbicans) were investigated.

Keywords:Synthesis, Zic(II) complexes, Antibacterial, Antifungal

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A novel Palladium(II) complex of α-keto arsonium ylide: Synthesis, characterization, and application in the Suzuki−Miyaura cross-coupling reaction

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A new Palladium(II) complex having α-keto stabilized arsonium ylide ligand with the general formula $[Pd(\mu\text{-}Cl)(Ph_3AsCHC(O)C_{10}H_7)]_2$ was synthesized and applied as a performance catalyst to achieve palladium (II)-catalyzed Suzuki-Miyaura reaction of arylboronic acid with aryl bromides. This complex was characterized by CHN analysis,FT-IR and multinuclear (^{1}H and ^{13}C) NMRspectroscopic techniques. For more than 30 years, Pd-catalyzed homogeneous bonding reactions have been used in C-C coupling reactions such as Heck, Sonogashira, Suzuki, Kumada, Negishi, Hiyama, etc. [1–3].Suzuki-Miyaura reactions are environmentally benign, have a high tolerance to different functional groups, are easily available, have high stability of used substrates, and are widely used to form natural products, biologically active pharmaceuticals, and agrochemicals [4]. Based on this, we decided to evaluate and compare the catalytic activity of catalyst synthesized by Suzuki-Miyaura cross-coupling reactions. This catalyst showed high catalytic activity in the C-C cross-coupling reaction.

Keywords:Arsonium ylide, Homogenization,Pd(II) complex,Suzuki-Miyaura reactions

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Supramolecular frameworks of zinc-pyridine-2,6-dicarboxylic acid compound: synthesis and characterization

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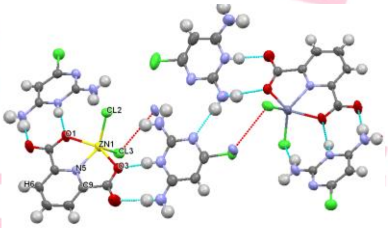
New Zinc-Pyridine-2,6-dicarboxylic acidsupramolecular compound was synthesized from zinc chloride and two ligands (pyridine-2,6-dicarboxylic acid and 2,4-diamino-6-chloropyrimidine) by using sonochemical and side branch tube methods. The compounds were characterized by X-ray diffraction and crystallography, FT-IR, XRD, TGA-DTA, ^{1}HNMR, ^{13}CNMR, EDS, SEM and TEM techniques. The compound is a supramolecule with five coordination in the monoclinic crystal system with space group $P2_1/c$. By examining the angles and bond lengths around the central atom, a distorted square pyramidal geometric shape has been proposed for the compound. Non-covalent intermolecular forces have a great contribution in creating the supramolecular structure of this compound. Intermolecular and intramolecular interactions, including hydrogen bonds such as (O...H) and π-π interactionsbetween aromatic ringssuch as (C...H, C...C, N...H and C...N). Particles of this compound has a cubic morphologyand the particle size is 300-500 nm.



Keywords:Supramolecular, Zinc, Pyridine-2,6-dicarboxylic acid, 2,4-Diamino-6-hloropyrimidine

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Synthesis and characterization of mercury(ii) supramolecular compoundfrompyridine-2,4-dicarboxylic acid

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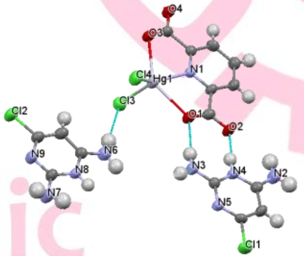
New supramolecular compound was synthesized frommercury (II) chloride and two ligands (pyridine-2,6-dicarboxylic acid and 2,4-diamino-6-chloropyrimidine) by using sonochemical and side branch tube methods. These compounds were analyzed using FT-IR, TGA-DTA,^{1}HNMR, ^{13}CNMR,EDS, SEM and TEM. Also, the structures of these complexes were determined by X-ray diffractionand crystallography. According to the analyzes performed and the investigations carried out, the compound is a supramolecule with five coordination in the monoclinic crystal system with space group P-1. By examining the angles and bond lengths around the central atom, a distorted square pyramidal geometric shape has been proposed for this compound.Also, intermolecular and intramolecular interactions that include hydrogen bonds such as (O...H and N...H) and π-π interactions between aromatic rings such as (C...H, C...C and C. ..N) have a great effect on the stability of the supramolecular structure. Particles of this compound has a rod morphology and the particle size is 200-300 nm.



Keywords:Supramolecular, Mercury (II), Pyridine-2,6-dicarboxylicacid, 2,4-Diamino-6-chloropyrimidine

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Synthesis and catalytic applications of metal-organic framework nanocomposite modified by ferric ions containing sandwich polyoxometalate

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In this thesis, B-type sandwich polyoxometalate of $[(PW_9O_{34})_2Fe_4(H_2O)_2]^{6-}$wasimmobilized into porous composite cavities of Cr-MIL-101 by simple anion exchange[1,2]. The formation of $P_2W_{18}Fe_4$@MIL-101 nanocomposite was confirmed by FT-IR, TGA, BET, SEM, EDX, ICP, BET and powdery XRD methods. The catalytic activity of nanocomposites was investigated in oxidation of sulfides to sulfons with H_2O_2 at room temperature[3]. The effect of temperature on stability and catalytic activity of the $P_2W_{18}Y_3$@MIL-101 was investigated. The effects of different dosages of catalyst, type of solvent, reaction time, amount of oxidant in this catalytic system were investigated. The new $P_2W_{18}Fe_4$@MIL-101 nanocomposite exhibited well recyclability and reusability in at least five consecutive reaction cycles without significant loss of activity or selectivity.

Keywords:B-typesandwich polyoxometalate,Cr-MIL-101,Sulfides, Homogeneous and heterogeneous catalysts

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A theoretical study on the anionic metal bis(ditholate) complexes $[M(S_2C_2R_2)_2]^{2-}$(M=Zn(II), Cd(II), Hg(II); R=H, CH_3, CN)

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Metal bis-dithiolene complexes have indeed been the subject of extensive study by chemists in both the inorganic and organic fields in recent decades. This is due to their wide range of applications in various areas, including conducting and magnetic molecular materials, as well as their relevant optical properties [1]. Dithiolenes exist in three different forms with varying charges, which contribute to their redox activity and ability to form highly electron-delocalized complexes. However, the term dithiolene is used without taking into account the formal oxidation state of ligands to describe their noninnocent character in several metal complexes [2]. In this work, the interactions between the fragments in metal bis(1,2-dithiolate) complexes complexes $[ML_2]^{2-}$ (M=Zn(II), Cd(II), Hg(II); L= $S_2C_2H_2^{2-}$ (edt^{2-}), $S_2C_2Me_2^{2-}$ (dmedt^{2-}), $S_2C_2(CN)_2^{2-}$ (mnt^{2-})) have been investigated,at BP86/def2-TZVP and M06/def2-TZVP levels of theory. Four types of interaction energies between the fragments as well as the total interaction energies of the complexes [3–5] were calculated and compared. An Energy Decomposition Analysis-Natural Orbital for Chemical Valence (EDA-NOCV) was also performed to study the nature of metal−bis(dithiolate) interactions in these complexes.The results showed that among the metal complexes studied here, the Zn(II) complexes have the largest values of interaction energies. On the other hand, the values of total interaction energies of $[M(edt)_2]^{2-}$ and $[M(dmedt)_2]^{2-}$ complexes are similar or close together and both are larger than those for $[M(mnt)_2]^{2-}$ complexes. The EDA-NOCV results showed that the electrostatic interactions have considerably more contribution to the total attractive interactions compared to orbital interactions and, as expected, the contributionof dispersion forces in all complexes is inconsiderable.

Keywords: Interaction Energy, Nature of Bond, 1,2-Dithiolate Ligands, Metal Complexes.

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Strength and nature of metal-dichalcogenolate bond in homoleptic metal bis(1,2-dichalcogenolate) complexes $[M(C_3E_5)_2]^{2-}$(E=S, Se; M=Ni(II), Pd(II), Pt(II)); A theoretical study

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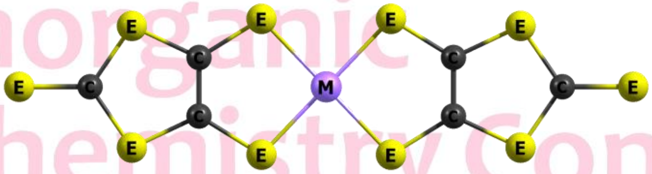
"Dichalcogenolene" is a general term used to describe unsaturated bidentate ligands in the form of $E^\wedge E^{x-}$ units with chalcogen donor atoms (E=S, dithiolene; Se, diselenolene; Te, ditellurolene) and different charges (x=2, 1, 0) [1]. This class of ligands includes ene-1,1- and ene-1,2 dichalcogenolates(where x=2) and also the corresponding oxidized species (neutral and monoanionic). However, the study of 1,2-dichalcogenolene ligands in coordination chemistry has been more extensive, resulting in a greater number of reported complexes [2].In this work, the interactions between the fragments in homoleptic square-planar d^8 metal bis(1,2-dichalcogenolate) complexes $[M(C_3E_5)_2]^{2-}$(E=S, Se; M=Ni(II), Pd(II), Pt(II)) have been investigated,at BP86/def2-TZVP and M06/def2-TZVP levels of theory. Four types of interaction energies between the fragmentsas well as the total interaction energies of the complexes [3–5] were calculated and compared. An Energy DecompositionAnalysis-Natural Orbital for Chemical Valence (EDA-NOCV) was also performed to study the nature of metal–bis(dichalcogenolate) interactions in these complexes. The results showed thatthe total interaction energiesare decreased by changing the chalcogen atom from sulfur to selenium. The analysis of metal–bis(dichalcogenolate) interaction showed that the orbital interactions have less contribution to the total attractive interactions compared to electrostatic interactions.



$[M(C_3E_5)_2]^{2-}$
E = S, Se
M = Ni(II), Pd(II), Pt(II)

Keywords:1,2-Dichalcogenolate, Metal Complexes, Interaction Energy, Nature of Bond.

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Investigating the effect of pressure and concentration on permeability of methylene blue through a geopolymeric membrane based on phosphorus slag

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The effluent from textile factories carries various types of hazardous chemicals through a few stages of manufacturing processes and also known to contain highly coloured species[1].Not only colours, the break down products are toxic and harmful to human and living organisms, raising attention to the worldon the importance of removing the dyes from the wastewater.Recently, membrane separation techniques which used polymeric and inorganic materials have also been introduced for dye removal[2].In this article, 3 pre-prepared membranes p1, p2 and p3 were tested to test the permeability and removal of methylene blue effluent. Each of the membranes were compacted with distilled water for 25 minutes before starting the effluent test. In the next step, the membranes were tested at 3 pressures of 1, 2, and 3 bar and concentrations of 20, 30, and 40 ppm for 30 minutes. All 3 membranes are based on phosphorus slag and compounds of mullite and microsilica with sodium hydroxide and sodium silicate alkaline activators. The results showed that all 3 membranes have a rejection rate of over 85% in all 3 tested pressures and concentrations. By comparing the results in order to obtain the best result, taking into account the optimal permeability of the membrane, p2 is the selected membrane with a separation rate of 97% and a permeability of $69\times 10^{-7}\ m^3/m^2s$ at 3 bar pressures and 20 ppm concentrations. According to the results obtained from the BET analysis, the selected membrane has a pore size of 12.42 nm and a porosity of 20.84%.In the spectrum of the sample analyzed by FT-IR, there is a broad and strong main absorption band that appeared in the range of $979 cm^{-1}$, which is related to the asymmetric stretching vibrations of Si-O(Al) in the tetrahedronSiO4 and asymmetric stretching of Al [3].

Keywords: Membrane, Phosphorus Slag, Mullite, Geopolymerization

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Enhancing Oxygen-Evolution Reaction in Alkaline Conditions with Anodized FeNi Alloy

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The efficient and durable catalysis of the oxygen-evolution reaction (OER) is crucial for the conversion of energy through the water-splitting process. The OER, which involves the oxidation of water, can provide electrons for reduction reactions of H_2O, CO_2, and N_2, leading to the production of valuable compounds. In this study, a FeNi alloy foam with a Ni:Fe ratio of 1:1 was anodized at 50 V in a two-electrode system in a KOH solution (1.0 M). The resulting material was characterized using various techniques including Raman spectroscopy, diffuse reflectance spectroscopy (DRS), X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive X-ray spectrometry (EDX), transmission electron microscopy (TEM), and high-angle annular dark-field imaging (HAADF)-scanning transmission electron microscopy (STEM). This FeNi alloy foam was found to be an efficient and durable electrocatalyst for the OER in a KOH solution (1.0 M). The onset overpotential for the OER, based on extrapolation of the Tafel plot, was 225 mV, while the overpotentials for current densities of 10 and 30 mA/cm^2 were observed at 270 and 290 mV, respectively. Additionally, a low Tafel slope of 38.0 mV per decade was observed for the OER. To investigate the mechanism of the OER, in situ surface-enhanced Raman spectroscopy was employed to detect high-valent Fe and Ni species formed on the electrode surface.

Keywords: Artificial Photosynthesis, Nickel, Iron, Oxygen-evolution Reaction

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Adsorption of Metronidazole Drugin MOF by Monte Carlo Simulation

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Metal-organic frameworks (MOFs) are a new type of nano-porous [1] coordination networks [2] which composed of metal ions or clusters linked by organic ligands [3]. Metal-organic frameworks due to the characteristics of both groups, are considered as suitable materials in drug delivery [4, 5]. Generally, in recent years, MOFs have received much attention which is attributed to their unique surface areas and permanent porosity. MOFs are showed great promise in various applications such as gas storage, gas separation, shape/size selective catalysis, drug storage and delivery, imaging, and sensing [6]. Therefore, grand canonical Monte Carlo (GCMC) simulations were used in this work to investigate the adsorption behavior of metronidazole in MOF-5 as a carrier of drug [7].A typical GCMC simulation was carried out for 1000000 step, in which the first 200000 step were used for equilibration followed by 800000 steps to sample the desired properties. All the simulations are performed at 36.5 and 37.5 °C and at pressures varying between 0-100 kPa. The results showed that the maximum adsorption of metronidazole in MOF-5 is 43 units per cellat 100 kPa and 37.5 °C. In general, metronidazole adsorption on MOF-5 in the aqueous environment is similar to the adsorption in pure MOF-5 at the all ranges of investigated temperatures and pressures. Also, metronidazole uptake in other metal organic frameworks showed that MOF-177 has the highest drug adsorption than MOF-5. Finally, the results of the present study suggested MOF-5 has a suitable potential as a carrier of metronidazole.

Keywords: Metal Organic Framework, Metronidazole, Drug Carrier, Simulation

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Selective Carbon−Carbon Bond Forming Reductive Elimination from Cycloplatinated (IV) Complexes

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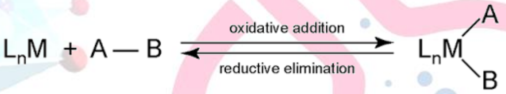
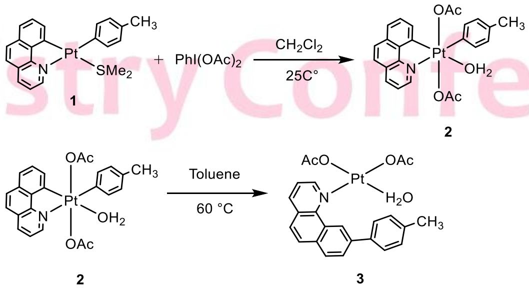
Oxidative addition involves the attachment of two groups A−B to a metal complex of relatively low oxidation state. This produces a new complex with an oxidation state two units higher than before.Reductive eliminationreaction is exactly the opposite of the oxidative additionreaction during which A and B are removed from metal center, during this process the oxidation number of the central metal decreases by two units.Since oxidative addition and reduction-elimination reactions are among the basic steps in many catalytic cycles,mechanistic investigations need to be studied more in depth to provide a useful basis for further developments.



In the present work, complex[Pt(bhq)(*p*-Me-C_6H_4)(H_2O)($(OAc)_2$)], **2**, in which bhq = deprotonated benzo[h]quinolineis prepared through the reactionof [Pt(bhq)(*p*-Me-C_6H_4)(SMe_2)], **1**with 1 equiv of PhI$(OAc)_2$ via anoxidative addition (OA) reaction.Complex **2** was fully characterized by means of^{1}H, ^{13}C, ^{195}Pt NMR and ESI-Mass spectroscopic techniques. Density functional theory (DFT) calculationssignify that the OA reaction initiated by a nucleophilic attack of the platinum (II) central atom of **1**, on the Iodine(III) atom of PhI$(OAc)_2$while ithad commenced by a nucleophilic substitution reaction of coordinated $SMe_2$with H_2O.In the next step **2**undergoselective C(sp^2)−C(sp^2)bond forming reductive elimination reaction at elevated tempreture to form new Pt(II) complex **3**. DFT calculations showed that the reductive elimination reaction occurs through three-center concertmechanism (Scheme 1).



Scheme 1. Oxidative addition and reductive elimination reactions of cycloplatinated complexes.

Keywords: Platinum Complexes, Oxidation-addition Reactions, Reductive Elimination Reactions

The Study on Structural and Optical properties of Binuclear Platinum Complexes with various bidentate Ligands

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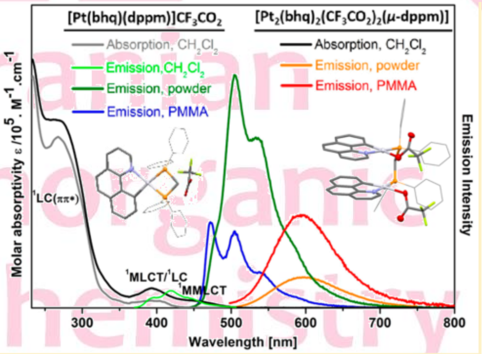
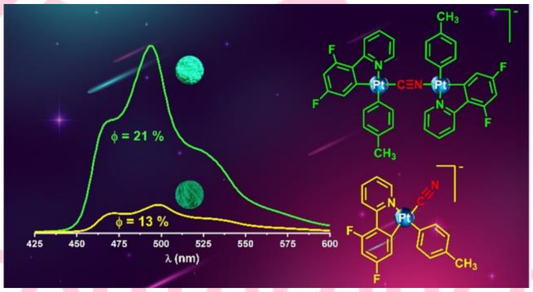
The cyclometalated organometallic compounds have been extensively investigated by many research groups because of their catalytic reactivity in organic synthesis, diverse medical and industrial applications. In particular, cyclometalated platinum(II) complexes have been widely developed for their applications in organic light-emitting diodes (OLEDs), vapor sensing, oxygen sensing and DNA applications. However, most applications are restricted to mononuclear cyclometalated organoplatinum(II) complexes; in which different kind of electronic transitions, such as metal to ligand charge transfer (MLCT), ligand centered (LC) and ligand to ligand charge transfer (L′LCT), are involved in any related emission operation. Furthermore, binuclear platinum complexes have drawn attention on account of their particular photophysical properties [1-4]. There are metal-metal to ligand charge transfer (MMLCT) transitions in binuclear platinum(II) complexes, when Pt···Pt distance is less than 3.5 Å (sum of two platinum van der waals radius), leading to marked red shifts compared to the corresponding emission peaks of mononuclear platinum complexes.





Keywords: Platinum, Binuclear, Luminescence, Phosphine, Cyanide

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Preparation of Ni-Fe layered double hydroxide/ graphitic carbon nitride nanocomposite for enhanced sonocatalytic degradation of tetracycline hydrochloride

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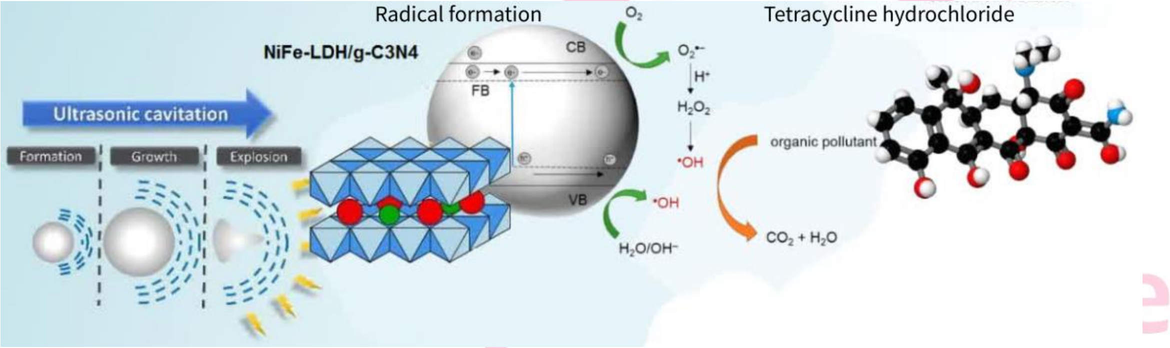
Pharmaceutical compounds, including antibiotics, are a major source of micropollutants in water, leading to antibiotic-resistant pathogens and human health problems. Advanced Oxidation Processes (AOPs) [1] and sonochemistry are effective methods to remove these pollutants. Layered Double Hydroxide (LDH) [2] and graphitic carbon nitride ($g\text{-}C_3N_4$) are promising materials for adsorption and degradation of heavy metals and pollutants. However, $g\text{-}C_3N_4$ has low efficiency due to its structure and low utilization of visible light. To overcome this, researchers have loaded $g\text{-}C_3N_4$ [3]with metal atoms and non-metallic elements, and fabricated microstructures. The synthesis of NiFe_LDH/$g\text{-}C_3N_4$ double layered hydroxide nanocomposite shows potential for efficient sonocatalytic degradation of pharmaceutical pollutants. A NiFe-LDH/$g\text{-}C_3N_4$ nanocomposite was synthesized and used for sonocatalytic degradation of tetracycline from solution. The green conditions, simple catalyst preparation, and straightforward separation and recovery of the nanocomposite from the reaction mixture are the significant points of interest of this study.



Keywords: Graphitic Carbon Nitride, Layered Double Hydroxide, Sonocatalytic Degradation, Tetracycline Hydrochloride

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Synthesis, Characterization and Catalysis by Highly Active CationicCopper(I) Complexes in the Cycloaddition of Azides and Alkynes

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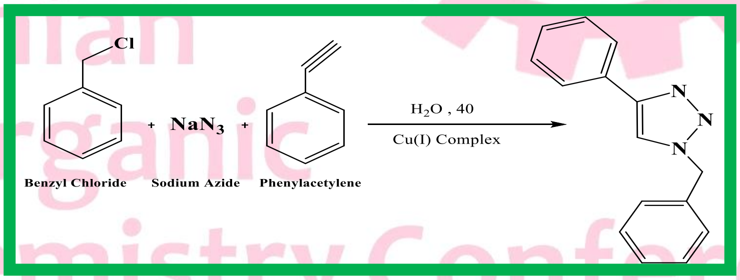
Huisgen 1,3-dipolar azide–alkyne cycloaddition is an important reaction in click chemistry and is applied to the preparation of biologically active compounds and biomolecules toward preclinical and clinical applications.3 Meldal and coauthors4 and Sharpless and coauthors5 independently reported the copper-catalyzed azide–alkyne cycloadditions (CuAAC), in which a Cu(I) catalyst promotes the reaction regioselectively to afford 1,4-substituted 1,2,3-triazols[۱].Among the most genuine examples of “click chemistry”thecopper-catalyzed Huisgen 1,3-dipolar cycloaddition of azidesand terminal alkynes (CuAAC)(Scheme 1) has found widechemical applications in many fields,3,4rendering 1,2,3-triazolesunder mild and neutral conditions with high efficiency[۲]. After many years of research, it was proven that the Cu(I)-catalyzed azide-alkyne cycloaddition (CuAAC reaction) could be performed under various conditions according to the need of click chemistry using the catalysis of various copper salts that generate Cu(I) sources in situ [3,4].In this work, we have investigated the synthesis, characterization and catalysis by highly active cationic complexes of copper (I) in the cycloaddition of azides and alkynes.



Keywords: CuAAC Reaction, Cycloaddition of Azides and Alkynes, Click Reaction, Cu(I) Complex

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Tris(2-aminoethyl)amine-based metal complexes as newpH-sensitive drug vehicles

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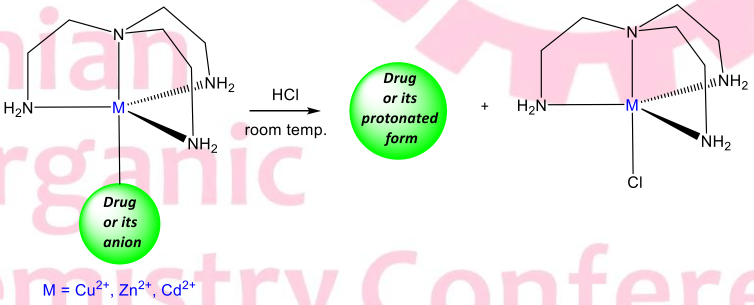
Transition metal complexes can be designed as prodrugs that are inactive under normal physiological conditions but become unstable with changes in the environment such as changes in pH and redox status. By deactivating the drug before reaching the target, side reactions can be reduced, and adverse side effects can be avoided [1]. The delivery of drug favipiravir (FAV) is challenging due to its limited solubility in water and common organic solvents [2]. Given that the safety of FAV has already been demonstrated by its widespread use as an anti-influenza drug in Japan [3] further research into the more effective delivery of this drug is warranted. In an attempt to solve the delivery problem, we have used the biocompatible tris(2-aminoethyl) amine (tren) as a basic ligand for the preparation and characterization of a highly water-soluble drug-carrier complex with a zinc center that can carry the drug FAV, as an anion, and then release the molecule at a site where the pH is in the range of 3 to 5.5. We also report a theoretical study that shows the same nature of metal−ligand bonds for *N/O*-coordinated FAV and supports experimental observations indicating that FAV can easily leave the drug carrier in acidic conditions [4]. Our results indicate that this drug vehicle is suitbale for delivery of some other drugs, specially drug amifampridine.

Keywords: Tris(2-aminoethyl)amine, Favipiravir, Drug Carrier, COVID-19.



Scheme 1. The release of drug or its protonated form, from adrug-carrier complex and formation of [M(tren)Cl]cation(M = Cu^{2+}, Zn^{2+}, Cd^{2+}) as a drug vehicle, in the acidic conditions.

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Synthesis modulation as a useful tool to improve oxidation desulfurization in POM@UiO-66 nanocomposite

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Sulfur-containing compounds in petroleum products cause environmental pollution. Therefor, environmental concerns make restrictions to the sulfur content of fuels more and more exigent. Among the desulfurization processes, the oxidative desulfurization (ODS) technology has become as one of the most propitious techniques for obtaining fuel oil [1]. Porous metal-organic frameworks (MOFs) are a new porous crystalline materials have attracted significant attention as efficient catalysts ODS [2,3]. Defect engineering is as an advantageous synthetic tool for the introduction of structural point defects into MOFs to tune the physical-chemical properties and to modify their structure in oder to superior catalytic properties [4,5]. In this study, POM@UiO-66 nanoparticles were synthesized by encapsulation of polyoxometalate (POM) particles into a modulated-UiO-66 as catalyst. For this purpose, a monocarboxylic acid was used as the modulating agent to promote defect formation in UiO-66 and then was employed to investigatec atalytic activity. The experimental results showed that the novel POM@UiO-66 nanocomposite exhibits excellent efficiency for oxidative desulfurization in comparison with neat UiO-66 and some typical catalysts.

Keywords: Metal-Organic Frameworks, Polyoxometalate, Defect, Desulfurization

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Fabrication of Novel WO_3 /$NiCo_2O_4$ magnetic photocatalysts **with UV-light driven photocatalytic activity in MB degradation in an aqueous solution**

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This work presents the preparation and characterization of a novel synthesized Tungsten trioxide and Nickel Cobaltite hybrid(WO_3/$NiCo_2O_4$) and investigates its photocatalytic activity for Methylene Blue (MB) decomposition under UV radiation. The nanopowder of WO_3/$NiCo_2O_4$was synthesized by hydrothermal method. The samples using various mass ratios (1:1, 1:2, and 2:1) of WO_3 and $NiCo_2O_4$ were prepared under the same conditions. Several techniques, such as XRD,SEM,TEM,BET,DRS, and VSM were used to characterize the structure and morphology of the products.The WO_3/$NiCo_2O_4$photocatalysts exhibit enhanced photocatalytic removal efficiency towards the target pollutant in comparison to pristine $NiCo_2O_4$ and WO_3. Although The valence band potential (EVB) of WO_3 reaches approximately 2.7–3.4 eV which is a suitable potential for oxidation but single component WO_3 has displayed low photocatalytic performance despite UV light or visible light range because of its low conduction band edge position (+0.5 V vs. NHE at pH = 0) [1]. $NiCo_2O_4$ is used as a valuable candidate for photocatalysis as it provides a redox couple of Co^{3+}/Co^{2+} and Ni^{3+}/Ni^{2+}which provide considerably more catalytic active sites when compared with NiO and Co_3O_4. However, the practical use of $NiCo_2O_4$ as photocatalytic material is minimal due to its low efficiency and long-term stability [2]. The aim of the synthesis of WO_3/$NiCo_2O_4$hybrid samples is to improve the photocatalytic properties of semiconductors and to solve the challenges that were discussed. The advantage of the above research is the use of this photocatalyst to increase the efficiency of wastewater treatment and lower the costs to remove colored pollutants. The synthesized material must have magnetic properties to reuse the synthesized sample for multiple cycles in the photocatalytic process.The magnetic separation of WO_3/$NiCo_2O_4$ nanocomposite dispersed in an aqueous solution by employing a permanent magnet to provide a magnetic field is possible [3].

Keywords: Dye, Nanocomposite, $NiCo_2O_4$, Photocatalyst, WO_3

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Zif-67 Drivate Nanocomposite as Efficient Peroxymonosulfate Activator for Degradation of Sulfamethoxazole

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The importance of clean water to human health necessitates the development of cutting-edge techniques for the elimination of all organic contaminants [2, 3]. One of the most promising strategies for getting rid of resistant organic pollutants is the employment of persulfate-based advanced oxidation processes (AOPs), which are commonly employed in the degradation of organic pollutants[3, 4].In order to promote catalytic activity and activate peroxymonosulfate (PMS) to degradation sulfamethoxazole (SMZ), N-doped porous carbon (Co_3O_4@N-C) materials were prepared by one-pot pyrolysis of a ZIF-67 powder under N_2 atmosphere, followed by oxidation under air atmosphere (200 °C). Co_3O_4@N-C were synthesized using 2-methylimidazole as a nitrogen source and a competitive ligand, which not only affects nucleation and development of the crystal but also stimulates the creation of active Co-N sites. Co_3O_4@N-C nano-architecture is a non-toxic, efficient, and stable PMS activator with a large specific surface area (250 m^2 g^{-1}). The presence of Co_3O_4@N-C was studied in relation to a number of operational factors, such as SMZ concentration, catalyst dose, temperature, and pH. Complete degradation of SMZ (50 M, 100 mL) was accomplished in 15 minutes using the Co_3O_4@N-C composite, which shown improved effectiveness in activating PMS over a broad range of pH (2-10) and varied temperatures.The catalyst was observed to retain its catalytic activity for at least 5 cycles.

Keywords: Degradation, Sulfamethoxazole, ZIF-67, Co_3O_4, Peroxymonosulfate

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Preparation of SBA-16/g-C_3N_4/Fe_3O_4magnetic nanocomposite and kinetic investigation of absorption of cefazolin and cefixime antibiotics on it

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In this research, the absorption kinetics of cefazolin and cefixime antibiotics on SBA-16/g-C_3N_4/Fe_3O_4magnetic nanocomposite as adsorbent was studied. For this purpose, SBA-16/g-C_3N_4/Fe_3O_4magnetic nanocomposite was synthesized in the first step. XRD, SEM and FT-IR analyzes were prepared from the synthesis sample. Then, the absorption kinetics of cefazolin and cefximber antibiotics on the synthesized nanocomposite was investigated. In the second step, the effect of effective parameters on the drug absorption process, including pH, contact time, temperature, drug concentration and adsorbent dose, was studied by using the design of experiments (DOE) software using the response surface method (RSM) and the central composite model (CCD). and the optimal value for each parameter was obtained. Finally, to find the best kinetic model, four kinetic models of zero order, pseudo first order, pseudo second order and Higuchi model were studied under optimal conditions and the obtained results showed that the process of cefazolin and cefixime antibiotics on SBA-16/g-C_3N_4/Fe_3O_4magnetic nanocomposite corresponds to the pseudo-second-order kinetic model.

Keywords: Adsorption; Response Surface Methodology; Cefixime; Cefazolin; SBA-16/g-C_3N_4/Fe_3O_4

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Fabrication and characterizationof new Co(II)-MOF/polyvinylidene fluoride (PVDF) bead composites as visual sensors for detection of industrial acid vapours

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Visual sensors based on Metal-Organic Frameworks (MOFs) in the detection of gases and vapors are known as vapochromic systems. The color change of MOFs is easily visible with the naked eye and is the simplest answer in sensing and detecting gaseous species [1]. In this work, a cobalt-organic framework (Co(II)-MOF) has been perpared by the reaction of mixed bis-pyridyland dicarboxylate linkers under ultrasound irradiation.The composite mixture of these nanocrystals with organic polymer polyvinylidene fluoride (PVDF) was prepared using phase inversion method and the resulting mixture was shaped into composite beads.The sensing properties of the prepared bead composites toward vapors of concentrated industrial acids such as hydrochloric acid (HCl), nitric acid (HNO_3), and sulfuric acid (H_2SO_4), as well as thionyl chloride ($SOCl_2$) vapors were investigated. The color change of nanoparticles was observed from purple to green, yellow, blue-violet and dark green, respectively.

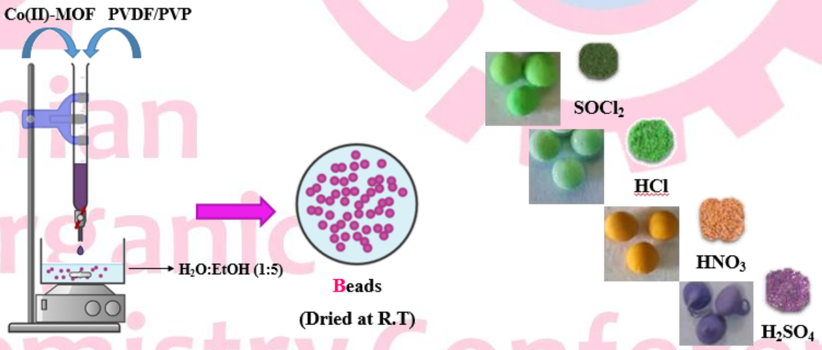

Fig. 1. Preparation and colour change of the composite beads after exposure to acid vapors.

Keywords:Metal–organic Framework (MOF), Sensing, Bead composite

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Cooperative effect between the chalcogen (Ch…N) and dihydrogen (H…H) bonds in the series of XHTe…NCH…HY (X=F, Cl, Br, I, H, Y=Li, Na, BeH, MgH) and FHCh…NCH…HNa (Ch=Te, Se, S) triads

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Focus on the bonds between molecules instead of bonds between atoms, results in the creation of large molecules with unusual structures and different physical and chemical properties, which are useful for various applications [1]. Such interactions lead to a tremendous increase in the variety of crystal architectures and thus properties to be discovered [2].There are some well-known methodologies for evaluating the degree of cooperativity of noncovalent bonds, but herein we emphasize on our proposed methodology that evaluates the origin of the cooperativity of bonds. Cooperative energy of chalcogen and dihydrogen bonds in some ABC triad systems of the typesXHTe…NCH…HY (X=F, Cl, Br, I, H, Y=Li, Na, BeH, MgH) and FHCh…NCH…HNa (Ch=Te, Se, S) were computed and compared at MP2/TZVPPD, BP86/TZVPPD, BP86-D3/TZVPPD, and BP86-D3/QZVP levels of theory. The cooperative energies were evaluated using two different equations/methods, on the basis of interaction energies versus stabilization energies of the triads and corresponding dyads. In addition, a number of good to excellent correlations were observed between the interaction, stabilization, and cooperative energies and change in Te…N and H…H bond lengths upon the formation of triads from the corresponding dyads. All resulting data showed that the strengths of chalcogen (Te…N) and dihydrogen (H…H) bonds increase in the order of H< I < Br < Cl < F, and Be < Mg < Li < Na, respectively. Thus, the shortest Te…N and H…H bond lengths and the largest values of interaction, stabilization, and cooperative energies were observed for FHTe…NCH…HNa triad. Then, the resulting data for the above triad were compared with those for FHSe…NCH…HNa and FHS…NCH…HNa triads. The data showed that the interaction, stabilization, and cooperativity energies decrease in the order of Te > Se > S. Also, it was shown that the more electronegative fluorine atom bonded to chalcogen atom would have no meaningful effect on the strengths of the Ch…N bond and its cooperativity with the H…H bond in present triad complexes, when F−Ch bond is not along Ch…N bond. Finally, the nature of both dihydrogen and chalcogen bonds and the origin of the cooperativity of bonds were evaluated by NBO and EDA analyses [3].

Keywords: Cooperativity, Dihydrogen Bonds, Chalcogen Bonds, Stabilization Energies, Interaction Energies

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The First Row Transitional Metals Effects on Stabilization of Biliverdin Complexes, Theortical Study

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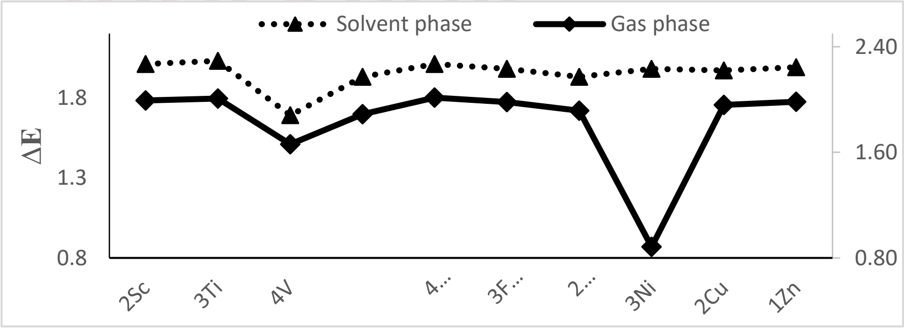
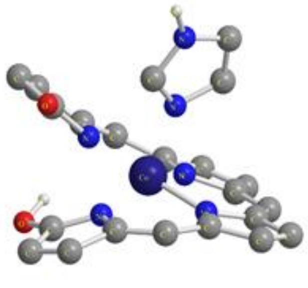
Biliverdin is a product of heme catabolism. It is the pigment responsible for a greenish color sometimes seen in bruises. Biliverdin has been found in excess in the blood of humans suffering from hepatic diseases. Structure of biliverdin from catabolism process of heme is one of the cases that has been less discussed. In this research characterization of biliverdin analogues in the presence of hydroxide as a nucleophile and imidazole as axial ligands was investigated using the B3LYP method and the 6-31G basis set both in gas and solvent phases. Theoretical studies have shown that the absolute energy of the metal biliverdins increase with atomic mass both in gas and solvent phases. By changing the central metal in the structure of billiverdin, some features such as gap energy, hardness and softness, electrophilicicity index and exact polarizability were studied and copmared with iron. the nickel and vanadium biliverdin have the least stability in gas and solvent phases respectively and the titanium biliverdin has the most one in both gas and solvent phases. Calculation of hardness (η) of these complexes confirms these stabilities in which the titanium is the hardest among the other metals. Electrophilicity calculation shows the nickel biliverdin in gas phase and copper in solvent phase are the most electrophile.

Keywords: Hemeoxygenase, B3lyp, First Row Transitional Metal Biliverdin, Heme Degradation




Cobalt Biliverdin

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Investigation of Spin-Charge-Structure in Human Verdoheme Using The DFT Method

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The enzyme heme oxygenase (HO) plays an essential role in the destruction of heme molecules. Heme oxygenase uses dioxygen to open the specific orientation of the porphyrin ring at the position of the α-meso carbon. This enzyme catalyses the degradation of heme to biliverdin IX*α* through three distinct intermediates, *α*-hydroxyheme, *α*-verdoheme, and ferric biliverdin–Iron chelate, at the expense of O_2 and electrons. To elucidate the mysterious mechanism of the oxygenation steps, the atomic-resolution structure of the verdoheme–HO complex has been needed. In this work the structure of Iron verdoheme in complex with Human Heme Oxygenase according to the structure of verdoheme that was solved by Lad et all (PDB Id: 1TWN) (Fig. 1), was studied by density functional theory based B3LYP method and 6-31G basis set. Herein we regard the central metal of the five coordinated human verdoheme as ferrous (Fe^{2+}) and ferric (Fe^{3+}). Many parameters such as the charge of verdoheme and Iron as a central metal, electron distribution, spin multiplicity of the molecule, and proximal substituents effect on the verdoheme ring stabilization and their arrangement were discussed

Keywords: Verdoheme, Human, Density Functional Theory, Structure Optimization

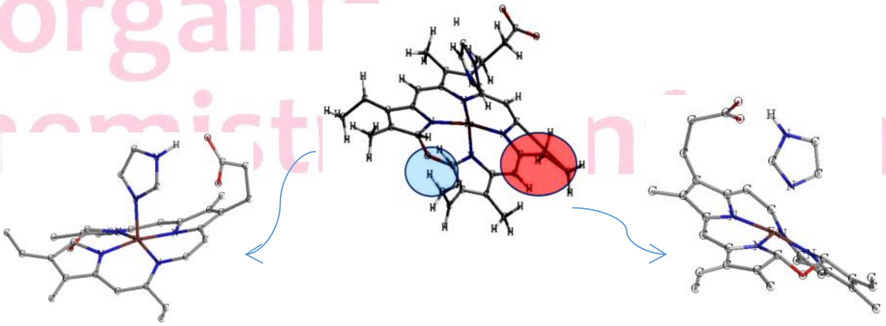

Fig. 1. Input and calculated human verdoheme structures.

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Introduction of a new member of bipyridine-based molten salt containing copper as an efficient and reusable catalyst for the synthesis of isoxazole derivatives

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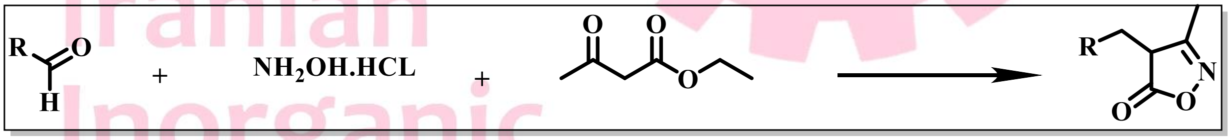
Isoxazoles constitute a crucial class of heterocyclic compounds composed of five-membered rings, with one oxygen and one nitrogen atom located in adjacent positions. The distinctive structural motif of isoxazole confers diverse non-covalent interactions. The transformations of their derivatives encompass electrophilic substitution reactions, nucleophilic substitution, as well as side-chain substitution reactions in isoxazoles. Also hold particular significance, exhibiting a diverse range of biological activities and therapeutic potential. Specifically, isoxazole has demonstrated promising anticancer, antituberculosis, anti-inflammatory, and acetylcholinesterase inhibitory properties in pharmaceutical applications [1,2]. One of the used methods forit preparation of isoxazoles is the reaction between aromatic aldehyde, hydroxylamine, and ethyl acetoacetate, which is carried out in a water solvent and in the presence of an acid catalyst.[3]In this work, a novel approach utilizing a *Lewis* acidic molten salt based on bipyridine was employed for the synthesis of isoxazole derivatives(Scheme1). The preparation of this catalyst is uncomplicated. Moreover, use of this catalyst presents various benefits such as effortless and facile separation, considerable product yield, and brief reaction time.



Scheme 1. Synthesis of isoxazole derivatives in the presence of Bipyridine-based molten salt.

Keywords: Isoxazole, Hetrocyclic, Bipyridine,Molten Salt

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Theoretical Kinetics and Thermodynamics study peripheral substituent effects on the hydrolysis of verdoheme

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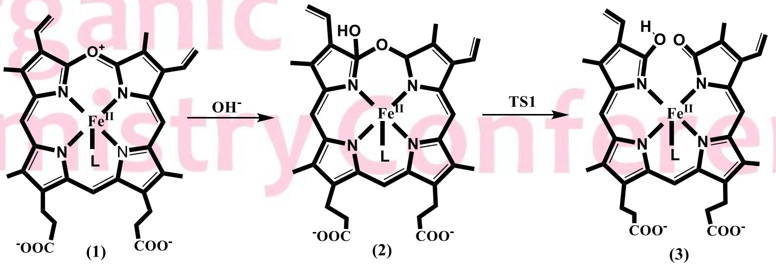
The heme oxygenase enzyme is a free heme protein that binds to heme in the body. Heme acts as both a substrate and a cofactor in this enzyme. The heme oxygenase enzyme (HO) plays a key role in destroying heme molecules. Studies of the reaction of 5-oxaporphyrin iron complexes (verdohemes) with peripheral substituent on the heme ring have been undertaken to provide models and largely unknown for the initial step in hydrolysis of verdohemes. In this work a theoretical kinetics and thermodynamics study of degradation reaction of verdohemes was performed, and calculations show that $\Delta G_{Reaction}$ in hydrolysis of verdohemes non- peripheral substituent is more negative than hydrolysis of verdohemes with peripheral substituent. In the other words, hydrolysis of verdohemes with non- peripheral substituent is more energy efficient than verdohemes with peripheral substituent. The equilibrium constant calculation shows that hydrolysis of verdohemes non- peripheral substituent is much faster than verdohemes with peripheral substituent, which it is due to more convenient nucleophilic attack to cationic ring than anionic. In order to obtain a better molecular understanding of peripheral substituent effects on the hydrolysis of verdoheme inhibitory role of have been studied using DFT method.

Keywords: Heme Oxygenase, Peripheral Substituent, DFT Method, Hydrolysis, Ring Opening of Verdohemes.



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Evaluation of photocatalytic performance based on nanomaterials as an effective advanced oxidation process (AOPs) in oil pollution treatment

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Refinery wastewaters are significant contributors to water pollution due to their non-biodegradable and toxic nature. Phenolic compounds, classified as priority pollutants by the US EPA, are particularly problematic. Photocatalytic techniques based on nanomaterials, like titanium dioxide (TiO_2) nanostructures, have emerged as effective and versatile solutions for wastewater treatment. TiO_2 nanoparticles offer advantages such as increased surface area, enhanced reaction rates, non-toxicity, biocompatibility, and ease of preparation, making them popular in photocatalysis [1]. They exhibit high photocatalytic activity under ultraviolet light, ensuring efficient degradation even in low-light conditions. Importantly, TiO_2 can undergo oxidation state changes without decomposing, making it a desirable catalyst for complete mineralization, serving as an alternative to chemical oxidation [2]. The specific surface area of TiO_2 allows photocatalysis to proceed unaffected by the presence of other molecules, such as water [3]. This article investigates the effective parameters in the purification of p-nitrophenol, a hazardous phenolic compound, using TiO_2 nanoparticles in the photocatalytic method. The study reveals that within the studied range, lamp power and pH positively influence the purification efficiency, while pollutant concentration negatively affects it. Increasing the amount of TiO_2 nanoparticles initially improves efficiency, but further increases lead to decreased process efficiency due to increased turbidity.In summary, this study demonstrates the effectiveness of TiO_2 nanoparticles in the photocatalytic purification of phenolic compounds. It highlights the positive impact of lamp power and pH, along with the negative influence of pollutant concentration on the efficiency of the photocatalytic process. Moreover, the findings emphasize the importance of controlling nanoparticle concentration to avoid diminishing process efficiency caused by turbidity. Overall, this research contributes to the understanding of the photocatalytic method's potential for wastewater treatment and optimization.

Keywords: Photocatalyst, p-nitrophenol, TiO_2

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Investigating the effects of operational parameters on the electrochemical treatment of water containing p-nitrophenol

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Nitrophenols are widely used in the production of various chemical products but can pose significant threats to ecosystems and human health when released into the environment. The United States Environmental Protection Agency recognizes nitrophenols as priority organic pollutants due to their high toxicity, persistence, and bioaccumulation[1-2]. Electrochemical methods have shown high efficiency in mineralizing organic pollutants, with electrolysis being the most common and cost-effective technique for decomposing these pollutants in wastewater. Electrolysis is an advanced oxidation process facilitated by the hydroxyl radical, a strong oxidizer that helps remove organic molecules from water. Organic pollutants can be eliminated during electrolysis through direct electron transfer to the anode (direct electrolysis) or by reacting with oxidants produced through electromagnetic reactions, such as the hydroxyl radical (OH) generated during water discharge at the anode (indirect electrolysis) [3]. This study aims to provide an efficient technology for wastewater treatment and investigate the key parameters of the electrolysis process. The research findings reveal that the reaction flow directly impacts the removal efficiency of p-nitrophenol (PNP), while the initial concentration of the pollutant and the pH of the solution have opposite effects. PNP decomposition is more efficient in an acidic environment compared to alkaline and neutral conditions. The increased efficiency in acidic conditions can be attributed to the enhanced production of H+ ions, resulting in the formation of H2SO4, a strong acid that improves pollutant decomposition. Conversely, at higher pH levels, the formation of polymer intermediate products hampers PNP degradation due to interactions with the hydroxyl group. In conclusion, this study highlights the potential of electrolysis as an efficient technology for wastewater treatment. The findings contribute to a better understanding of nitrophenol removal and offer insights for the development of optimized treatment systems.

Keywords:Electrolysis, Graphit, p-nitrophenol

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Synthesis and characterization of bimetallic metal-organic frameworks based on Cu and Zr for absorption and photocatalytic degradation of organophosphorus compounds

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Metal-organic framework (MOF) is a new class of porous crystalline materials featured with regular pores, open channels and high surface area [1,2]. In particular, a few bimetallic MOFs can be obtained when two kinds of metal ions are coordinated with ligands among the MOF structures[3]. Adsorption desulfurization is very effective for the removal of organophosphorus compounds from the environment. The metal-organic frameworks have emerged as a new type of adsorbents because of their porous nature and large specific surface area [4]. In this study, Cu^{2+} was covalently introduced into the UiO-66 framework at the defective sites with H_2BDC as a ligand by the solvothermal method. Then, the structure of the synthesized compounds is investigated by using SEM, TEM, EDX, XRD, DRS, and FT-IR. The photocatalytic activities were investigated via the degradation of organophosphorus pesticides using the Cu/Zr MOFs under UV light irradiation. On the basis of the results, a possible photocatalytic mechanism of the prepared samples was proposed. The results indicate that the Cu/Zr bimetallic metal-organic framework has great application potential in pollutant degradation.

Keywords: Metal-Organic Framework, Bimetallic MOF, Photocatalyst, Photocatalytic Degradation, Organophosphorus Compounds

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Synthesis and characterization of bimetallic metal-organic frameworks based on Zr and Cdand composite it with g-$C_3N_5$for absorption and photocatalytic degradation of organophosphorus compounds

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Metal–organic frameworks (MOFs) are a new group of molecular networks arranged in a three-dimensional skeleton with metal centers and bridged organic ligands around them [1]. The MOFs have a remarkable performance in the fields of adsorption [2], separation [3], photocatalysis [4], and drug delivery [5].On the other hand the adsorption and photocatalytic degradation of hazardous materials such as organophosphorus compounds by adsorbents with high adsorption capacities and easy separation from sample solutions are highly desirable. In this research, the photocatalytic degradation of organophosphorus compounds in real specimens was developed using an bimetallic metal-organic frameworkcompositewith the addition of C_3N_5 as an adsorbent. The adsorption of organophosphorus compounds on Cd/Zr-MOF/C_3N_5 was optimized by considering various factors including pH, amount of adsorbent, contact timeand sample concentration.Results with scavengers allowed concluding that $O_2^{\bullet -}$ radicals are the main reactive species, although photogenerated$^{\bullet}$OH radicals and electrons also contribute to the degradation.

Keywords: Bimetallic MOF, MOF/C_3N_5, Photocatalyst, Photocatalytic Degradation, Organophosphorus Compounds

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Cs@MCM-41 network as a organocatalyst for the reduction of nitro compounds to amines

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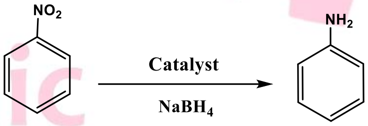
In recent years, applying nanoparticles as high efficient catalysis has been attracted a great deal of interest. On the other hand, Hydrogels as three dimensional, flexible and polymeric networks, based on natural and synthetic materials with extensive features such as hydrophilic nature, desired functionality, elasticity, reversibility and biocompatibility, are one of themost ideal andmultipurpose substances in catalytic system. In this regard, chitosan (Cs) and MCM-41(Mobil Composition of Matter-41), as lexible networks can physically and chemically cross-link by non-covalent or covalent interactions or combinations of both [1].We report a novel green procedure for immobilization of Ni on MCM-41 grafted to chitosan with EDTA as a cross-linker was accomplished in order to fabricate three dimensional. here is a plenty of both acidic and basic sites on the surface of this bio-based and biodegradable network, as a multifunctional organocatalyst, for the reduction of nitro compounds with sodium borohydride ($NaBH_4$) in green conditions. Easy separation of catalyst by using filtration , excellent catalytic activity, efficiency and proper reaction time, and reuse are some of the advantages of catalyst used [2]. In this work, reduction of various nitro groups to the corresponding amines with $NaBH_4$as reducing agent in the presence of Cs@EDTA@MCM-41 catalyst investigated. The resulting nanocomposite was studied by EDX, FESEM and FT-IR techniques.



Schem 1. A general procedure for reduction of nitro compounds with $NaBH_4$.

Keywords: Catalysis, Chitosan, MCM-41

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Synthesis, spectral characterization and thermal study of some biological active Zinc(II) halide complexes

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Schiff base complexes are an important group of inorganic coordination compounds due to their ready availability, synthetic flexibility and facile structural modification. Coordination of of Schiff base ligands have attracted the attention of the researchers because of their diverse applications in molecular recognition, catalysis, and as components of luminescent and magnetic materials. In recent years, Schiff base coordination compounds have also been shown to display a variety of useful biological properties. Structural and spectral properties of these complexes are strongly dependent on the nature of the ligand structure . As a d^{10} metal ion, zinc is an essential trace element and plays a considerable role in maintaining human health. Zinc is a relatively abundant trace metal present in biological systems, second only to iron, and is present in more than 300 enzymes of living organisms [1-5]. In this research, a new bidentate ligand entitled as *N,N'*-Bis-(3-(2methoxyphenyl-2- allylidene)-hexane-1,6-diamine and its Zn(II) complexes were synthesized and identified by analytical and spectral data(FT-IR, UV-Visible and ^{1}H and ^{13}C-NMR). Moreover, thermal analysis of ligand and its complexes were studied in the range of room temperature to 1000 °C with a heating rate of 20 °C min^{-1} and then some thermokinetic data were estimated for all thermal decomposition steps. Moreover antibacterial and antifungal properties of the ligand and its mercury complexes were evaluated *in vitro* by well diffusion method.

Keywords: Zinc(II) Complex, Schiff Base, Thermal, Antibacterial, Antifungal.

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Copper-functionalized magnetic mesocellular foams: as a magnetically recoverable nanocatalyst for carbon-selenuim bonds formation

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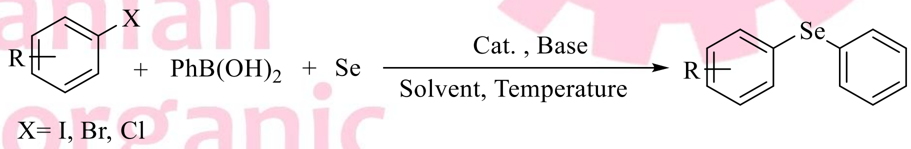
With the development of nanoscience and nanotechnology, chemists achieved the various catalytic reactions due to a wide variety of nanostructured catalysts or immobilization of homogeneous catalysts on nanostructured supports[1]. Among the various nanoparticles, mesoporous silica compounds especially siliceous mesocellular foams (MCFs) due to a three-dimensional mesoporous structure with internal connectivity, large pore size (diameter 20–50 nm), uniform pore size ranges, large pore volumes, high surface areas (>1000 m^2 g^{-1}), a large number of silanol groups that contribute to high catalyst loading and high thermal and chemical stability are good candidates for catalyst supports[2, 3]. The formation of C–Se bonds using catalytic methods is very popular in diverse fields including organic synthesis, the pharmaceutical industry, and materials science[4]. In this work, we report a new system for the synthesis of phenyl aryl selenides in the presence of copper-modified-MCF as a novel magnetically reusable nanocatalyst (Scheme 1). The significant advantages of the designed system include simple separation, reusable for several times, eco-friendly, high stability and good to excellent yields of products in relatively mild conditions.



Scheme 1.Copper complex supported on magnetic MCF nanoparticlesfor carbon-selenuimbondsformation

Keywords: Nanostructure, Mesoporous Silicas, C–Se Bond Formation

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Utilization of a new ionic liquid based on tropine as an efficient catalyst for the acceleration of the synthesis of spiro-2-amino-4*H*-pyran-oxindoles

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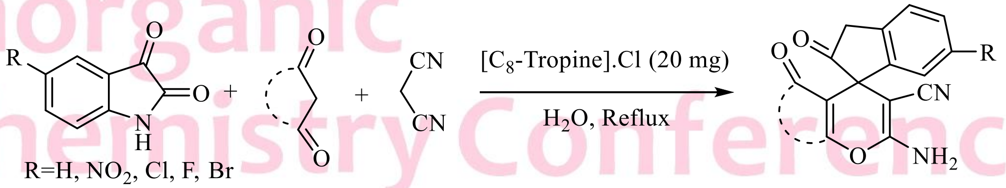
In recent years ionic liquids(ILs) have become a promising area of concern for organicchemists due to their distinctive properties such as high thermalstability, low vapor pressure, high load capacity, ease ofrecycling and environmental friendliness[1]. Tropine, a bicyclo structured compound, is one of the important tropane alkaloids which under the influence of special features in main structure such as having a nitrogen atoms and hydroxyl group and its ability to form hydrogen bonds has a high potential for the synthesis of ionic liquids with high biocompatibility. Heterocyclic systems containing pyran rings specially spiro-2-amino-4*H*-pyrans have received considerable attention due to their various biological and pharmacological activities [2]. These compounds form the structural unit of many natural products and are potential calcium channel antagonists, also having various activities such as anti-allergy, anti-tumor, and anti-bacterial [3].In this work, we wish to introduce a efficient ionic liquid based on tropine**(**[C_8-Tropine].Cl) for the acceleration of the synthesis of thespiro-2-amino-4*H*-pyran-oxindoles. The green conditions, simple catalyst preparation, straightforward separation and recovery of the catalyst from the reaction mixture, simple work-up method requiring no special separation procedure, use of water as a reaction media, short reaction times, and high yields of the products are the significant points of interest of this study.



Keywords: Ionic Liquid, Spiro-2-amino-4*H*-pyran-oxindoles, Tropine, [C_8-Tropine].Cl.

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Synthesis, characterization, computational study and covalent immobilization of H_2saldien ligand on dendrimer functionalized magnetic nanoparticles fordrugdeliveryapplication

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Novel pH-sensitive, biocompatible and biodegradable magneto-dendrimers with imine and hydroxyfunctional groups based on polyamido-amine were synthesized for drug-delivery system that can enhance the therapeutic effects of drugs[1]. In this study, $MnFe_2O_4$ magnetic nanoparticles (MNPs) with a diameter of 35 nm were prepared by using the hydrothermal route. MNPs were coated by tetraethoxysilane (TEOS) to obtain core/shell of $MnFe_2O_4/SiO_2$. Core–shell nanoparticles were modified by (3-aminopropyl) triethoxysilane (APTES) to fabricate amine-functionalized magnetic nanoparticles (zero generation(G0)). The half generation (G0.5) of the magneto-dendrimer with *methyl ester*groups were produced by Michael addition reaction using the required amount of methylacrylate (MA). The first generation (G1) of nanocarrier was synthesized by the amidation reaction using the necessary amounts of N,N'-bis(salicylidene)diethylenetriamine (H_2saldien)(obtain from the reaction betweensalicylaldehyde (2 equiv.)and diethylenetriamine(1 equiv.)). The characterization of synthesized ligand and nanoparticles were performed by Fourier Transform Infrared spectroscopy (FT-IR),*Nuclear magnetic resonance spectroscopy (NMR)*,X-Ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FESEM), Energy Dispersive X-Ray Analysis (EDX), Elemental Mapping Directily from FESEM (MAP), Thermogravimetric Analysis (TGA) and Vibrating-Sample Magnetometer (VSM). Magnetic dendrimer was*used*as novel drug*nanocarrier*.Ibuprofen was chosen as model drug, which directly conjugated to imine, hydroxyandaromatic groups of terminated dendrimer by hydrogen bond and π-π stacking interaction. Drug content and drug entrapment efficiency were determined for drug-loaded nanocarrier by UV-Vis spectroscopy and in vitro drug release studies were done in simulated gastric fluid (pH=1.2), colonic media (pH=5.5), blood environment (pH=7.4) and others (pH=8.5) at 37 ºC. Such unique properties enable maintenance of the bioactivity of the drugs. Therefore, the findings in this study showed magneto-dendrimer is a promising oral drug delivery nanocarrier. This improvement could enhance the potential of magnetic targeting therapy in clinical applications of cancer treatments. Also, full optimization of the geometries of *drug*-loaded nanocarrier, natural bond orbital (NBO) analysis, vibrational frequencies, the HOMO–LUMO energy gap and Molecular electrostatic potential (MEP), were calculated by using density functional theory (DFT) by Gaussian software. Finally, a comparison has been made between computational and experimental results. The theoretical spectral properties show good agreement with the experimental ones.

Keywords*:* Magnetic Nanoparticle, Magneto-dendrimer, Nanocarrier, Drug Delivery, DFT Study

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Functionalization of chitosan to prepare an appropriate catalyst and investigation of its catalytic properties

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Every year around the world, a vast amount of organic waste is produced from aromaticnitro compounds and their derivatives due to their wide application in the production of pesticides,herbicides, insecticides, and synthetic dyes. They have a huge adverse effect on theenvironment due to their difficult degradation process. In the same direction, developing heterogeneous catalysts using chitosan (CS) and magnetic (Fe_3O_4) as supports has attracted enormous interest due to their availability, low cost, and non-toxicity [1-3]. In this work, a heterogeneous catalyst was fabricated as a result of facile modification of NH_2 groups of the chitosan on the Fe_3O_4/CS surface and subsequent metalation of the obtained NS donors. The prepared catalyst was characterized using Fourier transform infrared (FT-IR) spectroscopy, thermogravimetric analysis (TGA), X-rayDiffraction (XRD), vibrating sample magnetometer (VSM), CHN elemental analysis, inductively coupled plasma optical emission spectroscopy (ICP/OES), field emission scanning electron microscopy (FE-SEM), and energy dispersive X-ray spectroscopy (EDX). The performance of the synthesized catalyst on the reduction of various nitroarene compounds to corresponding amino arenes was evaluated at ambient conditions. UV–vis absorption spectra were recorded in different intervals to monitor the reactionchanges at room temperature. The reduction of 4-nitrophenol in optimized reaction conditions reached 91% conversion. The catalyst was easily separated by an external magnet and the recovered catalyst was reused without significant loss of catalytic activity [4].

Keywords: Chitosan; Magnetic Nanoparticles; Catalyst; Reduction Ofnitroarene

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Modification of Clay Mineral Montmorillonite via Graphene Quantum Dots for Use as a Nanofiller in Bio-Based Hydrogel for Wastewater

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The use of dyes in industries for coloring products is a major cause of environmental pollution [1].This study explores the potential of semi-interpenetrating polymer networks (semi-IPN) for the removal of dyes from water. Dyes are a significant contributor to environmental pollution and are commonly used in various industries for coloring products. Semi-IPN hydrogels were synthesized by blending a cross-linked polymer with another polymer to create a new network. The resulting hydrogels exhibit excellent absorption capacity, high resistance to water and salt, and superior mechanical strength. These properties make semi-IPN hydrogels a promising candidate for the removal of dyes from water. The semi-IPN hydrogels were tested for their ability to remove dyes from water, and the results showed that they were highly effective in removing various types of dyes. The high removal efficiency of semi-IPN hydrogels is attributed to their unique structure, which provides a large surface area for adsorption and a porous structure for the diffusion of dyes [2]. GQDs can serve as novel adsorbents for removing pollutants from wastewater. However, the lack of good water penetration of GQDs in an aqueous solution makes their separation difficult. Therefore, some researchers have focused on the immobilization of GQDs on the surface of materials such as gold and bilayer hydroxides. Montmorillonite (MMT) clay is a flaky silicate material that has layers consisting of an alumina octahedral sheet and two silica tetrahedral sheets. It has many interesting properties, including a large surface area, excellent cation exchange capacity and strong hydrophilicity [3]. This study synthesized a semi-IPN network using GQD, and MMT as nanofillers in different amounts to obtain a hydrogel nanocomposite structure. In addition, the above hydrogel nanocomposite was prepared through the solution polymerization method, and safranin (SA), methylene blue (MB), methyl green (MG), crystal violet (CV), malachite green (MlG), and concord (CR) were used to remove dyes. FTIR, FESEM, Mapping, TGA, and XRD analysis were used to check the chemical and structural properties of the hydrogel samples. Dye absorption was investigated by measuring swelling, the effect of adsorbent dose, and the effect of contact time.

Keywords: Graphene Quantum Dot, Montmorillonite, Hydrogel, Dye Removal, Semi-IPN

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Copper oxide on graphene oxideaerogel (CuO/rGO) nanocomposite as catalyst forhydrogen generation from hydrolysis of sodium borohydride

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In this study, copper oxide on graphene oxide aerogel (CuO/rGO) was synthesizedby a facile method using sodium borohydride as a reducing agent[1, 2].The structure of the as-synthesized composite was characterized byultraviolet–visible spectroscopy (UV–vis), Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), X-ray Energy Dispersive Spectroscopy (EDS) and field emission scanning electron microscopy (FE-SEM). The catalytic activity of the nanocomposite was examinedfor sodium borohydride hydrolysis.The effects of different parameters such as catalyst amount, sodium borohydride concentration, temperature, and pH were investigated. The activation energy, enthalpy, and entropy for sodium borohydride hydrolysis were determined. The CuO/rGO catalyst performed best at neutral pH, room temperature, and the minimum amount of catalyst producing hydrogen at a rate of 61.11 L. min^{-1}.g^{-1}.

Keywords: Copper Oxide, Graphene Oxide, Aerogel, Sodium Borohydride, Hydrolysis

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Pumicepowdersupportedbimetallic Fe-Ag nanoparticles: as a new, powerful magnetic nanocomposite for the aqueous reduction of nitro compounds to amines

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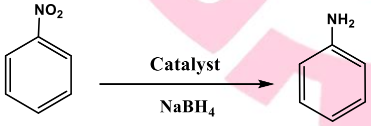
As time goes on, microscale and nanoscale heterogeneous catalytic systems are gaining increasing attention for a variety of reasons [1]. silver nanoparticles (Ag NPs) are among the best competent candidates in the catalytic processes due to including impressive electronic and optical properties. Also, Pumice is a volcanic stone that includes numerous voids in its structure, and since it is fallen into the category of the light- weight materials, it can be well dispersed/submerged in the reaction mixture [2]. Herein, for the first time a novel magnetically retrievable nanocomposites of pumice powder andFe/Ag is prepared, characterized and its catalytic system application for reduction of various nitro groups to the corresponding amines with $NaBH_4$ as reducing agent inH_2O is investigated.The efficiency and proper reaction time, recyclability of the catalyst, reaction conditions (H_2O as green solvent) coupled with activity and stability of the nanocomposite make the described heterogeneous catalyst highly desirable from the green chemistry point of view. The resulting nanocomposite was studied by SEM, XRD, VSM and FT-IR techniques.



Schem 1. A general procedure for reduction of nitro compounds with $NaBH_4$.

Keywords: Magnetic Nanocatalyst, Pumice, Bimetallic

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Construction of Organoplatinum(II) Complexes by a Tripod Phosphine Ligand: A Joint Experimental and Computational Investigation

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The chemistry of 1,1,1-tris(diphenylphosphino)methane (tppm) as a ligand is less explored [1] in comparison with bis(diphenylphosphino)methane (dppm) [2], and only a handful of studies are documented in the literature. This ligand opens up an opportunity for systematic investigation of the steric and electronic effects on chemical and physical properties, in which, by purposeful variation of the substituent groups on phosphorus, a wide array of properties can be "fine-tuned"[3]. Taking this considerable potential into account, two organoplatinum(II) complexes [PtR_2(tppm)] (R = Me, **1**, *p*-MeC_6H_4, **2**) were synthesized starting from the well-known precursor [$PtR_2(SMe_2)_2$] (R = Me, **A**, *p*-MeC_6H_4, **B**) through ligand substitution in acetone. The structures of the obtained Pt(II) complexes were characterized by NMR spectroscopy, HR ESI-MS(+), and X-ray crystallography (Fig. 1). In these Pt(II) complexes, the tppm ligand is bound to the Pt center *via* monodentate-chelating mode, rendering one of the tppm's P atoms uncoordinated.In the following, computational calculations using density functional theory (DFT) and time-dependent DFT (TD-DFT) were carried out in order to gain deep insight into experimental observations.

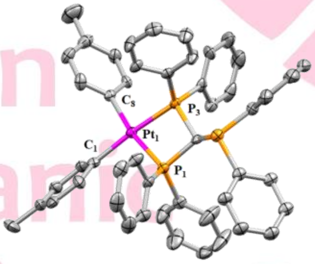

Fig. 1. Crystal structure of **2**.

Keywords: Ligand Substitution Reaction, Organoplatinum Complexes, Phosphine Ligand, Theoretical Calculations

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Synthesis, Spectroscopic Characterization and Crystal Structure of$(EtO)_2P(S)[1\text{-}(NHCH_2)C_6H_4\text{-}3\text{-}(CH_2NH)]P(S)(OEt)_2$

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Bisphosphoramidothioates are widely used as additives in polymers,pesticides in agricultureand drugs inpharmaceutics[1,2].In this research, we report on the synthesis of $(EtO)_2P(S)[1\text{-}(NHCH_2)C_6H_4\text{-}3\text{-}(CH_2NH)]P(S)(OEt)_2$,belonging to bisphosphoramidothioate family.Characterization was performed byFTIR,NMR (^{1}H, ^{13}C, and ^{31}P),elemental analysis, Mass spectroscopyand X-ray crystallography.The crystallization solvent was chloroform and n-heptane (4:1 *v*/*v*), andthe compound crystallizes in the triclinic system, and space group $P\bar{1}$with a= 10.0962 (2) Å, b= 10.5568 (2)Å, c= 11.5523 (2)Å, α= 83.6620 (16)^o, β= 74.3410 (18)^o,γ= 71.0050 (18)^o, V= 1120.68 (4)Å^{3}and Z= 2.The asymmetric unit consists of one complete molecule. In the crystal structure, the molecules are aggregated through N—H…S═P hydrogen bonds (which appears as red spots on the Hirshfeld surface) in a one-dimensional chain along the *b*-axis. The weaker contacts are C—H…S═P, C—H…π, and CH…HC, manifested as pale red spots on the Hirshfeld surface. The phosphorus signal appears at 72.82 ppm and molecular weight is441.In the IR spectrum, the band centered at 3275 cm^{-1} is attributed to the NH stretching frequency.

Keywords: Crystal Structure, Bisphosphoramidothioate, NMR, Synthesis

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Catalytic oxidation of alcoholsby new Fe(III) oxazolidine complex

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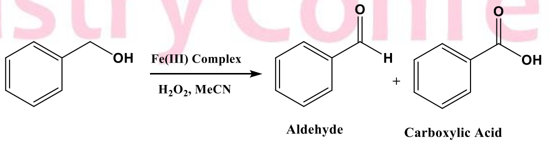
Iron complexes are known as one of the attractive catalysts for many chemical reactions [1]. The exceptional catalytic properties of iron complexes is mainly related to its several oxidation states which can act as active intermediate in the oxygen transfer reactions and redox prcoesses [2]. Selective oxidation of alcohols to aldehydes or carboxylic acids is one of the crucial classes of organic reactions, and iron complexes can act as effective catalysts for this process [3]. In this context, a new dinuclear iron complex, $[Fe(\mu\text{-}L)(NCS)_2]_2$ (where HL is (4-ethyl-2-methyl-2-(pyridin-2-yl)oxazolidin-4-yl)methanol), was synthesized by the reaction of $Fe(NO_3)_3.9H_2O$, HL and KSCN in methanol. The complex has been characterized by using spectroscopic methods and elemental analysis. The crystal structure of the synthesized iron complex has been determined by single-crystal X-ray diffraction analysis which revealed it is alkoxido bridged dinuclear iron complex and the SCN ligands act as teminal monodentate ligand. The catalytic activity of this complex in the oxidation of benzyl alcohol derivatives to their corresponding benzaldehyde and benzoic acid derivatives has been studied in the presence of H_2O_2 as the green oxidant. In this study, the effects of several parameters such as the molar ratio of oxidant to product, temperature, and solvent on the reaction conditions have been investigated to find the optimal conditions for the selective oxidation of alcholos. Additionally, the effect of different substituents on the phenyl group of benzyl alcohol derivatives in this catalytic system has been examined. The results show that the selectivity and activity of this dinuclear Fe(III) complex depend on the steric and electronic properties of chemical substances and reaction conditions.



Keywords: Complex, Catalyst, Oxidation, Iron

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Synthesis and Characterization of a New Copper Complex with Oxime Ligand as a Catalyst for Alcohol Oxidation

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Oximes are a significant class of bioactive organic compounds that possess a functional group consisting of an imine connected to a hydroxylamine (C=N-OH) group. The amphoteric nature of the oxime functional group arises from a slightly basic nitrogen atom in the imine group and a slightly acidic hydroxyl group, giving rise to excellent ligands for coordination chemistry [1]. Copper is a crucial metal in mineral and complex chemistry and is widely used as a catalyst in many chemical reactions due to its unique properties, including stability under different conditions, catalytic activity in oxidation and reduction reactions, and antibacterial and antifungal properties. Copper complexes based on oxygen-containing ligands are particularly advantageous for these applications [2,3]. In this work, a new copper complex was synthesized by the reaction of copper nitrate trihydrate with an oxime ligand in methanol solvent. The obtained complex was characterized by spectroscopic methods and its structure was determined by single crystal X-ray analysis. SC-X-ray analysis idnicated that the obtained compound is a mononuclear copper complex with general formula of $[Cu(L)_2(NO_3)_2]$ (where L is (*Z*)-2-amino-N'-hydroxybenzimidamide). $[Cu(L)_2(NO_3)_2]$ is crystallized in the Triclinic *P-1* space group, exhibiting octahedral geometry around the copper ion and z-out Jan-Teller distortion can be clealy obsereved in the axial positions. This complex was used as a catalyst for the oxidation of benzyl alcohols by using H_2O_2 as an oxidant. The catalytic reactions were carried out under air condition and the results indicated the synthesized copper complex has high catalytic activity in the oxidation of benzyl alcohol. The electronic effects of the substituents in the catalytic process were studied, concluding that strong electron-withdrawing groups indeed facilitate the catalytic reaction.

Keywords: Copper, Catalyst, Complex, Oxime, Ligand

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Comparison of the Antiitch Activity of Avenanthramidesin OatsUsing Molecular Docking Study

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Ancient literature describes the anti-inflammatory and antiitch properties of oat extracts. Medical texts by Pliny andother notables promoted the topical application of oatmeal flour for a variety of dermatologic conditions [1]. Avenanthramides (AVAs) are a group of unique, low-molecular-weight hydroxycinnamoyl anthranilate alkaloids uniquely present in oats. AVAs, besides affecting the flavor of oat products, have been reported to improve health parameters in animal and human studies.They have antiproliferative, antioxidant, anti-inflammatory, and anti-atherogenic properties [2]. While 25 distinct Avnshave been identified in oats, the most plenteous forms are N-(3′,4′-dihydroxy-(E)-cinnamoyl)-5-hydroxyanthranilic acid (2c;AvnC), N-(4′-hydroxy-3′-methoxy-(E)-cinnamoyl)-5-hydroxyanthranilic acid (2f;AvnB), and N-(4′-hydroxy-(E)-cinnamoyl)-5-hydroxyanthranilic acid(2p; AvnA), which differ by a single moiety on the hydroxycinnamicacid ring. It is widely believed that AvnA, AvnB, and AvnCare mainly responsible for the antioxidant functions of oats [3]. In this work, a molecular docking study was performed to investigate the antiitch activity of avenanthramides (AvnA, AvnB, and AvnC). Also, the results were compared with gabapentin,an effective antiitch-approved drug.Since one of the most important treatments for itching isκ-opioid antagonists [4], threeκ-opioid receptors are selected for the study. Ligands are docked to the target proteins, and the best binding modes are analyzed. Among the results, AvnC showed better binding affinity against the receptors, with docking scores ranging from -7.72 to -8.40 kcal/mol. Besides, the number of hydrogen bindings created by AvanC is remarkably higher than other AVAs and also gabapentin.

Keywords: Antiitch, Avenanthramides, Molecular Docking, Oat

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Antiitch Efficacy of Henna Bioactive Components by Inhibition of Kappa-Opioid Receptors

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In recent times, focus on plant research has increased all over the world and a large body of evidence has been collected to show the immense potential of medicinal plants used in various traditional systems. Nowadays, we are seeing a great deal of public interest in the use of herbal remedies. One of these plants, *Lawsonia Inermis Linn* (Family: Lythraceae) which is commonly known as henna, is mainly present in subtropical and tropical areas and is used all over the world. Henna attracts the care of scientists for its therapeutic activities ranging from antiinflammatory to anticancer activities [1]. Phytochemical studies in the henna plant have indicated the presence of several bioactive molecules like isoplumpagin, lupeol, 30-norlupan-3-ol-20-one, betuhennan, betuhennanic acid, and n-tridecanoate phenolic glycosides, lawsoniaside, β-sitosterol and stigmasterol in leaves and roots. Lawsone (2-hydroxy-1,4-naphthoquinone), the red-orange dye present in the henna leaf paste, is being used in modern pharmacopeia as a starting molecule for the synthesis of clinically important anticancer drugs such as atovaquone, lapachol, and dichloroallyl lawsone [2]. This study is an in-silico approach to investigate the antiitch activity ofsome bioactive molecules of Henna. Isoplumpagin, lawsaritol, lawsone, lupeol, and stigmasterol were docked against thekappa-opioid receptor (PDB ID: 4DJH),and the results were compared with the antiitch-approved drug, gabapentin.All the selected ligands revealed better efficacy than gabapentin.The results showed that the best binding affinity is in the sequence stigmasterol>lawsaritol> lupeol >isoplumpagin> lawsone > gabapentin, with lots of convergence points. Stigmasterol, with a docking score of -11.54 kcal/mol and an inhibition constant of 3.46nMexhibited the best antiitch activity and can be considered an effective frame to design new antiitch drugs.

Keywords: Antiitch, Henna, Kappa-opioid Receptor, Molecular Docking

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Preparation, identification and investigation of catalytic activity of sandwich polyoxometalates nanohybrids with graphene oxide

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Polyoxometalates have been considered a class of metal cluster complexes consisting of oxide anions of intermediate metals due to their high potential in chemistry.[1] In this study, in the first stage, graphene oxide (GO), amine graphene oxide (GO/NH_2) as well as Keggin-type sandwich polyoxometalateswith abbreviation (POM) were synthesized and then synthesized polyoxometalateson amine graphene oxide (GO/NH_2-POM) is fixed.[2] The synthesized GO/NH_2-POM catalyst was characterized via Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM), X-ray energy diffraction spectroscopy (EDAX), BET, and Thermal gravimetric analysis (TGA).The results of these analyzes showed that the stabilization of POM on graphene oxide was successfully performed.Methylene blue dye was used to evaluate the adsorption and degradation activity of the final synthesized catalyst.The results showed that maximum dye removal and degradation occur when using 10 mg catalyst, 20 ppm initial concentration of methylene blue at pH 9.Finally, according to the obtained results, it can be said that GO/NH_2-POM catalyst can have a good function as an effective adsorbent for removing methylene blue dye molecules from the effluent.

Keywords:Polyoxometate, Graphene Oxide, Absorption Process, Dye Removal, Methylene Blue, H_2O_2

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Plant-mediated synthesis and characterization of iron oxide nanoparticles using Tribulus terrestris

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The plant *Tribulus Terrestris*locally named “Sadeng” is one of the nativemedicinal plants of the Baluchestan region of Iran. The plant is traditionally used as an anti-infective agent and kidney stone treatment [1]. Many types of organic compounds, such as alkaloids, phenols, and flavonoids have been reported in phytochemical investigations of this medicinal plant [2]. Iron oxide nanoparticles (Fe_3O_4-NPs) is an important nanoparticle with exclusive physicochemical behaviors, such as specific surface area, magnetic segregation properties, and unique lattice plane [3]. Several physical and chemical techniques have been applied for the preparation of Fe_3O_4-NPs([3]). However, these techniques need high energy and solidly built equipment to prepare the Fe_3O_4-NPs. In recent years, researchers have been focused on the plant-mediated synthesis of Fe_3O_4-NPs instant of previous methods, because of the economical and environmentally-friendly processing approach. In the current study, the aqueous extract of *Tribulus terrestris* was employed for the phyto-fabrication of iron oxide nanoparticles.The biosynthesized extract-mediated iron oxide nanoparticles (INPs) was characterized through different methods containing FT-IR (Fourier transform infrared spectroscopy), FESEM (Field emission scanning electron microscopy), EDS (Energy-dispersive X-ray spectroscopy), and XRD (X-ray diffraction).The results demonstrated that the average size of Fe_3O_4-NPs nanoparticles was found to be 30-40 nm with spherical morphology.

Keywords: Green Synthesis, Nanoparticles, Plant Extract, Iron Oxide

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SiO_2 nanoparticles catalyzed the synthesis oftetrahydro-2,6-dioxopyrimidin-4-yl)-2,3-dihydrophthalazine-1,4-diones

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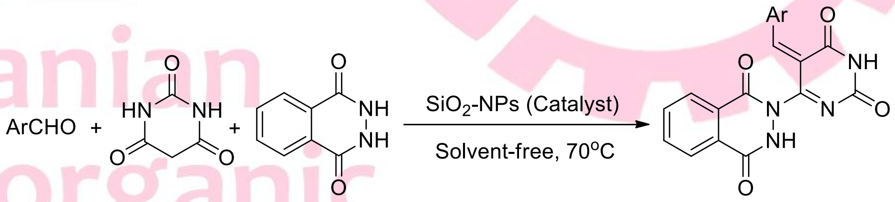
Multi-component reactions (MCRs) have been considered as asuperior synthetic approach for the preparation of libraries of biologically active compounds [1]. MCRs offer environmentally friendly methods by reducing the number of waste production, steps of the reactions, and energy consumption [1]. Silica gel is one of the most widely used solid support for various catalytic applications, due to its non-toxicity, high surface area, excellent thermal stability, and ready availability [2]. Based on silica as an efficient catalyst and support, numerous silica-supported catalysts have been developed in recent years [3]. Also, these catalysts catalyzed the various Multicomponent reactions [3]. In this work, silica nanoparticles (SiO_2-NPs)were applied for the one-pot synthesis of tetrahydro-2,6-dioxopyrimidin-4-yl)-2,3-dihydrophthalazine-1,4-diones scaffolds. These compounds were prepared via the three-component reaction ofaromatic aldehydes, phthalhydrazide, and barbituric acid (Scheme 1). After completion of the reaction, the simpleand rapid separation and facial recovery of the SiO_2-NPs was accomplished.



Scheme 1. The synthesis of tetrahydro-2,6-dioxopyrimidin-4-yl)-2,3-dihydrophthalazine-1,4-diones.

Keywords: Nanoparticles, SiO_2, Solvent-free, Barbituric Acid, Synthetic Methodology

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Nanocomposite based molecular sieve, a green, highly efficient and recyclable catalyst for the reduction of medicine

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Water pollution has led to various diseases that have resulted in severe health issues and increased mortality of humans and aquatic life [1]. Therefore, to solve the problems that emanated from wastewater contamination, pharmaceutical industries came up with different classes of drugs that could improve the deteriorating health conditions of the affected population. Meanwhile, the untreated discharge of effluents from pharmaceutical industries, hospitals, and sewers, has increased the contamination of surface and groundwater [2, 3]. Different materials have been used for treatment of pharmaceutical drugs in wastewater. We used highly ordered mesoporous molecular sieves AlMCM-41 and its new nanocomposite with mixed metal nanooxideto remove and degradation of this pollution.The nanocomposite was charachterized by Fourier transform infrared (FT-IR) spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), and N_2 adsorption desorption analyses were used to examine the structure, morphology, size and phase composition of the synthesized nanocomposites. The results show the successful deposition of metal oxides nanoparticles onto the framework of AlMCM-41. AlMCM-41 provides enormous benefits such as environmentally safe, economic viability and porosity when used as support for metal oxide nanoparticles. The excellent catalytic activities of nanocomposites were investigated for the reduction of metronidazole and tetracycline in water at ambient temperature.The best observed performance of reduction of these contaminants with 100% conversion occurred within 6 min. The nanocomposite could be recycled and reused up to five times without noticeable change in its structure and activity.

Keywords: Nanocomposite, Mesoporous Compound, Metronidazole, Tetracycline

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Synthesis of allylic esters using phenyl glycine-functionalized metal-organic framework and copper salts

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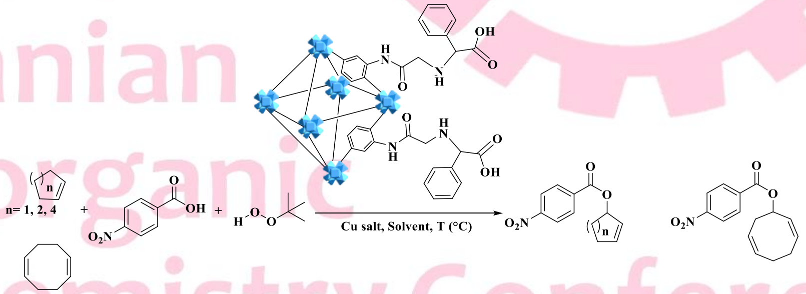
Metal-organic frameworks (MOFs) are a class of catalysts which have attracted the attention of many researchers, due to their different structural and physical advantages such as the ability to adjust the pore size, high biocompatibility, relatively high mechanical and thermal stability. These structures are used in many fields such as adsorption and separation, chemical sensors, drug carriers, heterogeneous catalysts, etc. [1, 2]. Direct activation of C-H bonds is one of the most important reactions in organic synthesis. The oxidation of these bonds in the allylic position of alkenes is known as the Kharasch-Sosnovsky reaction [3]. In this work, Metal-organic framework UiO-66-NH_2 is prepared from the reaction of $ZrCl_4$ with 2-aminoterphthalic acid in DMF by solvothermal method and then functionalized with 2-chloroacetyl chloride. After ensuring the functionalization of the metal-organic framework, the phenyl glycine (2-amino-2-phenylacetic acid) was immobilized on it and the heterogeneous ligand was obtained. The products of each step were characterized with SEM, EDX, BET, TGA, XRD and FT-IR techniques. Finally, the copper complex of the synthesized heterogeneous ligand was used in the allylic oxidation of alkenes and the resulting allylic esters were obtained in good to excellent yields (Scheme 1).



Scheme 1: Synthesis of allylic esters using synthesized heterogeneous ligand and copper salts.

Keywords: Metal-organic Frameworks, UiO-66-NH_2, Kharasch-Sosnovsky Reaction, Allylic Esters

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Adsorption performance of Cerium-based MOF toward malachite green removal

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These days tension of clean water has become a major issue for most of the countries in whole world. the footprint of water is followed everywhere, all the living species, most of the chemical and biochemical reactions are dependent on water. In parallel to improvements of human life, new water pollutants are developed and removing these contaminants from water is one of the most concerning issues for the human of 21'st century [1]. These pollutants are toxic and they harm to ecosystem, environment and human health [2]. Metal-Organic frameworks (MOFs) are a novel class of highly porous and crystalline materials that have catched a lot of attentions for past 10 years [3]. These materials are constructed from metal ions and organic ligands that play the role of connectors through coordination bonds. Because of their great porosity, large specific surface area (typically more than 10000 m^2/g), large pore volume, great affinity to specific molecules, ability for tuning the pore size as well as structural controllability. MOFs are known as a new class of highly porous materials for gas storage and adsorption, photocatalysis, bio medical imaging, ion exchange, water purification, drug adsorbent and sensing [4]. In this research the (MG) is used as model pollutant and the high crystalline and porous Ce-based UiO-66 (Ce-UiO-66) MOFs as adsorbent. Various factors which influence on adsorption capacity had been investigated. The aim of this work was to use green synthesis method to synthesize Ce-UiO-66 MOF. According to the results, this MOF can successfully adsorb this dye from water. Based on the obtained results, the pseudo-second-order kinetic model matched well for the elimination of the MG from aqueous media through adsorption onto the Ce-UiO-66. Adsorption capacity of this adsorbent changes with the initial pH solution, which demonstrates that the adsorption mechanism could be electrostatic interaction among dye and MOFs.

Keywords: Ce-UiO-66, Malachite green, Green synthesis, Dye removal.

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Synthesis of ETS-10 and its modification

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The objective of this study is to synthesize ETS-10 and modify its surface area, pore volume, and pore size. ETS-10 adsorbent, with a Si/Ti ratio of 5.5, was synthesized without seeds using the hydrothermal method[1]. To modify ETS-10, organic templates such as tetrapropylammonium bromide and P123, as well as a specific weight percentage of isopropanol as a solvent, were used. ETS-10(Na, K) was synthesized using hydrothermal methods as previously reported. The final gel composition was $3.5Na_2O:1.5K_2O:TiO_2:5.5\ SiO_2:131\ H_2O$ [1]. During the synthesis of ETS-10, sodium silicate and deionized water were mixed, and then sodium hydroxide and potassium chloride were added to the mixture. After achieving a homogeneous mixture, titanium trichloride was added, and the pH level was set to 10-11. The resulting gel was then transferred to a Teflon-lined autoclave and heated at 230°C for 60 hours. Finally, the ETS-10 powder obtained was washed and dried for 24 hours at 110°C. In comparison to the ETS-10 synthesis, the synthesis of ETS10 (10 wt% isopropanol) and ETS-10 (20 wt% isopropanol) involved substituting 10 wt% and 20 wt% of deionized water, respectively, with isopropanol solvent in the first step of the synthesis. The synthesized adsorbents were named ETS10 (10 wt% isopropanol) and ETS-10 (20 wt% isopropanol). The synthesis of organic templates followed the same procedure as the ETS-10 synthesis: after adding sodium hydroxide and potassium chloride, organic templates such as TPABr and P123 were added to the mixture. The resulting mixture was dried and then calcined [2]. XRD, SEM and BET analysis were used to identify the synthesized compounds.

Keywords: Synthesize, Titanosilicat, ETS-10, Hydrothermal Method.

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Theoretical investigation of the elastic and structural properties of the $LaLi_3Sb_3$ compound by the pseudo-potential method

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In this research, the structural and elastic constant properties of the $LaLi_3Sb_3$ compound, with a trigonal crystal structure (space group p31m) have been discussed [1]. The calculations have been done in the framework of the density functional theory and with the pseudo-potential method in the generalized gradient approximation (gga) by the quantum espresso software [2], and further, the elastic constants were investigated based on the density functional theory. Elastic constants give information about the hardness, stability, ductility, and brittleness of compounds. Moreover, obtaining the elastic constants subsequently gives information about elastic properties such as volume modulus B, shear modulus G, Young's modulus, and Poisson's ratio. Therefore, studying elastic constants is a functional and fundamental tool to understand the physical, chemical, and mechanical properties of the structure and can be used as *a measure criterion of* the resistance of a crystal to an externally applied stress. The amounts of bulk modulus B = ([40.8]) G, Young's modulus = ([80.7]) GPa and shear modulus = ([34.5]) GPa have been obtained. The value of Poisson's ratio ν=([0.17]) has been obtained for this crystal structure, which indicates the existence of a covalent bond between the two atoms. The Poisson's ratio is in the range of [*(0. 1-0.25)]* among solids implies the presence of a covalent bond [3]. The structure of this compound shows a small and indirect band gap between L and Γ, and also the examination of the partial density of states determined that the maximum contribution of the conduction band is related to the d orbital of the La atom and in the valence band is related to the p orbital of the Sb atom and the d orbital of the La atom. In this work, the elastic properties of this compound have been investigated for the first time.

Keywords: Band structure, $LaLi_3Sb_2$, DFT, Elastic calculations

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Synthesis magnetic nanoparticles of Fe_3O_4 for the harvesting of native microalgae *Chlorella sorokiniana.pa91* from municipal wastewater by using RSM

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Microalgae are valuable organisms due to their ability to produce various beneficial products for human utilization [1].Understanding the interface interactions between microalgae cells and magnetic nanoparticles (MNPs) is essential for effective magnetic harvesting of microalgae using MNPs.In order to make large-scale microalgae cultivation economically viable, it is crucial to enhance the harvesting process. Magnetic separation is a straightforward process involving the use of a magnetic separator to remove magnetic contaminants or selective magnetic adsorbents for the recovery of desired products [2].Magnetic nanoparticles show great potential as they can effectively attract and bind to microalgal cells, facilitating their separation through a magnetic field and enabling efficient harvesting. This technology holds promise for streamlining microalgae production and expanding its applications in various industries. This method enables rapid and cost-effective harvesting of microalgae for various industrial purposes. magnetic nanoparticles consisting of Fe_3O_4 were synthesized using the co-precipitation. The researchers utilized the surface response method (RSM) in conjunction with a central composite design (CCD) to thoroughly investigate the impact of three key factors: time, nanoparticle concentration, and pH in the culture medium. RSM, a statistical technique, enabled the simultaneous evaluation and optimization of multiple variables, providing a comprehensive understanding of their interactions.These significant findings highlight the effectiveness and feasibility of the magnetic nanoparticle-based harvesting method [3]. Moreover, the utilization of municipal wastewater as a cultivation medium offers significant advantages in terms of cost-effectiveness and sustainability. The use of magnetic nanoparticles and the application of RSM with CCD led to the optimization of harvesting conditions for native microalgae *Chlorella sorokiniana.pa91*. The achieved harvesting efficiency of 79% under the optimized conditions demonstrates the efficacy of the magnetic nanoparticle-based method and sets the stage for economic and efficient microalgae harvesting techniques.

Keywords: Fe_3O_4 nanoparticles, municipal wastewater, microalgae harvesting, RSM-CCD.

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The effect of calcination temperature on the characteristics and properties of titanium dioxide

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In this study, ilmenite soil particles in Gharaghaj Urmia were measured using the leaching method with hydrochloric acid to obtain high-quality and pure titanium dioxide pigment. The study involved several stages, including leaching with 37% HCL acid, hydrolysis, crystallization, and calcination. The calcination stage was investigated in this study, which is one of the most important stages in producing this white pigment. Calcination is a thermal operation on solid materials that is used for thermal phase decomposition or removal of volatile substances. Temperature, pressure, and calcination conditions can all affect the structural and photocatalytic properties of the particles obtained from ilmenite soil. Different methods exist for ilmenite calcination, depending on the specific conditions and process requirements. XRF, SEM, EDX, and XRD analyses were performed on the primary concentrate and final calcined product under different conditions.

Keywords: Ilmenite, Calcination Temperature, Titanium Dioxide.

Cu(I) Complex of N-benzoyl, N´, N″ -bis (tert-butyl) Phosphoric triamide as an anti cancer agent

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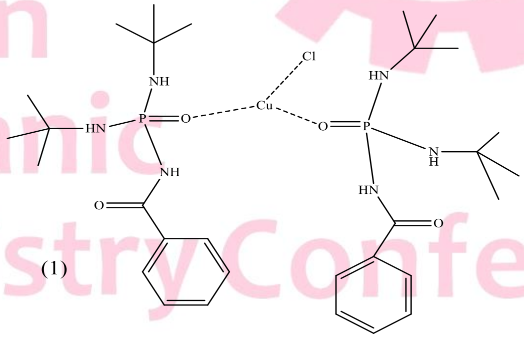
Drug resistance and lack of selectivity are major problems in the treatment of diseases such as cancer and microbial infections. Considering this, the design and development of new bioactive agents devoid of many of the unpleasant side effects has become a serious challenge to medical chemists. Due to steric, electronic, and conformational properties, the structures of phosphorus derivatives allow them to interact easily with the biopolymers of the living systems [1,2]. In this study, a Cu(I) complex of phosphoric triamde ligand, $C_6H_5C(O)NHP(O)[NHC(CH_3)_3]_2$.CuCl (**1**), was synthesized according to the procedure of our previous work [3]. Cytotoxic activities of (**1**) were assayed against A549 (lung cancer) and MCF-3 (breast cancer) cell lines by applying the MTT colorimetric assay. Results showed that the effective doses of compound (**1**) that inhibited 50% growth (IC$_{50}$) of A549 and MCF-3 cells were 24.65 and 41.53 µM respectively According to IC$_{50}$ values, the (**1**) was much more active against the lung cell than breast cell. In other words, it has a greater interaction with the lung cancer cell membrane than breast cells. Thus it has a better anti-proliferative effect on the lung cancer cell.



(1)

Keywords: Cu(I) complex, Phosphoric Triamide, Cytotoxicity, Cell Proliferation.

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N-nicotine-N', N''-bis (cyclopentyl) phosphoric triamide as an anti-bacterial agent

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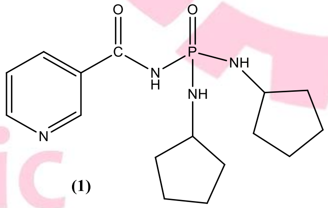
The emergence of multi-drug resistant strains of bacteria is a problem of ever-increasing significance. Consequently, the development of new antimicrobial agents will remain an important challenging task for medicinal chemists[1]. Carbacylamidophosphate compounds with the formula $RC(O)NHP(O)R_1R_2$ are one important class of organophosphorus compounds that have high antibacterial activities due to the existence of peptide-like group –C(O)NHP(O)– in their skeleton [2]. In this study, a Phosphoric triamide compound with the formula $NC_5H_4CONHPO(NHC_5H_9)_2$ (**1**) was synthesized according to the procedure of our previous work [3] and was confirmed by FTIR and ^{31}PNMR. The antibacterial properties of compound (**1**) were evaluated against Staphylococcus aureus and Escherichia coli bacteria. The inhibition zones measured for the antibacterial activities against S.aureus and E.coli were 18.36mm and 10.33 mm respectively, which means this compound has greater antibacterial effects against the Gram-positive bacteria than the Gram-negative one.



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Keywords: Carbacylamidophosphate, Antibacterial, Staphylococcus Aureus, Escherichia Coli.

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Synthesis and characterization of copper bismuth oxide nanostructure by sonochemical method

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In recent years, with the development of technology and the need to use different sources of energy, the exploitation of unusual sources of oil, which mainly contain a lot of sulfur, has become common. Considering problems such as corrosion and poisoning of catalysts caused by sulfur during petrochemical processes, it is inevitable to remove them using methods such as photocatalytic desulfurization. In this research, copper bismuth oxide nano/microstructures were synthesized using new precursors and characterized by XRD, EDS, and FESEM analyses. The sonochemical method was used for the synthesis of nano/microstructure due to the ease of the reaction, low temperature, high speed, and the ability to control the effective factors in the reaction. The mentioned nano/microstructure has a high efficiency in carrying out photocatalytic processes, for example, photocatalytic desulfurization of petroleum derivatives, and finally, by examining the photocatalytic performance of this nanocomposite in desulfurization of petroleum derivatives, its efficiency was confirmed.

Keywords: Copper Bismouth Oxide, Desulfurization, Photocatalyst, Nano/microstructure, Sonochemical.

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The effect of doping zinc ions on the antibacterial activity of nitrogen-carbon quantum dots

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Recently, carbon quantum dots (CQDs) have become a very valuable material that exhibits excellent properties, such as electrical, optical, and antimicrobial. The shape and high active sites on their surface (hydroxyl, carbonyl, and carboxyl groups) are the response to CDs solubility, biocompatibility, and bio-activity [1] also these groups are causes of CDs surface charges. death bacteria via the interaction of charged CDs with bacteria, electrostatic interaction is an important factor in the control of bacteria growth[2]. metal ions can be doping to the CDs that can exchange electrons with the CDs matrix, leading to simplified change electrons which can be the cause of improving the deterrence bacterias property of CDs[3]. In this work, by the hydrothermal method synthesized nitrogen-carbon quantum dots and zinc-doped nitrogen-carbon quantum dots (N-CQDs and Zn/N-CQDs) [4]. The N-CQDs and Zn/N-CQDs were characterized by EDX, UV-Vis, FT-IR, and PL techniques. also, They were evaluated for their bactericidal activity against representative Gram-negative and Gram-positive bacterial strains. All of the mentioned techniques confirm the successful synthesis of these quantum dots. According to the findings and comparison average halo zone of the anti-bactericidal activity of the prepared particles shows that doping of Zn improved the inhibitory effect against bacteria.

Keywords: Carbon quantum dots, Antibacterial, Doping

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Synthesis of Pt-Cu alloy nanoparticles on sulfur-modified graphene as electrocatalysts for methanol oxidation reaction

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The sources of electric power are mostly derived from fossil fuels, which has a negative impact on the environment, and also population growth and the importance of tecchnology in socity have both contributed to the upsurge in the demand for energy. Recently, research in the field of direct alcohol fuel cells due to advantages such as low cost, portability, high-energy density, low operating temperature, and relatively significant efficiency, has attracted much attention from researchers[1]. Direct methanol fuel cells (DMFCs), compared with hydrogen-powered fuel cells, are widely used as mobile and portable power sources due to their portability and high efficiency. Although the current research on DMFCs has made great progress, due to the unavailability of suitable catalysts for methanol oxidation reaction (MOR), it still cannot be widely commercialzed. Up to now, a number of catalysts based on supported noble metal including Pt, Ru, and Pd for MOR have been designed, synthesized, and extensively studied [2]. However, supported Pt-based catalysts are the most active electrocatalysts for MOR in practical DMFCs. The support can promote the formation of highly distributed catalyst nanoparticles with small size and narrow size distribution [3]. Recently, graphene (G) is regarded as a novel and promising support for the preparation of noble metal/G hybrids. The hybride of noble metal and graphene show better activity and stability for alcohol oxidation due to the increasing electrochemical active surface area (ESA) and effectively accelerating electron transfer during the alcohol oxidation reaction. Based on this view, we choose graphene as support to prepare PtCu/G hybrids in our work [4]. In this work, the sulfur-modified graphene supported Pt–Cu alloy nanoparticles have been synthesized and used for MOR in acidic solutions. The catalysts were prepared by impregnation of the catalyst precursors on the graphene support and then alloying at high temperature under an atmosphere of H_2/N_2. The improved electrochemical response and facile synthesis make the present method promising for the preparation of graphene-supported well-dispersed pure metal and alloy nanoparticles of small size and narrow size distribution.

Keywords: Methanol Oxidation Reaction, Geraphene, PtCu, alloy.

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Theoretical studies on nature of bond in some pharmaceutical N-heterocyclic carbene complexes with general formula [NHC(R)(R')MCl]; M=Cu, Ag, Au, R= $C_{12}H_{13}N_2O$; R'=$C_{12}H_{13}N_2O$, CH_3, $C_{15}H_{11}$, $C_{10}H_{12}N$, C_7H_7, C_5H_4N, $C_{14}H_{15}O_9$ and investigation of correlation between metal-ligand interaction energies and IC_{50} values.

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N-heterocyclic carbenes (NHCs) as ligands in organometallic chemistry are subjects of growing interest, and this is not surprising since they form highly stable complexes that result froma very strong bond with the metal centre [1]. Gold complexes bearing N-heterocyclic carbene are currently one of the most promising classes of substances for drug research [2].Complexes of silver and gold have been biologically evaluated most frequently but also platinum or other transition metals have demonstrated promising biological properties [3]. In this project, the nature of the metal-ligand bond in a number of medicinal complexes of N-heterocyclic carbon derivatives, as well as the formation and interaction energies of the metal-ligand in the mentioned complexes in gas phase will be investigated and compared. Also, the possibility of a linear relationship between the formation energies and metal-ligand interactions and the IC50 experimental data of the respective complexes will be investigated.

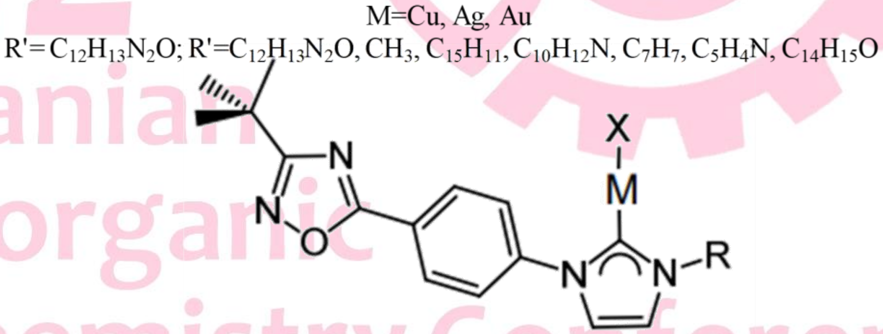

Fig. 1. Structure of ralated complexes NHC.

Keywords: NHC, IC50.

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PMo_{12}/PANI Supported on Activated Carbon Derived from Waste Tire Pyrolysis as Electrode Material in Supercapacitor

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Utilization of renewable sources and waste conversion processes is increasing in the world because of global warming. An estimated of 4 billion waste tire (WT) are currently in landfills and stockpiles worldwide. Scince waste tires do not decompose easily due to their cross-sectional structure and the presence of various additives. The best economic and environmental solution would be to recycle used tires and use them as materials for value-added products [1]. There are several methods for recycling worn tires. Pyrolysis as one of the most important methods is a thermal decomposition process performed at high temperature in an inert atmosphere [2]. Solid residues from tire pyrolysis are often called coal or carbon black. Black carbon is a carbon compound with a carbon content higher than 80 %wt, but the surface area of the resulting carbon is not large enough and its porosity is low, so in order to be used as an adsorbent and energy storage, it must be activated in certain ways. Activation of carbon takes place in two ways: physical activation and chemical activation. Tire-derived activated carbon have numerous advantage such as a high surface area with porosity. Thus, this paves the way for the recycling of waste tires, and this porous activated carbon can be used as an adsorbent as well as promising materials as support in various electrochemical applications. Supercapacitors (SCs), also known as electrochemical capacitors, are some of the most promising energy storage devices due to their higher power density, longer lifespan, and better safety tolerance than batteries. In recent years, the design and fabrication of supercapacitors have become an important research area due to their high power density, relatively high energy density and long cycle life in power source applications. General electrode materials mainly involve carbon materials, transition metal oxides and conductive polymer materials. However, relatively low energy density of carbon materials often limits their large-scale application. Consequently, transition metal oxides and conductive polymer materials have attracted much more attention and have been extensively employed as electrode materials owing to their redox pseudo-capacitance. The purpose of this research is to prepare activated carbon with high surface area and porosity from the pyrolysis of domestic car tire in a chemical methode. Then, by depositing polyoxometalates and conductive polymers on activated carbon, composites will be prepared which used as electrodes in supercapacitors. The capacitance of these electrodes will be examined by electrochemical methods.

Keywords: Waste Tire, Pyrolysis, Activated Carbon, Supercapacitor.

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MXenes in separation science

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One of the factors that classify supramolecules is based on dimension, which is specifically the effect on the physicochemical properties of compositions. Two-dimensional compounds are the most well-known materials in this category. Graphene, Boron Nitride, and Transition Metal Dichalcogenides are examples of bi-dimensional materials. Metal carbides and nitrides which are called MXenes are the new members of this big family. These solid layered crystals with particular characteristics are widely applied in various fields such as biotechnology, medicine, and engineering. MXenes are lamellar crystals that are taken frequently by selective extraction of the A-portion sheets from the corresponding parent MAX phase bulk ceramics, with the general stoichiometric formula of $M_{n+1}AX_n$ where M stands for early transition metal (Ti, Mo, V, etc.), A mainly refers to a group IIIA or IVA element, X is Carbon and/or Nitrogen, and n = 1, 2, or 3. The MAX phase structure can be explained via strong mixed covalent/metallic/ionic M-X bond whereas the character of the M-A bond is metallic. Since for the etching process, hydrofluoric acid or solutions of fluoric salt are usually used, termination molecules (e.g., O, OH, or F) as represented ‘’T’’ in Mn+1XnTx(n = 1, 2, 3) are placed on the flat sheet of MXene [1]. These different functional terminations make MXene extraordinary compared to other bi-dimensional materials. They also affect the role of MXene in adsorption applications. The porosity and high surface area are other important reasons which lead MXene to be applicable for the removal of specific kinds of pollutants and used as a kind of membrane to adsorb heavy metals, organics, and pigments from various media [2]. The large interlayer spaces in the stacked networks of MXenes, these porous materials exhibit high suitability for gas adsorption [3]. Also, the reusability of porous MXene leads this bi-dimensional material to be an environmental-friendly and economical sorbent among wide ranges of other sorbents [4]. Finally, it can be concluded that MXenes are interested significantly in the analytical chemistry field as sorbents because of their unique features.

Keywords: Bi-dimensional, MXene, Sorbent.

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Prussian blue analog-derived Fe-Co-P as excellent electrocatalyst for oxygen evolution reaction

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Due to the environmental deterioration caused by overuse of fossil fuels and generating large mounts of greenhouse gases, it is significant to develop efficient and economical techniques for producing green and renewable energy sources [1]. Among the competitive candidates, the rapid progress in hydrogen and oxygen production via electrochemical water splitting (ECWS) has made it a promising solution [2]. ECWS is composed of oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). However, the sluggish kinetics of OER due to its four-electron transfer process is still a challenge, which greatly limits the electrocatalytic efficiency [2]. In addition to, noble metal-based oxides, such as RuO_2 and IrO_2, are recognized as state-of-the-art OER electrocatalysts [3] and since these catalysts are expensive, thus extensive research is being done to replace them. In this regard, transition metal salts, organometallic compounds, metal-organic frameworks (MOFs), polyoxometalates (POMs), Prussian blue (PB) and other nanostructures have been investigated. Among them, PB and Prussian blue analogs (PBAs) are of special interest, as they are excelent catalysts and precursor materials due to their easy, robust and cost- effective synthesis, highly porous structure and designed morphology, improved electron transport and accessible catalytic sites [1]. The PB, termed ferric ferrocyanide, is a polynuclear complex including transition metal (Fe) and cyanide group (CN) and as a MOF has had industrial applications since the 18th century, which initial structural forms discovered by Keggin and Miles. Their proposed form showed that PB comprises iron ions including ferrous (Fe^{2+}) and ferric (Fe^{3+}) located at the corners of a cube which is linked by cyanide ligands with the general formula of $Fe^{3+}_4[Fe^{2+}(CN)_6]_3$, their assembly can be achieved by mixing ferric or ferrous with hexacyanoferrate ions and different oxidation states of iron [4]. Which, PB-based catalysts it has shown broad application in different disciplines especially OER based on publications since 1986. Herein, FeCoP nanocages have been obtained from FeCo-PBA nanocube precursor via a facile phosphorization route. The porous hollow structure and unique multi-void interior provide exposed active sites and a large surface area. In the FeCoP catalyst, both P and metals (Fe and Co) serve as active sites, and the synergism between them induces an optimized electronic structure. Finally, these nanocage structures showed good catalytic activity for OER.

Keywords: Prussian blue , Water splitting, Oxygen evolution reaction.

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Theoretical studies on the cooperative effects of π…M-X bonds in complexes [{μ_2-$E_2(NHC(R)_2)_2$}$(MX)_2$](E=B , Al; R=H, CH_3, SiH_3, Dipp, F, Cl, Br, Ph; M=Cu, Ag, Au; X=F, Cl, Br) containing E≡E fragment stabilized by *N*-heterocyclic carbene

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Transition metal (TM)-alkyne π complexes are key compounds in organic synthesis and catalysis [1]. Such complexes form during catalytic processes and are important intermediates in many metal-catalyzed reactions in inorganic chemistry [2]. The structure optimization of the complexes has been done at the M05/def2-SVP level of theory, and the bond analysis and related structural investigations have been done at the M05/def2-TZVP level of theory. This study contains theoretical studies on the three metal complex structure, silver, gold and copper with triple bond B_2 and Al_2 stabilized by NHC ligands. Changing The structural characteristics of the complex will be reviewed when the R group attached to the NHC ligands and the halogen group attached to the metal are changed. Also, the cooperative effects of the bonds in the structure of this complex will be investigated. In all sections, different bonds have been investigated using Natural Bond Orbital (NBO), Energy Decomposition (EDA) and (ETS-NOCV) analyses.The stability energy of the complexes shows a better trend in the structures containing boron atom Based on the stability energy of the structures, the value of cooperativity (E_{Coop}) ($E_{COOP} = SE_{(ABC)} - SE_{(AB)} - SE_{(BC)}$, (AB) and (BC) fragments of (ABC), SE is stabilization energy) [3] was calculated for some B structures and the results showed that the investigated structures do not have cooperativity.

E=B , Al

M=Cu, Ag and Au

X=F, Cl, Br

R=H, CH_3, SiH_3, Dipp, F, Cl, Br, Ph

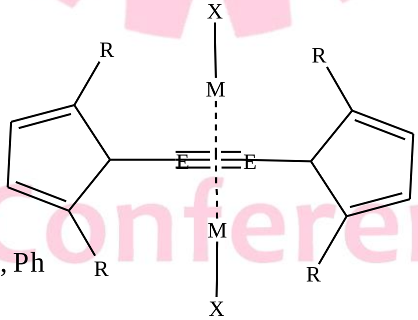

Fig. 1. structure of related complex.

Keywords: NHC complexes, Cooperativity, (TM) Alkyne π Complexes , Boron-Boron Multiple Bonding.

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Effect of addition of indium on corrosion resistance of AZ63-1.5La anode for seawater batteries

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Developing anodes for seawater batteries need to control anodic reaction kinetics, cathodic reaction kinetics, and self-peeling discharge product films. Alloy AZ63-1.5RE is a suitable choice as anode in seawater batteries. In spite of its impressive corrosion resistance, AZ63-1.5RE alloys cannot satisfy the increasing demands for higher corrosion resistance, especially for submersion in seawater. The addition of indium can improve the properties of AZ63-1.5RE anode. In this study, corrosion resistance of AZ63-1.5RE-0.5In is compared with the AZ63-1.5RE alloy. The open circuit potential, potentiodynamic polarization, and electrochemical impedance spectroscopy tests were used to examine the corrosion resistance of alloys. As can be seen in Fig. 1a, the corrosion potentials (E_{corr}) of AZ63-1.5RE alloy is –1.590 V vs. SCE, which the addition of In element causes a shift in the potential towards a more positive value (-1.632 V vs SCE). The 1.5RE alloy has a lower corrosion current (i_{corr}) (7.58×10^{-5} mA cm^{-2}) and a lower anodic slope (β_a) (0.11 mV dec^{-1}), therefore it has higher corrosion resistance. The EIS plot (Fig. 1b) shows that with an R_{ct} of 1552 Ω cm^2, the AZ63-1.5RE-0.5In alloy has a higher corrosion resistance than AZ63-1.5RE alloy. There are two essential factors that determine the corrosion resistance, namely the β-$Mg_{17}Al_{12}$ phase continuity along the grain boundary, the number of β-$Mg_{17}Al_{12}$ phase and rod-like Al-RE phase particles in the α-Mg grains (Fig. 1c). The addition of In element helps in increasing the corrosion resistance of the alloy by reduction of contribution of β-$Mg_{17}Al_{12}$ phases.

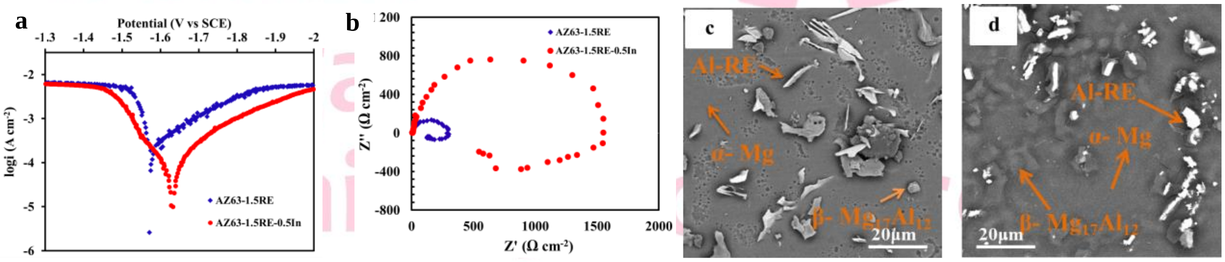

Fig. 1. (a) The potentiodynamic polarization curve, (b) the Nyquist plot of the AZ63-1.5RE and AZ63-1.5RE-0.5In alloys, FESEM images of (c) the AZ63-1.5RE alloy and (c) the AZ63-1.5RE-0.5In alloy.

Keywords: Seawater Battery, Anode, Corrosion, Alloy.

Synthesis and characterization of Bismuth / Bismuth Sulfide / Bismuth Vanadate nanocomposite by hydrothermal method

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Recently, there has been growing interest in the development of efficient photocatalysts for various applications, such as environmental remediation and optoelectronics. the synthesis of nanocomposites has received attention due to their unique properties and potential applications in various fields. Bismuth vanadate ($BiVO_4$) and bismuth sulfide (Bi_2S_3) are two promising materials with strong visible light absorption capabilities. in this article, bismuth / bismuth sulfide / bismuth vanadate nanocomposite is prepared by hydrothermal method using ammonium metavanadate, bismuth nitrate, and thioacetamide reagents and was synthesized in the presence of hydrazine. The purity, structure and morphology of the produced nanocomposite were identified by XRD and FT-IR analyze. This nanocomposite can have high photocatalytic capability and can be used for desulfurization of petroleum derivatives, and finally, by examining the photocatalytic performance of this nanocomposite in desulfurization of petroleum derivatives, its effectiveness was confirmed.

Keywords: Bi / Bi_2S_3 / $BiVO_4$, Nanocomposite, Photocatalyst.

Synthesis and crystal structure of a dinuclear Cu(II) complex with multidentate Schiff base ligand

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In this research we report synthesis, characterization, crystal structure and spectroscopic properties of a new dinuclear copper(II) complex with polyamines ligand. The complex was synthesized by the reaction of $Cu(NO_3)_2.3H_2O$ and multidentate Schif base ligand (H_4L) and sodium azide in methanol solvent. The reaction mixture was heated to reflux for 12 hours and the green precipitates were obtained. The resutling precipitates were filtered off and washed with cold methanol and finally dried in air. The complex was characterized by FT-IR and UV-Vis spectroscopic methods and elemental analysis. Comparing FT-IR spectrum of complex with free ligand (see Fig. 1) confirmed the coordination of both azide and Schiff base ligands to the metal ion. The strong peak at 2038 cm^{-1} is related to azide ligand [1] and the band located at 1600 cm^{-1} is related to the C=N group of Schiff base ligand [2]. The single crystals of this complex was obtained in methanol by slow solvent evaporating during one week. Structural studies indicated that a dinucelar structure has been obtained and its general formula is $[Cu_2(L^{'1})(N_3)_2]$ where H_4L is 2,2'-{ethane-1,2-diylbis[3-(2-{[(*1E*)-(2-hydroxyphenyl)methylene]amino}ethyl)imidazolidine-1,2-diyl]}diphenol. H_4L, is coordinated to the Cu(II) ion as $(H_2L)^{2-}$ ligand by elimination of two phenolic hydrogen during the formation of complex.

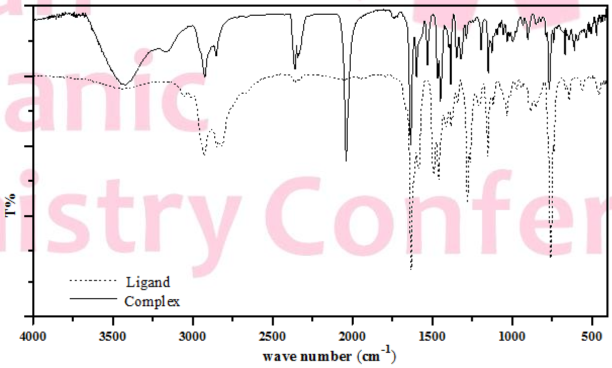

Fig. 1. FT-IR spectrum of ligand (dashed line) and complex (solid line).

Keywords: Cu complex, Crystal Structure, Spectroscopic Studies.

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Zinc cobalt telluride@nickel cobalt selenide as a battery type electrode in asymmetric supercapacitor

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In recent decades, the fossil fuels have engendered climate changes and environmental pollution. Energy conversion and storage devices with low cost, high-efficiency and environment-friendly replaced the immoderate traditional energy [1,2]. Additionally, metal chalcogenide have been used as an electrode materials for supercapacitor applications [3]. Zinc cobalt telluride@nickel cobalt selenide were prepared by two step hydrothermal and electrodeposition method. Zinc cobalt telluride@nickel cobalt selenide electrode achieved highest specific capacitance of 800 F g^{-1} at 2 A g^{-1} current density. As fabricated electrode exhibited the retention of 93.5% after 5000 GCD cycles, confirmed the good stability and reversibility. An asymmetric device showed a high energy (55 W h kg^{-1}) and power density (560 W kg^{-1}).

Keywords: Asymmetric Supercapacitor, Metal Chalcogenide,

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Effect of catalyst on benzene chlorination process

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Chlorobenzene is an aromatic organic compound with the chemical formula C_6H_5Cl. This colorless and flammable liquid is a common solvent and a widely used intermediate in the manufacture of other chemicals. Benzene chlorination is of considerable commercial importance and has therefore received wide attention. Chlorobenzene is used as a raw material in the production of a new safe explosive based on 2,4-dinitroanisole (DNAN) and pesticides dichlorodiphenyltrichloroethane (DDT), and also as an intermediate in the preparation of pharmaceutical raw materials, herbicides. The choice of a catalyst for liquid phase chlorination of benzene depends on the desired product, operating conditions and cost. Considering the risks of the chlorination process, choosing the right catalyst can save the time of the process and the amount of chlorine gas consumed. For this reason, the available and widely used iron chloride catalyst was used. And the effect of this catalyst on the time and efficiency of the chlorobenzene preparation process was investigated. And the result of these experiments is that with increasing time in the amount of catalyst and constant temperature, the production efficiency of chlorobenzene is reduced and the reaction is carried out towards the production of higher chlorinated benzenes. Also, with the increase of the catalyst, the amount of chlorobenzene production decreases.

Keywords: Catalyst, Iron Chloride, Chlorobenzene, Liquid Phase.

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Synthesis of a green magnetic nanocatalyst through the functionalization of 2,4,6-trichloro-1,3,5-triazine and boric acid

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In contemporary times, the fabrication of green nanocatalysts has garnered considerable interest among numerous scholars [1]. The synthesis and investigation of Fe3O4@SiO2@APTES@TCT magnetic nanoparticles have been previously documented [2]. This study involves the synthesis of a nano catalyst that is both environmentally friendly and green. The synthesis process involves functionalizing 2,4,6-trichloro-1,3,5-triazine and boric acid on magnetic nanoparticles that are coated with silica and APTES. The synthesis of 4-chlorobenzylidene malononitrile involved the utilization of a novel catalyst. This catalyst was employed due to its significance in the field of organic compounds. The characterization of this catalyst was conducted using FT-IR and NMR analyses. The magnetically recoverable nanocatalyst exhibited the ability to be reused multiple times without experiencing a substantial decline in its catalytic activity.

Keywords: Green Catalysts, Nanocatalysts, Magnetic Nanoparticles, Recovered.

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Synthesis and characterization of bismuth iron oxide nanostructure by sonochemical method

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So far, considerable attention has been paid to the construction of potential photocatalysts to deal with issues related to environmental degradation and energy crises. Among the multitude of photocatalysts, the photocatalyst based on bismuth iron oxide is flourishing as an adsorption center due to its good chemical stability and easy extraction. This article presents the synthesis and properties of bismuth iron oxide nanocomposite using sonochemical method as well as different techniques for desulfurization of petroleum derivatives. The synthesis of iron oxide bismuth nanocomposite includes preparation of precursor solutions, sonication of solutions, addition of a surfactant, etc. The purity, structure and morphology of the produced nanocomposite were identified by X-ray diffraction (XRD) analysis.Desulfurization of petroleum derivatives is a vital process to reduce sulfur content, which helps to develop efficient and environmentally friendly technologies in this field

Keywords: Bis Bismuth Iron Oxide, Nanostructure, Photocatalyst, Sonochemistry, Desulfurization Muth Iron Oxide, Nanostructure, Photocatalyst, Sonochemistry, Desulfurization

Synthesis, Characterization, and spectral properties of new Schiff base ligand derived from “(E)-4-((nitrophenyl) diazenyl)-2-hydroxy-3-methoxy benzaldehyde” with amine and its metal complexes

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In view of recent developments and increasing applications of transition metal complexes with Schiff base ligands, in this research work the novel azo Schiff base of Cu(II) and Ni(II) have been synthesized by reaction of $Cu(OAC)_2.1H_2O$, $Ni(OAC)_2.4H_2O$ and $NiCl_2.6H_2O$ with “methyl2-((2-((E)-(2-hydroxy-3-methoxy-5-((E)-(4-nitrophenyl)diazenyl)benzylidene)amino)ethyl)amino)cyclopent-1-enecarbodithioate” novel azo Schiff base ligand. The new products were characterized by IR, UV-Vis, ^{1}HNMR and fluorescence spectroscopies. The spectroscopic data suggest that in these complex the azo Schiff base ligands are coordinated as deproton form through oxygen, nitrogen and sulfur atoms with metal [1]. The coordination around metal in these complex was essentially square-planar with a small tetrahedral distortion [2,3].

Keywords: Schiff-base Compound, Azo Compound, Square Planar Complex, Transition Metal Complex

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Synthesis and Characterization of new Azo-Schiff Base Ligand and its complexes derived from N-aminonaphthalimide with azo-aldehyde and investigation of photophysical properties

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The azo–Schiff base compounds 2-(((E)-(2-hydroxy-3-((E)-(4-nitrophenyl)diazenyl)naphthalen-1-yl)methylene)amino)-1H-benzo[de]isoquinoline-1,3(2H)-dione (H_2L) were prepared from the reaction of N-aminonaphtalimid with (E)-2-hydroxy-3-((4-nitrophenyl)diazenyl)-1-naphthaldehyde. Mononuclear complexes of H_2L with Ni(II), Cu(II), Pb(II), Mn(II) and Cd(II) transition metal were also prepared. The structures of all compounds were then characterized by NMR, IR and fluorescent spectroscopy. Our result show that reactions of $M(OAc)_2.XH_2O$ and $M(NO_3)_2.XH_2O$ with H_2L resulted to $M(L)(NO_3)_2$ in which coordination to M carried out through O and N atoms of ligand. The influence of metal cations such as Na^+, Mg^{2+}, Al^{3+}, Pb^{2+}, Cr^{3+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+}, Cu^{2+} and Cd^{2+} on the photophysical properties of ligand were investigated by means of emission spectrophotometry, which the ligand was found to be as an effective fluorescent sensor for Cd^{2+} or Al^{3+} ions.

Keywords: Schiff Base, Fluorescent Spectroscopy, Photophysical Properties

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Synthesis and characterization of a new nano complex derived from (E)-2-hydroxy-5-(2-nitrophenyl)diazenylbenzaldehyde and $Fe_3O_4@SiO_2$ and investigation of its catalyst and photophysical properties

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Synthesis of a heterogeneous nanosized catalyst with a coating of a branch of the dioxo-molybdenum(VI) complex on the shell structure of $Fe_3O_4@SiO_2$. Properties and the nature of the surface of the complex were investigated using methods such as infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), X-ray diffraction analysis (EDX) and vibrational sample magnetometer (VSM)[1]. The prepared composition of the nanocatalysis effect was used for the selective epoxation of alkenes in the presence of tert-butyl hydroperoxide[2].The results showed that this catalyst has a good ability to produce various epoxies..

Keywords: Nanocatalyst, Epoxidation, Selectivity, Heterogeneous

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Synthesis and spectroscopic characterization of two new phosphoramides

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Recently, phosphoramide compounds have received considerable attention as a key factor for many biologically active molecules. They also show good performance as organic dyes, flame retardants and extractants. Therefore, developing an efficient and practical method to synthesize phosphoramides is of great importance [1]. Furthermore, Phosphoryl-based compounds, can be good representatives for complex reactions as well [2]. Consequently, in this work, the synthesis of two new phosphoramide compounds, $P(O)(OC_6H_5)_2(NHCSNHC_7H_{13})$ (1) and $P(O)(NHC_6H_{11})_2(NHCH(CH_3)(C_6H_5))$ (2) are reported. Characterization was performed by IR, NMR (^1H, ^{13}C, ^{31}P) and Mass spectroscopies. Some carbon atoms with two and three bonds separations from phosphorus appear as doublets, due to the coupling with phosphorus. Typical values of coupling constants are $^2J(P,C) = 6.1$ Hz, $^2J(P,C) = 5.3$ Hz and $^3J(P,C) = 4.5$ Hz in (1) and $^2J(P, C) = 3.0$ Hz and $^2J(P,C) = 6.1$ Hz in (2).

Keywords: Phosphoramide, Synthesis, Charactrization.

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Crystal structure and Hirshfeld surface analysis of a new Eu(III)/Cr(III) double-complex salt

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Hirshfeld surface analysis and two-dimensional fingerprint plot are used to study the intermolecular interactions in a new double-complex salt: diaqua pentakis (tetramethylurea) europium(III) hexa (isothiocyanato) chromate(III) tetrakis (tetramethylurea) solvate, $[Eu(H_2O)_2(C(O)(N(CH_3)_2)_2)_5][Cr(NCS)_6].4C(O)(N(CH_3)_2)_2$ (I). The contacts received by the four symmetry-different components in the structure, including cationic complex, counter-anion complex and two symmetry-independent tetramethylurea molecules are discussed, with considering the relative contributions percentages of all contacts existing in the crystal packing. The highlighted interactions are S…C contacts (between cation and anion) and relatively strong Eu—O—H···O hydrogen bonds, which are manifested as red spots in the related Hirshfeld surface maps. These highlighted contacts in the title structure are compared with those found from the Cambridge Structural Database (CSD) [1] in the structures including similar contacts.

Keywords: Double-complex Salt, Hirshfeld Surface Analysis, Crystal Structure

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Synthesis and Characterization of Mononuclear Cobalt(II) and Binuclear Copper(II) Complexes with Tetradentate Ligand(L)

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This research describes the synthesis and charactrization of new mononuclear cobalt(II) and binuclear copper(II) complexes with the tetradentate ligand: N,N'-bis(ortho-carbonyl, benzoic acid) 1,3-diaminopropane dihydrochloride (L), which is divided into the following two parts: In the first part, the ligand (L) is synthesized from the reaction of trimethylene diamine compound (tn) with phthalic anhydride and then partial hydrolysis of its product using alkaline sodium hydroxide solution, under completely controlled conditions, which is similar to the synthesis of Schiff base ligands. In the second part, by the McCarthy method, two complexes $[Co(L)(H_2O)_2]$ and $[Cu_2(L)(MeO)_2(MeOH)_2]$ are synthesized using this ligand and salts of cobalt(II) nitrate hexahydrate and copper(II) nitrate trihydrate in methanol solvent and pH adjustment by sodium methoxide. The structure of the synthesized products has been characterized through the analysis of spectra obtained from IR, FT-IR, 1H NMR, ESR spectrometers, as well as the results of elemental analysis, and the study of their electron absorption spectrum has been done by UV-Vis device.

Keywords: Complex, Ligand, Spectroscopy, Elemental Analysis, Mononuclear

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Easy synthesis of highly fluorescent carbon dots from tomato lycopene and their biological imaging applications

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Fluorescent carbon dots (CDs), a new member of the carbon nanomaterial family, have drawn considerable attention in the fields of optoelectronic devices, biological labeling and biomedicine.Typically, CDs are small oxygenous carbon nanoparticles with sizes blow 10 nm, displaying size and excitation wavelength dependent photoluminescence (PL) behavior.A simple and green approach was developed to synthesize highly fluorescent carbon dots (CDs) using lycopene as a carbon source.The CDs were characterized by excellent monodispersion, superior photostability, pH-independent emission, long fluorescence lifetime and high quantum yield (QY).CDs could be considered as a potential substitute for organic dyes or semiconductor quantum dots (SQDs) in biological imaging[2-3].

Keywords: Fluorescent Carbon Dots, Lycopene, Green Synthesis

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Electron flux at the Schottky junction of Bi NPs and MoS_2-supported RGO for degradation of Tetracycline

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In this work, a heterostructured metallic Bi/MoS_2 photocatalyst (MBi_x) was prepared via uniform decoration of plasmonic bismuth nanoparticles onto the surface of MoS_2 nanosheets. MBi_x catalysts were then loaded onto the surface of reduced graphene oxide (RGO) using a simple hydrothermal method to form RGO/MBi_x nanocomposite. RGO/MBi_x heterostructures demonstrated significantly improved photocatalytic performance for the removal of tetracycline (TC) under visible-light irradiation. The enhanced photocatalytic activity was found to be dependent on the level of Bi and RGO in the catalyst. The degradation rate over the optimum catalyst (RGO-2.5/$MBi_{1.0}$) was six-fold higher than that of pristine MoS_2. The results indicated the dual roles of the Bi nanoparticles in the RGO/MBi_x nanocomposite in improving the light-harvesting ability and charge separation attributed to the plasmon-mediated activation of the metallic Bi nanoparticles under visible light, followed by efficient electron migration among Bi/MoS_2 interfaces. The intimate interfacial contact of the metal and semiconductor allows only the electron transport from the semiconductor to metallic nanoparticles and hinders electron movement back across the Schottky barrier, resulting in significantly accelerating the carrier pairs separation and restricting the mobile charges recombination. Therefore, the built-in electric field at the junction of the Bi nanocrystals and MoS_2 can provide an interesting and efficient pathway for the photocatalytic oxidation of TC. Both of these features in synergy with the inherent characteristics of RGO as a competitive acceptor component, which provided a conduction path for the photo-induced charges, led to remarkable enhancement in the photocatalytic activity of the nanocomposite. The trapping experiments showed •OH and $•O_2^-$ played a crucial role in TC photocatalytic degradation. Additionally, RGO-2.5/$MBi_{1.0}$ exhibited stable activity during the photodegradation of TC over multiple cycles. The present study could not only present a novel strategy for increasing the photocatalytic performance of MoS_2 but also display great potential for the feasibility of utilizing the abundant and low-cost Bi nanoparticles to replace the precious noble metals to promote the spectral response in the visible region.

Keywords: MoS_2, Metallic Bi, Nanoparticles, Light-harvesting, Charge Separation

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Visible-light-induced In,S-TiO_2@rGO with enhanced photocatalytic activity for detoxification of atrazine

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The visible-light activated In,S-TiO_2@rGO nanocomposite was prepared using an innovative ultrasonic-assisted solvothermal method. The XRD patterns indicated the anatase structure for TiO_2 co-doped with indium and sulfur elements. FT-IR and Raman spectra analysis confirmed the presence of rGO in nanocomposites. In addition, SEM and HRTEM images confirmed the presence of mono-dispersed TiO_2 nanoparticles on rGO sheets. A considerable red shift in absorption edge of TiO_2 was observed after co-doping with In and S. Co-doping of TiO_2 with In and S elements and compositing with rGO significantly enhanced its visible-light photocatalytic activity which was strongly affected by the amount of In, S and rGO to TiO_2 ratio in the nanocomposite. The complete degradation and 95.5% mineralization of 20 mg/L atrazine (ATZ) was attained in the photocatalytic oxidation (PCO) process within 20 min with In,S co-doped TiO_2@rGO nanocomposite. The rate of ATZ degradation in the PCO process with In,S co-doped TiO_2@rGO nanocomposite was 80 times of that with pure TiO_2 as catalyst under visible-light irradiation. The enhanced photocatalytic activity of the In, S co-doped TiO_2@rGO is related to the synergistic effect of dopants contributing to improved visible light absorption and decreased recombination rate of the charge carriers. The degradation studies using various scavengers showed that hydroxyl radical was the main active species that contributed in the photocatalytic degradation of ATZ under the selected conditions. In addition, the rate of ATZ degradation and mineralization in the photocatalytic process with the TiO_2@rGO nanocomposites as catalyst was 0.248 and 0.169 min^{-1}, respectively, which was remarkably greater than TiO_2. The prepared nanocomposite was found to be a reusable and durable catalyst for visible light photocatalytic degradation of ATZ. As-made In,S co-doped TiO_2@rGO nanocomposite could preserve its catalytic activity during four consecutive recycles for the ATZ removal process. The cytotoxicity of fresh and photocatalytic-treated ATZ solutions assessed using the human hepatic cells (HepG2) indicated that treating ATZ solution in the developed PCO process could be considerably detoxified.

Keywords: TiO_2 doping, Graphene Oxide, Nanocomposite, Photocatalytic Process

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Photocatalytic wastewater purification under visible light irradiation using multi-doped TiO_2/rGO cross-linked 3D aerogel; Mechanistic catalytic experiments and cytotoxicity assessment

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In this work, the 3D Ga, N and F multi-doped TiO_2@rGO aerogels as an efficient visible-light activated and easily separable catalyst have been successfully prepared trough simple one-pot hydrothermal method using ascorbic acid as the cross-linker and reducing agent. It can be seen that multi-doping and coupling with GO decrease the growth of TiO_2 crystals. The band gap of TiO_2 was reduced from 3.21 eV to 2.73 eV with the use of 1 mol.% of Ga and 3 mol.% of NF. SEM images indicated an interconnected porous 3D network structure contain of 2D graphene oxide sheets, with uniform dispersion of TiO_2 nanoparticles on the rGO plane. The reduction of GO was clearly confirmed based on the results from FT-IR and Raman spectroscopy analysis. 3D porous structure of prepared aerogels resulted in large specific surface area and high pore volume and present good adsorption capacity as well as excellent photocatalytic activity for the degradation of ATZ molecules. Mixed-doped TGA samples showed higher photocatalytic activity than mono-doped and un-doped samples under visible light irradiation. The 100% degradation and 77% mineralization of 40 mg/L ATZ were attained in the PCO process within 60 min using the Ga_1NF_3@TGA sample. The enhanced photocatalytic activity of the Ga_1NF_3@TGA is due to the synergic effect of high visible light absorption, short band gap (Ga and N doping), surface acidity (F doping), ATZ adsorption (electrostatic attraction), efficient charge excitation and transfer (mid bands/defect levels/vacancies) and generation of more hydroxyl and superoxide radicals for the photocatalytic degradation of ATZ. The degradation studies using various scavengers showed that hydroxyl radical was the main active species that contributed to the photocatalytic degradation of ATZ under the selected conditions. The cytotoxicity of the fresh and photocatalytic-treated (under optimum conditions) ATZ solutions was evaluated as skin fibroblast cells (Hu02) viability. The results indicated excellent detoxification of ATZ upon photocatalytic treating under visible light irradiation. Accordingly, the GaNF@TGA sample prepared for this work could be an excellent visible-light photocatalyst for the degradation, mineralization, and detoxification of organochlorine pesticides in contaminated water.

Keywords: TiO_2 Modification, Nanocomposite, Aerogel, Cytotoxicity

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Preparation and application of alginate-graphene oxide magnetic beads to remove Zn^{2+} cation in aqueous solutions

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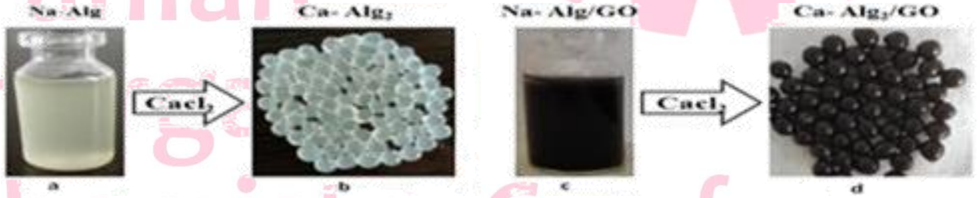
In this study, alginate has been used as a magnetic particle of graphene oxide absorbents to remove Zn2+ ions from aqueous solutions. The results demonstrated the following: At pH 6 in 180 min, zinc removal effectiveness was found to be optimal. [1]. The effectiveness of the removal process was also enhanced by increasing the initial concentration and adding more adsorbents. The Langmuir adsorption isotherm The model of zinc removal has been more closely matched to the test results. Conversely, the adsorption kinetics of zinc were in accordance with a model called Pseudonquadratic. Thermodynamic studies showed that the removal of zinc on the alginate-graphene oxide magnetic composite nanofibers is endothermic and the adsorption rate increases with increasing ambient temperature [2]. To identify the appearance and properties of absorbent nanocomposites, an analysis was performed on XDR, TEM, FESEM and VSM with a view to confirming the synthesis steps. TEM and FESEM analysis showed that the mGO/Alg Beads nanocomposite was a porous nanoabsorbent and a magnetite nanoparticle with an average diameter of 33.69 nm could be easily seen on the surface of the nanocomposite. Results from desorption tests show that, at the end of 5 absorption and desorption cycles, 90% of nanomaterials are able to be effectively used. Finally, these nanocomposites are very promising because of being easy, fast, healthy, cost-effective, and highly efficient separation of pollutants[3].



Keywords: Magnetic beads, Alginate, Graphene oxide, Zinc, Removal, Aqueous solution

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New bisphosphinamide: X-ray crystallography, spectroscopy and thermogravimetry

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Phosphinamides, with a $C_2P(O)N$ fragment, are well-known for flame-retardancy properties [1]. In this work, the synthesis, spectroscopy, thermogravimetry and X-ray crystallography of N, N'-(cyclohexane-1,4-diyl)-bis(P, P-diphenylphosphinic amide) are studied. The compound crystallizes in the monoclinic space group *C*2/*c*. The asymmetric unit is composed of one half of the molecule, and the complete molecule is generated by an inversion element. The P atom has a distorted tetrahedral $C_2P(O)N$ enviroment, and the maximum and minimum bond angles at phosphorus are related to N—P═O (120.23 (6)°) and N—P—C (101.95 (7)°). The bond-angle sum at nitrogen (about 353°) confirms its sp^2 character. The P═O bond length (1.4864 (11) Å) is slightly longer than the typical phosphorus-oxygen double bond length and is comparable to those in analogous compounds [2, 3]. The P—N bond length (1.6407 (13)Å) is standard for structures with a $C_2P(O)N$ skeleton [3]. The NH unit adopts a *synclinal* orientation with respect to the P═O group. In the crystal structure, the molecules are aggregated through N—H…O hydrogen bond in a two dimensional assembly along the *bc* plane. The ^{31}P NMR spectrum shows one signal at 19.91 ppm indicating the high purity of the compound. In the IR spectrum, the band centered at 3133 cm^{-1} corresponds to the N—H stretching. The TGA exhibits the starting decomposition point at about 250 °C.

Keywords: Bisphosphinamide, Crystal Structure, Thermogravimetric Analysis

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Synthesis and Structural Characterization of Two-dimensional Metal-organic Framework by Using BTZ Ligands

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Metal-Organic Frameworks are a new category of porous materials that have been extensively used in various applications such as gas separation process, gas storage and catalysis due to their unique properties such as high porosity, crystallinity, high surface area, designability, favorable thermal, chemical stability, adjustable pore properties and so on. In this work, new two dimentional Zn metal-organic framework was designed and synthesized by applying new BTZ ligands with different functional groups. The structures which were characterized by single crystal X-ray crystallography, XRD, and FT-IR spectroscopy. The thermal stability of compound has been studied by thermal gravimetric (TG) and differential thermal (DTA) analyses.This study is a new report of increasing Metal-Organic Frameworks by a simple method.

Keywords: Synthesis, Characterization, Metal-organic Framework, BTZ

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Synthesis of new Co-MOFs with bithiazole ligands

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To design and make new MOFs with desired structure and consequently spatial properties, there need to choose both metal ion as a node and ligands as their linkers. MOFs are a new category of porous materials that have been extensively used in various applications due to their unique properties such as crystallinity, high surface area, designability, favorable thermal and chemical stability, and so on. Here, a new MOF with molecular formula [Co (btz)(X)n]. Compound is based on a Co (II) unit complexed by bridging bidentate ligand, 4, 4'-bithiazole. This MOF was obtained by the reaction of zinc (II) nitrate with 4, 4'-bithiazole as the linker and the N-donor ligand. The thermal stability of compound has been studied by thermal gravimetric (TG) and differential thermal (DTA) analyses. The structure was determined by single-crystal X-ray diffraction and Fourier-transform infrared spectroscopy (FT-IR).

Keywords: MOF, Synthesis, Co, Bithiazole.

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Sono-synthesis of a new Pb complex based on 4,4′-bithiazole

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It is well-established that ultrasound irradiation is a key technology in fast synthetic approach for many materials [1]. Ultrasonic irradiation on reaction combination constructs a huge number of cavitation bubbles which grow up quickly and eventually undergo drastic collapses which result in the formation of micro-jets that can generate fine emulsion between the reactants. Besides, the local temperature within the reaction mixture rises with these vigorous collapses of cavitation bubbles and ultimately results to cross the activation energy barrier [2]. Hence, in many cases, the usage of ultrasonic irradiation can support the catalysts in organic reactions through alteration in morphology, size, and energy supply. This article focuses on the simple synthetic preparation of a new Pb complex by sonochemistry method. The thermal stability of new complex was studied by thermal gravimetric (TG) and differential thermal analyses (DTA). The Pb compound was characterized by X-ray powder diffraction (XRD) and Fourier transform infrared (FT-IR) spectroscopy.

Keywords: Sono-synthesis, Pb, Complexe, 4,4′-bithiazole.

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Enhanced photocatalytic conversion of organic dyes using $CeFeO_3/MoS_2$ heterojunction as a highly effective visible-light-driven photocatalyst

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The $CeFeO_3/MoS_2$ heterojunction was successfully prepared through the hydrothermal method. The synthesized heterojunction structure was characterized by various techniques and applied to the conversion of methylene blue (MB) under irradiation of visible light. To characterize the new heterojunction structure, Fourier transformed infrared (FT-IR), field emission scanning electron microscope (FE-SEM), energy-dispersive X-ray spectroscopy (EDXS), Xray diffraction (XRD), photoluminescence spectroscopy (PL), differential reflectance spectroscopy (DRS), and transmission electron microscopy (TEM) analyses were used. The FE-SEM images illustrated the successful deposition of MoS_2 flower-like on the surface of $CeFeO_3$ perovskite with 46 nm as an average size. The influence of the amount of catalyst, temperature, pH, and electron acceptor were investigated. By $CeFeO_3/MoS_2$ heterostructures photocatalyst, the conversion rate of MB reached 98% within 20 min, whereas by $CeFeO_3$ perovskite no significant conversion was observed in MB. The higher photocatalytic performance of $CeFeO_3/MoS_2$ heterostructures is assigned to their lower charge recombination compared to $CeFeO_3$ perovskite. Moreover, the photocatalytic mechanism and recycling experiments of $CeFeO_3/MoS_2$heterostructures are discussed in detail. The $CeFeO_3/MoS_2$heterostructures are thus promising photocatalysts for the cleanup of polluted water.

Keywords: Conversion of Dyes, Heterojunction, Perovskite, Photocatalyst

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Immobilization of zinc complexes on magnetic nanoparticles and their applications as catalyst

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In this study, a novel zinc complex immobilized covalently on $CoFe_2O_4$ magnetite nanoparticles was synthesized. The nanocatalyst was characterized thoroughly using thermogravimetric analyses (TGA), Fourier Transform Infrared (FT-IR) spectroscopy, scanning electron microscopy (SEM), energy dispersive X-ray (EDX), inductively coupled plasma optical emission spectroscopy (ICP-OES), vibrational sample magnetometry (VSM), and powder X-ray diffraction (PXRD). $CoFe_2O_4$@4-Dimethylaminopyridine (Dmap)@Zn was found to be efficient for synthesis of tetrazole at mild reaction conditions in the green medium. The influences of reaction temperature, solvent, and the amount of catalysts were studied. The best results were obtained in water and without organic solvent condition for synthesis of tetrazole. The catalyst was easily collected via an external magnetic field and further reused at least 6 times without a significant decrease in catalytic activity. The wide applicability of the catalyst, ease of catalyst separation, its reusability capacity, and importantly reaction operation in a green medium and elimination of hazardous organic solvents are the advantages of this catalyst.

Keywords: 4-Dimethylaminopyridine (Dmap), $CoFe_2O_4$ Magnetite Nanoparticles, Synthesis of Tetrazole

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Synthesis and characterization of Ni complex supported on MCM-41 as an efficient and reusable nanocatalyst the synthesis of Polyhydroquinoline derivatives

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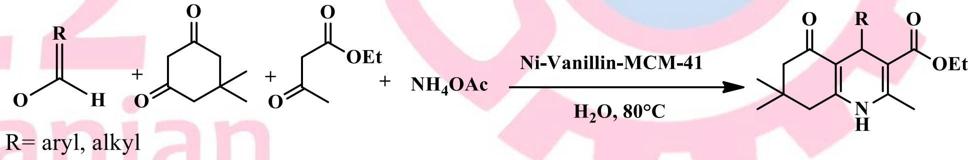
Polyhydroquinolines are important building blocks in the synthesis of many natural products with a wide range of pharmacological and biological activities including antifertility, anticonvulsant, antibacterial, anticancer, antifungal, antitumor, and also as a mono amine oxidase inhibitor [1-4]. An efficient heterogeneous catalyst has been synthesized by immobilization of nickel-vanillin complex on MCM-41 nanostructure and characterized by XRD, TGA, BET, EDS, SEM, ICP-OES and FT-IR spectroscopy. The catalytic activity and stability of the prepared compound have been studied for the synthesis of Polyhydroquinoline derivatives. The simple workup, mild conditions, excellent yield, and inexpensive and non-toxic catalyst; render this protocol both attractive and economically viable. More importantly, this catalyst can be reused several times without any significant loss of its catalytic activity. The synthesis of Polyhydroquinolines is shown in Scheme 1. The desirable product was synthesized in good to excellent yields.



Scheme 1. Synthesis of Polyhydroquinoline in the attendance of Ni-van-MCM-41.

Keywords: Polyhydroquinolines, MCM-41, Ni Complex, Recoverable Catalyst

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Synthesis of synthesis 1*H*-indazolo[1,2-b]phthalazine-trione derivatives catalyzed by Ni complex supported on MCM-41 as an efficient and reusable nano catalyst

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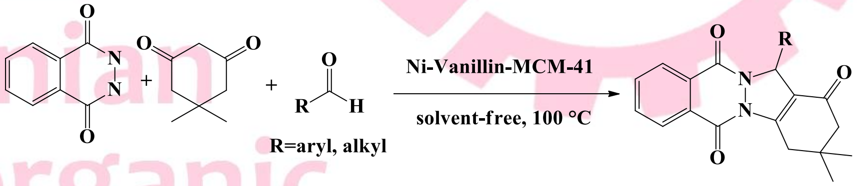
Development of efficient and selective synthetic transformations using inexpensive, available, and environmentally-benign catalysts and reagents is of great interest in modern organic synthesis [1]. Based on green chemistry desires, the development of new strategies for very low cost, relatively non-toxic and recycling of this catalyst, which minimizes the energy and time required in achieving separations, can result in significant economic and environmental benefits. [3-4]. An efficient heterogeneous catalyst has been synthesized by immobilization of nickel-vanillin complex on MCM-41 nanostructure and characterized by XRD, TGA, BET, EDS, SEM, ICP-OES and FT-IR spectroscopy. In this work, we report an efficient procedure for the preparation of 1*H*-indazolo[1,2-b]phthalazine-triones derivatives in solvent free conditions in good to excellent yields through a one-step reaction using various aromatic and aliphatic aldehyde in the presence of Ni-Vanillin-MCM-41 as an efficient, green, reusable and inexpensive catalyst.Also, The catalyst showed excellent stability and recyclability. The desirable product were synthesised in goog to exellent yeilds.



Scheme 1. Synthesis of 1*H*-indazolo[1,2-b]phthalazine-trione in the attendance of Ni-vanillin-MCM-41.

Keywords: 1*H*-indazolo[1,2-b]phthalazine-trione, MCM-41, Ni complex, Recoverable Catalyst.

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Theoretical studies on the nature of metal-ligand bonds in some cylinder-like trinuclear hexacarbene complexes of Cu(I), Ag(I), Au(I), Pd(II) and Hg(II) ions

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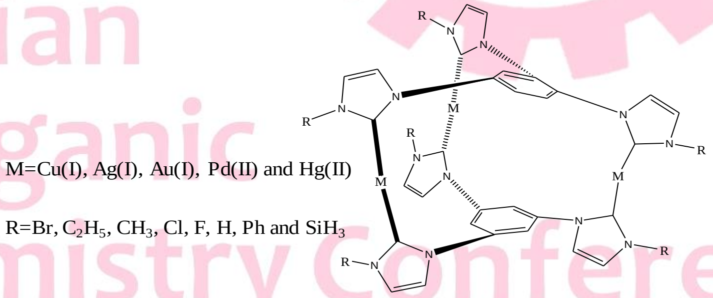
N-Heterocyclic carbenes (NHCs) have been extensively investigated over the last two cades due to their applications in various fields like as spectator ligands in catalytically active complexes, [1] in materials science, [2] as biologically active compounds [3] and very recently also in metallosupramolecular chemistry [4]. In the field of synthesis and investigation of trinuclear cylindrical hexacarbon complexes, various works have been done experimentallyTo the best of our knowledge, theoretical studies on the bonding nature of trinuclear-like cylindrical hexacarbon complexes have been performed less. In this structure project, the nature of the metal-ligand bonding of a number of cylindrical hexacarbon complexes such as trinuclears will be studied and the possibility of communicating between the theoretical and experimental data of these complexes will be investigated. By changing the central atom and replacing different d-block metals such as Cu(I), Ag(I), Au(I), Pd(II) and Hg(II) in the center of cylindrical hexacarbon complexes like trinuclears of these structural compounds , the stability and the nature of the bond in these compounds change significantly. To obtain the thermodynamic data of these compounds in the gas phase, calculations are performed on the optimized structures using the FREQ keyword. To investigate the nature of links and interactions, NBO, AIM and EDA calculations have been performed on the optimized structures with the PBEPBE methods and DEF2-TZVP basis set.



M=Cu(I), Ag(I), Au(I), Pd(II) and Hg(II)

R=Br, C_2H_5, CH_3, Cl, F, H, Ph and SiH_3

Fig. 1. structure of trinuclear cylindrical hexacarbon complex.

***Keywords**:* NHC, Trinuclear, Cylindrical, Theoretical, FREQ

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Structural, magnetic, and photocatalytic characterization of zinc-doped cobalt ferrite nanoparticles

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Spinel oxides (AB_2O_4) have garnered a long-standing reputation due to their intriguing electronic and magnetic properties, making them highly suitable for a wide range of industrial applications. These applications span from magnetic cores and high-frequency devices to medical diagnostics and environmental monitoring [1]. Cobalt ferrite and zinc ferrite, two specific ferrite spinels belonging to the AFe_2O_4 family, have emerged as subjects of significant interest in the scientific community. These materials exhibit exceptional properties and find numerous applications in fields such as photocatalysis, information storage, electronic devices, magnetic materials, and gas sensing. The remarkable potential and versatility of cobalt ferrite and zinc ferrite contribute to their widespread popularity and ongoing exploration in different industrial sectors [2,3]. In this study, we focus on the synthesis of zinc-cobalt ferrite magnetic nanoparticles using a sol-gel technique with natural gel as the precursor. The synthesized nanoparticles were thoroughly characterized using various analytical techniques, including Fourier transform infrared spectroscopy (FTIR), Brunauer-Emmett-Teller (BET) analysis, X-ray powder diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), and vibrating sample magnetometer (VSM). Furthermore, we evaluated the photocatalytic activity of the nanoparticles for the degradation of congo red dye under visible light irradiation. The efficiency of the photocatalytic process was investigated by varying the initial dye concentration, photocatalyst dosage, and irradiation time. The results demonstrated the remarkable ability of zinc-cobalt ferrite magnetic nanoparticles to effectively degrade congo red dye. This method offers various advantages, including cost-effectiveness, simplicity, shorter processing time, environmental friendliness, and the potential for scalable production.

Keywords: Dye Degradation, Green Synthesis, Magnetic Nanopaticles

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Zinc-cobalt ferrite magnetic nanoparticles as an environmentally friendly, cheap, and effective catalyst for solvent-free one-pot multi-component synthesis of 3,4-dihydropyrimidin-2(1h)-ones

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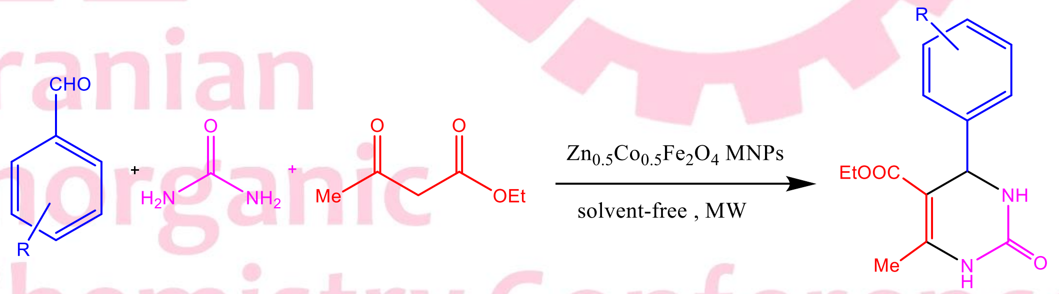
The synthesis of 3,4-dihydropyrimidin-2-(1H)-ones (Biginelli compounds) and their derivatives is of great interest due to their diverse therapeutic and pharmacological properties, including antiviral, antibacterial, antitumor, and antihypertensive activities. These compounds have also been utilized as calcium channel blockers, α-1a-antagonists, and neuropeptide Y (NPY) antagonists. Marine sources have provided various alkaloids with the dihydropyrimidine core unit, including batzelladine alkaloids, known for their potent inhibition of HIV gp-120-CD4 interaction. The Biginelli reaction is considered a crucial multi-component reaction for generating compounds with diverse medicinal applications [1,2]. In this work, we present a green and efficient method for the solvent-free synthesis of 3,4-dihydropyrimidin-2(1H)-ones through a one-pot three-component condensation of ethyl acetoacetate, an aryl aldehyde, and urea in the presence of zinc-cobalt ferrite magnetic nanoparticles as a high-performance magnetic catalyst (Scheme 1). The proposed methodology offers several advantages, including high yields, short reaction times, mild reaction conditions, straightforward work-up procedures, and the use of a highly recyclable catalyst.



Scheme 1. Synthesis of 3,4-dihydropyrimidin-2(1H)-ones by magnetic nanoparticles.

Keywords: 3,4-Dihydropyrimidin-2-(1H)-one, Solvent Free, Magnetic Catalyst

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Synthesis and photocatalytic investigation of zinc-doped nickel ferrite in the degradation of organic dye under visible light

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Nowadays, the act of releasing dyes and colored effluents into bodies of water poses a significant problem as it can lead to the formation of toxic and carcinogenic compounds, ultimately polluting the water [1]. Consequently, numerous techniques have been developed to address this issue. However, traditional methods like reverse chemical precipitation, ion exchange, adsorption, and filtration tend to be expensive and may inadvertently transfer dyes from primary pollutants to secondary pollutants, necessitating further treatment [2]. Among the available methods, the adsorption of dyes onto sorbents emerges as a cost-effective approach for removing pollutants. Its initial cost, simplicity, ease of operation, and sensitivity to toxic pollutants make it superior to alternative water reuse methods. Nonetheless, it is important to acknowledge that adsorption does transfer organic pollutants to secondary ones, which subsequently require additional treatment. Hence, researchers have made an important discovery a safe and environmentally friendly wastewater treatment method known as the photodegradation of dyes [3]. In this study, zinc-nickel ferrite magnetic nanoparticles were synthesized using the sol-gel method. The synthesized nanoparticles were characterized using various techniques including field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), X-ray diffraction (XRD), dispersive X-ray analysis (EDX), Brunauer-Emmett-Teller (BET), Fourier transforms infrared spectroscopy (FTIR), vibrating sample magnetometer (VSM), and UV-Vis diffuse reflectance spectroscopy (DRS). The X-ray powder diffraction analysis confirmed the formation of cubic spinel phase nanoparticles. Furthermore, the photocatalytic activity of the magnetic nanoparticles was assessed by measuring the degradation of reactive blue 21 dye under visible light irradiation. The study also investigated the effects of various process parameters such as catalyst dosage, initial dye concentration, and visible light irradiation on the degradation of the dye.

Keywords: Magnetic Nanoparticles, Photocatalysis, Dye Degradation.

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Microwave-assisted multicomponent reaction for the synthesis of 2, 4, 5-triarylimidazole derivatives using zinc-nickel ferrite magnetic nanoparticles as a catalyst

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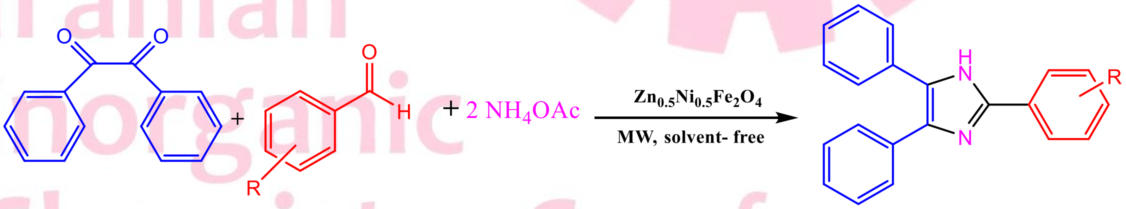
Imidazole derivatives have attracted significant attention in recent years due to their diverse therapeutic activities, including antibacterial, antifungal, antiviral, anti-inflammatory, antitubercular, antidepressant, and antitumor effects. Triarylimidazole compounds have gained notable significance owing to their broad range of biological activities and their utility in synthetic chemistry. The imidazole ring system is a crucial substructure that is commonly found in numerous natural products and pharmacologically active compounds. Examples of such compounds include the antiulcerative agent cimetidine, the proton pump inhibitor omeprazole, and the benzodiazepine antagonist flumazenil, all of which are derivatives of imidazole [1,2]. In this study, the synthesis of $Zn_{0.5}Ni_{0.5}Fe_2O_4$ magnetic nanoparticles by the sol-gel method was carried out. The resulting sample was characterized by FTIR, XRD, TEM, FESEM, EDX, and VSM. The catalytic activity of $Zn_{0.5}Ni_{0.5}Fe_2O_4$ MNPs was assessed for the synthesis of 2, 4, 5-triarylimidazole derivatives through a three-component reaction under microwave irradiation and solvent-free conditions. The obtained product was analyzed using ^{1}H NMR and ^{13}C NMR spectroscopy. This study offers several advantageous features, including the environmentally friendly and cost-effective synthesis of nanoparticles, utilization of microwave irradiation under solvent-free conditions, short reaction times, simple work-up procedures, and mild reaction conditions..



Scheme 1. Synthesis of 2, 4, 5-triarylimidazole derivatives

Keywords: 2, 4, 5-triarylimidazole Derivatives, Microwave Irradiation, Multi-component Reacion

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Green synthesis of copper-doped magnesium ferrite nanoparticles for the evaluation of their photocatalytic properties

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The contamination of water resources by industrial effluents, including organic dyes from sectors like textile, pharmaceutical, cosmetic, and paper, poses risks to human well-being and the ecological system. These dyes, which account for a significant portion of wastewater, contribute to concerns due to their mutagenic, carcinogenic, genotoxic, and teratogenic effects. Additionally, the coloration of water hampers sunlight penetration, reduces oxygen levels, disrupts photosynthesis, and negatively impacts aquatic life and the surrounding ecosystem [1,2]. Consequently, researchers have been actively seeking effective, low-cost, and reliable techniques for the removal of organic dyes from wastewater. Magnetic photocatalysts provide the advantage of recyclability by integrating catalytic properties with magnetism, enabling their effortless retrieval from the treated solution using an external magnetic field Among various magnetic nanoparticles, ferrite nanoparticles have garnered significant interest in the field of photocatalysis due to their electroconductivity, paramagnetic, optical, and chemical properties, high specific surface area, and environmental friendliness [3]. In this study, magnetic copper-magnesium ferrite nanoparticles were synthesized as an effective and recyclable photocatalyst using a sol-gel method. Characterization of the synthesized materials included XRD, FTIR, BET, FESEM, TEM, EDS, PL, and UV-Vis DRS analyses. The sample demonstrated a higher BET surface area due to the synergistic effect and interface between copper and magnesium metals. The photocatalyst effectively degraded malachite green dye under visible light irradiation. Notably, the magnetic nanoparticles could be easily separated using an external magnet, while the photocatalyst maintained its stable and high photocatalytic performance even after five consecutive runs under the same optimized conditions.

Keywords: Biosynthesis, Photocatalysis, Spinel Magnetic Nanoparticles

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Solvent-free one-pot synthesis of octahydroquinazolinone derivatives using copper-magnesium ferrite magnetic catalyst: an efficient approach

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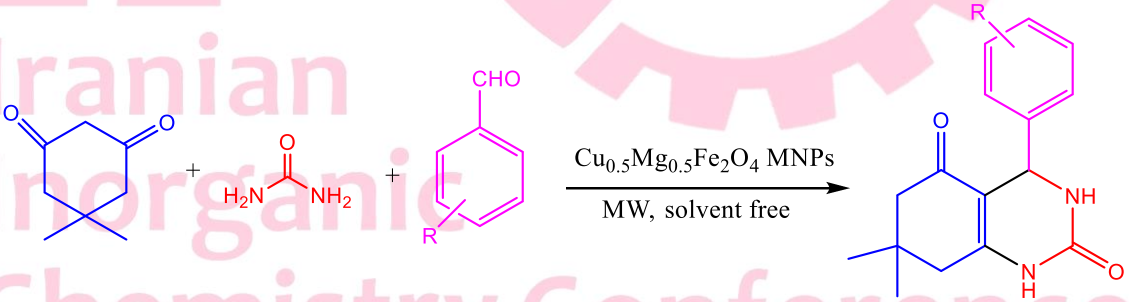
In recent years, there has been increasing interest in the Biginelli reaction for synthesizing octahydroquinazolinones. This reaction involves replacing open-chain dicarbonyl compounds with cyclic β-diketones and utilizing concentrated H_2SO_4 and HCl as catalysts. Octahydroquinazolinone derivatives synthesized through this method have garnered significant attention due to their diverse pharmacological properties [1]. The presence of the quinazolinone moiety in these compounds makes them valuable for applications such as hypnotic/sedative drugs and cancer treatment. Furthermore, quinazolinone derivatives exhibit a wide range of biological activities, including analgesic, anti-inflammatory, antimicrobial, anti-tubercular, anti-HIV, antimalarial, and antihistamine effects [2]. In this work, a simple, efficient and cost-effective method for the synthesis of octahydroquinazolinone derivatives using dimedone, urea and aromatic aldehydes using copper- magnesium ferrite as a catalyst under solvent free condition in microwave irradiation is reported. The present method does not involve any hazardous organic solvents. This catalyst has promising features for the reaction response such as the shortest reaction time, excellent product yields, simple work-up procedure and purification of products by non-chromatographic methods.



Scheme 1. Synthesis of octahydroquinazolinone derivatives

Keywords: Octahydroquinazolinone Derivatives , Magnetic Nanoparticles, Solvent Free Reaction

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Introduction of a bipyridine-based molten salt containing cobalt as an efficient and reusable catalyst for the Biginelli reaction

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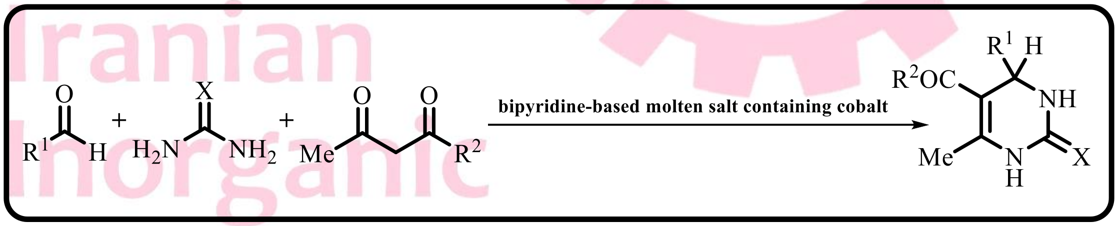
The research on one-pot multicomponent reactions has been an area of interest for the synthesis of *N*-containing heterocyclic scaffolds, such as 3,4-dihydropyridin-2-1*H*-(ones)/3,4-dihydropyridin-2-1*H*-(thiones) (DHPMs) and their derivatives. These heterocyclic compounds, particularly those with a DHPM core, have proven to have significant applications in biological and pharmacological fields, such as antibacterial, antihypertensive, calcium channel modulation, antiviral, antitumor, antifungal, anti-tubercular, mitotic kinesin Eg5 inhibition, anti-HIV, anti-HSV, and anti-inflammatory [1-2]. One of the most effective ways to synthesize DHPMs is the Biginelli reactions, which involves the condensation of an aldehyde, α *β*-ketoester, and urea under strongly acidic conditions. Despite several improved methods using different catalysts and reaction media to increase the yield and purity of the synthesized products, they suffer from disadvantages such as organic solvent use, long reaction times, low yields, high catalyst loading, and hard separation routes [3]. A new *Lewis* acidic molten salt based on bipyridine has been developed and used in this study to promote the synthesis of 3,4-dihydropyridin-2-1*H*-(ones)/3,4-dihydropyridin-2-1*H*-(thiones) compounds in a simple manner (Scheme1). The advantages of using this catalyst include ease of separation and high yield of products achieved in a shorter time.



Scheme1. Synthesis of DHPMs in the presence of Bipyridine-based molten salt containing cobalt.

Keywords: One-pot, DHPMs, Dihydropyrimidine, Biginelli, Multicomponent, Molten Salt

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Theoretical study of Kumada reactions on the formation mechanism of several p-carborane compounds

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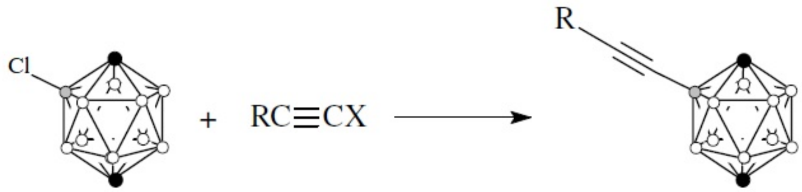
Cross-coupling is one of the most significant and extensively utilized methods in chemistry for linking two organic substrates using a metal catalystIn this method, two active groups (such as aryl or alkyl) are connected to each other via an alkyl radical or another reactive group. Kumada cross-coupling [1-3] is a specific type of cross-coupling that uses magnesium as a catalyst and connects an aryl group with another aryl or alkyl group. Carboranes are boron-rich compounds that have been synthesized through various cross-coupling reactions and hydrogen activation. Due to their unique chemical properties, these compounds are used as new ligands in metal catalysts in various fields of advanced chemistry. For example, in cross-coupling reactions, carboranyl ligands can serve as alternatives to phosphines in palladium and nickel catalysts. Herein, we have investigated the feasibility of obtaining heteroaryl derivatives of carboranes through Pd-catalyzed B–C cross-coupling reactions involving various organozinc heterocycle (See Scheme 1,). The molecular structures of the compounds studied here, such as reactants, transition states, intermediates and products, have been optimized using the Cam-B3LYP-D3 method in conjunction with the def2-SVP in solution. The Gaussian 09 (revision-D) program package is used for all quantum mechanical calculations. Based on the optimized structures obtained during the solution process,single point energies are determined using the IEF-PCM of the CamB3LYP-D3/def2-TZVP//Cam-B3LYP-D3/def2-SVP theoretical level. As seen in.



Scheme 1. General scheme for kumada reactions.

Keywords: Cross-coupling Reactions, Kumada Reaction, DFT Calculations, Palladium.

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Theoretical study of Sonogashira reactions on the formation mechanism of several p-carborane compounds

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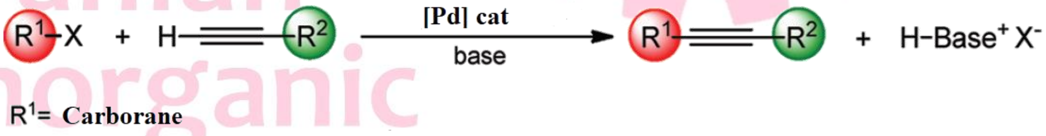
Cross-coupling is one of the most significant and extensively utilized methods in chemistry for linking two organic substrates using a metal catalyst. In this method, two active groups (such as aryl or alkyl) are connected to each other via an alkyl radical or another reactive group. The palladium-catalyzed Sonogashira reaction [1-3] is one of the most important and widely used methods for preparing arylacetylenes and conjugated enynes, which are precursors for natural products, pharmaceuticals, and materials with specialized optical and electronic properties. The general Sonogashira protocol for coupling terminal alkynes with aryl or alkenyl halides (or triflates) typically involves an organic solvent, a Pd(0)/Cu(I) catalytic system, and at least a stoichiometric amount of a base (Scheme 1). Herein, we have investigated the feasibility of obtaining heteroaryl derivatives of carboranes through Pd-catalyzed B–C cross-coupling reactions involving various organozinc heterocycle. The molecular structures of the compounds studied here, such as reactants, transition states, intermediates and products, have been optimized using the Cam-B3LYP-D3 method in conjunction with the def2-SVP in solution. The Gaussian 09 (revision-D) program package is used for all quantum mechanical calculations. Based on the optimized structures obtained during the solution process,single point energies are determined using the IEF-PCM of the CamB3LYP-D3/def2-TZVP//Cam-B3LYP-D3/def2-SVP theoretical level. As seen in.



Scheme 1. General scheme for Sonogashira reactions.

Keywords: Cross-coupling Reactions, Sonogashira Reaction, DFT Calculations, Palladium.

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Electronic structure and properties of a new series of fac-Re(I) tricarbonyl complexes: a DFT study

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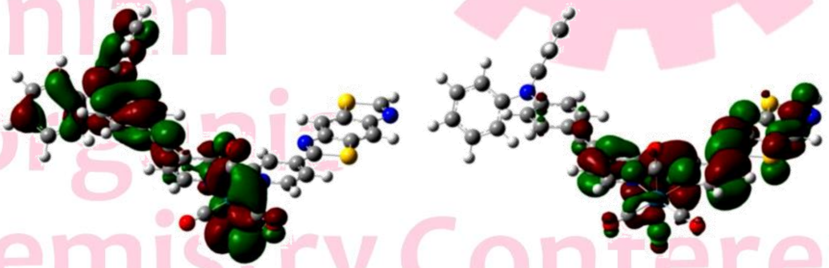
Luminescence of rhenium(I) tricarbonyl diimine complexes was first reported by Wrighton and Morse in 1974 [1]. Since the first report, syntheses, photochemistry and photophysics of fac-[Re(Cl)(CO)$_3$(α-diimine)] complexes have been widely studied. These complexes have been reported as promising materials for potential applications in catalysis, sensors, organic light-emitting diodes, solar energy conversion, photosensitizers and possible agents in bioimaging and cancer therapy [2,3]. Structural modification of α-diimine ligand broadly affects the character and energy of HOMO and LUMO in these complexes [4]. Electron donor-acceptor (D-A) systems have been extensively investigated in recent years. To realize high performance photocatalysis in the multichromophore ensembles, controlling the charge transfer (CT) process is essential [5]. Depending on the energy levels of the metal and ligand orbitals, different excited states, including MLCT, LLCT, IL and SBLCT can be generated. In this research work, electronic structure of four fac-[Re(Cl)(CO)$_3$(α-diimine)] complexes with electron acceptor-acceptor and donor-acceptor substituted α-diimine ligands are studied by DFT method. Benzothiazole derivatives (as electron acceptor) and triphenylamine groups (as electron donor) were introduced to the α-diimine core. The effect of donor and acceptor groups on the character and energy of HOMO and LUMO will be discussed in details. Moreover, TDDFT calculations results will be investigated to understand the electronic spectra and excited states of the complexes.



HOMO (MO 196) E = - 5.3938 eV   LUMO (MO 196) E = - 2.9628 eV

Keywords: Rhenium(I), α-diimine Ligands, Electron Donor-acceptor, Electronic Structure, DFT.

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A DFT investigation on the effect of ligand substitution on photophysical properties of some new cyclometalated Ir(III) complexes

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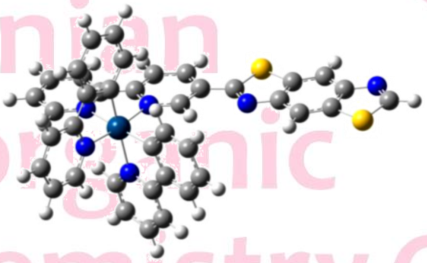
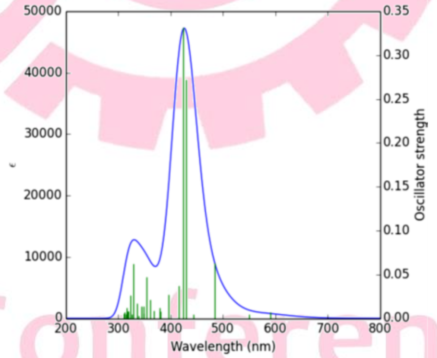
Cyclometalated Ir(III) complexes has attracted considerable attention due to their applications in electroluminescence, photocatalysis, phosphorescent molecular probes [1] and their potential for solid-state lighting and display utilizations [2]. The complexes are more promising because of larger d-orbital splitting and strong spin-orbit coupling (SOC) effect [3]. Phosphorescent cyclometalated Ir(III) complexes usually represent high quantum yields and emissive metal to ligand charge transfer (^{3}MLCT) excited states. Ir(III) ion, due to the high SOC, facilitates the intersystem crossing of the excited states. Moreover, the forbidden $T_1 \rightarrow S_0$ transition is activated in these complexes [4]. Here, electronic structure of four new cyclometalated Ir(III) complexes are studied at DFT/B3LYP level of theory. Previously, the method has been successfully applied to investigate Ir(III) complexes [5]. The effect of functionalization of ancillary ligand by benzothiazole derivatives (as electron acceptor) and electron donor groups on the electronic structure of the complexes are investigated. It is well known that, the electrochemical and photophysical properties of these complexes could be tuned by functionalization of the ancillary ligand [4]. Photophysical properties of the compounds are studied by TDDFT method at the same level of theory.





Keywords: Cyclometalated Ir(III) Complexes, Ancillary Ligand, Electron Donor-acceptor, DFT

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Preparation of amorphous MOF based biomimetic nanozyme (Me-Cu) with laccase-like activity for the aerobic oxidation of 1,4-dihydropyridine derivatives

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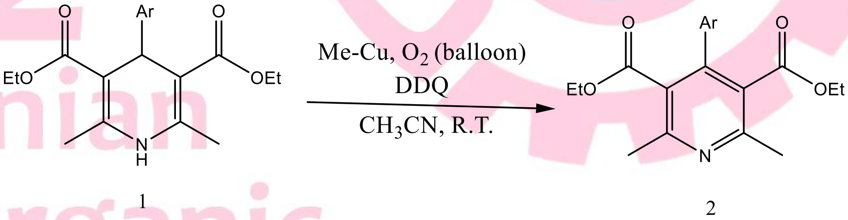
Recently, the rational construction of enzyme by mimicking the active site of natural enzymes has become a hot spot to endow the bioinspired enzyme with equal or even higher catalytic performance in comparison with natural enzymes. Generally, the biomimetic enzymes reported in previous studies were prepared based on precise multistep synthetic methods or complex ligand molecules. Hence, a facile synthetic method and simple ligand molecules in preparation of the biomimetic enzyme are required for its further development and application [1,2]. First, a new type of MOF (Me-Cu) amorphous enzyme with laccase activity was prepared. The synthesized compound was used as a recyclable catalyst in the aerobic oxidation of dihydropyridine derivatives. proper reaction time and efficiency, mild conditions, and reuse are some of the advantages of catalysts used. In this work, Arobic oxidation of 1,4-dihydropyridines 1 to pyridines 2 in the presence of Me-Cu catalyst and DDQ in Acetonitrile and at room temperature. The resulting nanocomposite was characterized by EDX, FESEM, and FT-IR techniques



Schem 1. Arobic oxidation of 1,4-dihydropyridines to pyridines.

Keywords: Nanozyme, Laccase, Amorphous MOF

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Photodegradation of organic compounds using MOF-74 nanocomposite

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Metal-organic frameworks (MOFs) are crystalline compounds that can form porous 1D, 2D or 3D structures. MOFs have attracted many researchers attention in drug delivery, catalysis, gas storage, and other applications because of their high specific surface area, large porosity, and adjustable chemical functions. MOF-74-type frameworks are considered one of the most promising metal–organic frameworks owing to their remarkable structural features and properties such as a high density of open metal sites, hexagonal channels along the *c*-axis, and high porosity[1,2]. In the present work, the synthesis of MOF-74 and MOF-74 nanocomposite was suggested. The new nanocomposite was prepared by solvothermal method at room temperature. MOF-74 nanocomposite was characterized by X-ray diffraction (XRD), field emission scanning electron microscopy (FESEM), transmission electron microscopy (TEM), diffusion reflectance spectroscopy (DRS), and nitrogen adsorption and desorption measurement. XRD results confirmed the successful synthesis of the MOF-74. FESEM results showed that the synthesized support has an almost spherical morphology. TEM images confirmed the presence of MOF-74 nanoparticles with an average length of 5.47 nm. Atomic absorption results showed that MOF-74 has good stability in water. The DRS spectrum of the nanocomposite shows an absorption edge at 465 nm, which corresponds to MOF-74. BET results also showed that the synthesized nanocomposite has a surface area of 600 m^2/ g and an average pore size of 13 nm. The photocatalytic activity of nanocomposites was evaluated under visible light irradiation for the removal of Congo red (CR) dye[3]. The removal rate of CR dye was performed under visible light irradiation.

Keywords: Metal-organic Frameworks, MOF-74, Photocatalytic, Nanocomposite, Visible Light

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Investigating the effect of active metal percentage composition on catalytic performance in the oxidative coupling reaction of methane

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The Oxidative Coupling of Methane (OCM) reaction [1] holds significant potential for the production of valuable products from methane. However, it is confronted with several challenges, including low selectivity towards the desired products and high energy requirements for the reaction conditions. As a result, ongoing research efforts are focused on developing more effective catalysts and optimizing reaction conditions to enhance the selectivity and efficiency of the OCM process [2-4]. In this investigation, we synthesized three distinct variants of Mn-Na_2WO_4/SiO_2 catalysts, employing different compositions ranging from 4% to 6%. The catalytic performance of these catalysts, designated as A, B, and C, was initially evaluated for the oxidative coupling of methane (OCM). The experimental conditions included a total flow rate of 480 mL/min, with methane-to-oxygen ratios of 2 and 4. Among the catalysts tested, catalyst A exhibited remarkable efficacy in generating C_2H_4 and C_2H_6 products compared to catalysts B and C. To further characterize the catalytic behavior, methane conversion and selectivity towards C_2 hydrocarbons were determined for catalysts A, B, and C at three distinct temperatures: 800, 825, and 850 °C. Notably, the desired catalysts displayed enhanced performance at elevated temperatures. Additionally, the highest conversion of reactants was achieved when the methane-to-oxygen feed ratio was set to 2, specifically at a temperature of 800 °C. To evaluate the properties of the synthesized catalyst, various characterization techniques such as X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), temperature-programmed reduction (TPR), Brunauer-Emmett-Teller (BET) surface analysis, and field emission scanning electron microscopy (FESEM) were employed.

Keywords: Methane, Oxidative Coupling of Methane, Mn-Na_2WO_4/SiO_2 Catalyst

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Tragacanth gum-stabilized Cobalt nano catalyst for hydrogen generation; Hydrolysis of Sodium borohydride

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Extraction of hydrogen gas from its compounds is necessary because hydrogen gas can be found rarely in its pure form. Fossil fuels, biomass and water electrolysis are the most resources for hydrogen generation. Sodium borohydride as a non-fossil inorganic energy sources has been suggested as a source for hydrogen gas under mild conditions. Among the certain catalysts, $NaBH_4$ can be hydrolyzed and hydrogen gas released. The hydrolysis of $NaBH_4$ is expressed as follows reaction (1):

$$NaBH_4 + 2H_2O \rightarrow NaBO_2 + 4H_2 \uparrow \qquad (1)$$

It is found that, $NaBH_4$ solution hydrolyzed only when certain suitable catalysts are added. As known, it is necessary to stabilize metal nanoclusters in an aqueous solution because of aggregation and agglomeration phenomenon. In this work, in order to reduce particles aggregation and then enhance the catalytic activity of nano powder, tragacanth gum (TGG) is used as a stabilizing matrix in preparation processes. Tragacanth gum-stabilized Cobalt nano catalyst was synthesized with chemical reduction method. XRD, FeSEM, EDS, XPS, FTIR and TGA/DTA techniques are used for characterization of powders. The catalytic activity of catalyst is tested for hydrogen generation through hydrolysis of alkaline sodium borohydride solution. Kinetics studies on the hydrolysis reaction of $NaBH_4$ are investigated through three factors: (i) initial concentration of $NaBH_4$, (ii) catalyst dosage and (iii) temperature. Arrhenius equation was used to calculate Ea of hydrogen generation reaction at different temperatures. The activation energy (Ea= 55 kJ/mol) was achievement indicated that the compound of Co/TGG has the lowest agglomeration and the highest rate of hydrogen generation. Catalytic hydrolysis of $NaBH_4$ is first order with respect to the catalyst dosage and also first order to $NaBH_4$ concentration in the case of Co/TGG.

Keywords: Tragacanth gum, Co Nanoparticles, $NaBH_4$, Hydrogen Generation, Kinetics.

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Removal of Dibenzothiophene from model diesel oil by adsorptive desulfurization using ZIF-8

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Sulfur-containing compounds in middle distillate fuels are known to have negative impacts on the environment because of SO_x emission from their combustion exhaust products [1]. In order to control and monitoring sulfur compounds a variety of removal techniques are available that well documented in the literature [2]. Among different desulfurization methods, ADS selective process is mainly considered as an appropriate approach for desulfurization, mainly due to its low energy consumption and cost and high efficiency [3]. In recent years, metal-organic frameworks (MOFs) and Zeolitic imidazolate frameworks (ZIFs) have shown better chemical and thermal stability compared with other adsorbent [4]. In the present work, the adsorbent ZIF-8 is used to reduce DBT in a model, and real gas oil fuel is synthesized in mild condition. To evaluate the efficiency and removal capacity of ZIF-8 adsorbent, various factors such as the amount of adsorbent, time, and temperature have been investigated. Structural characterization was performed by XRD, FT-IR, and BET. Studies were performed and complete desulfurization of model fuel was found after 4 h using 0.8 g of adsorbent at 50 ◦C, instead of the 105 mgS/g adsorption capacity of desulfurization obtained with the fresh ZIF-8 in the model fuel solution of DBT at 120 ppm. Moreover, the good selectivity of ZIF-8 indicated the absorption of non-saturation centers around Zn metal. The ZIF-8 reacted well to its excellent recycling capability to remove DBT under mild conditions 4 times.

Keywords: Adsorption, Desulfurization, Zeolitic Imidazolate Frameworks, Dibenzothiphene

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Synthesis of magnetic nanoparticles ZIF-8 to immobilize in ionic liquid for the adsorptive desulfurization of gas oil

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Over the past decades, the desulfurization of fuel oils has been known as one of the most challenging processes in petroleum refineries due to economic considerations. The presence of sulfur compounds results in SO_x emissions detrimentally affecting the equipment of refineries, the environment, and human health [1]. Due to the presence of unique characteristics, nanoparticles are used specifically as adsorbents, and in the meantime, magnetic separation has created a promising solution in the separation issue [2]. In the present work, by immobilize ionic liquid 1-Buty l-3-methylimidazolium methyl sulfate ([BMIM] [Me SO_4]) on the surface of Fe_3O_4@ZIF-8, a magnetic nano adsorbent was prepared to remove a mixture of gas oil sulfur. The structure of the nano adsorbent was investigated by different methods such as SEM, XRD and FTIR. The main factors on the performance of nano adsorbent were optimized and under optimal conditions, 90% of sulfur in model oil was reduced during four stages. The optimal temperature was 70 ˚C, optimal volume ratio(adsorbent/oil) was 1:6. It is possible to recycle and reuse this nano adsorbent for four consecutive cycles.

Keywords: Adsorption, Desulfurization, Ionic Liquid, Magnetic Nanoparticle, ZIF-8

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Hydrogen Generation via Tris(acetylacetonato)cobalt(III) as a Heterogeneous Nano Catalyst; Kinetics Study

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Hydrogen is a promising alternative energy source to conventional fuels, including fossil fuel. Several methods were reported for the generation of hydrogen but hydrolysis of aqueous sodium borohydride ($NaBH_4$) solutions is One of the non-fossil methods to generate hydrogen. $NaBH_4$ with high gravimetric hydrogen capacity of about 10.8 wt.%. is promising as a hydrogen storage material. This work reports the experimental results on synthesis and using $Co(acac)_3$ catalyst, Tris(acetylacetonato)cobalt(III) for hydrolysis of $NaBH_4$. The synthesized $Co(acac)_3$ catalyst was characterized by XRD, FESEM, TEM, XPS, and FT-IR techniques. The morphological and structural properties of the obtained materials were examined by FESEM and TEM images, Particle distribution histogram shows that the average particles size are 20 nm. The catalytic activity of catalysts was tested in the hydrolysis reaction of $NaBH_4$ in a semi-batch system. The volume of the evolved hydrogen gas was determined by a water displacement method. The effects of catalyst amount, $NaBH_4$ concentration and solution temperature on the hydrogen generation rate were investigated and partial order respect to $NaBH_4$ concentration and catalyst are 0.6584 and 0.6036, respectively. Arrhenius equation was used to calculate E_a of hydrogen generation reaction at different temperatures. The activation energy, 20.85 (KJ/mol) is calculated for hydrolysis of $NaBH_4$ which is a very promising amount.

Keywords: Tris(acetylacetonato)cobalt(III), Hydrogen Generation, Sodium Borohydrides, Nano Catalyst, Kinetics

Synthesis and characterization of nanocomposite hydrogel based on nanobead chitosan in the presence of $Fe_3O_4@SiO_2$-Ag nanoparticles and its use to study surface absorption of vitamin B12

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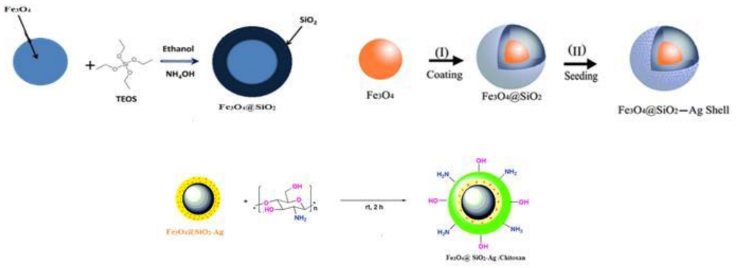
The use of nanoparticles in drug delivery systems has attracted a lot of attention over the last few years. Nanoparticles, which are made up of a mixture of Natural and Synthetic or Semisynthetic polymers, are colloidal particles. This study was conducted with the aim of developing an efficient catalyst, magnetic nanocomposite $Fe_3O_4@SiO_2$-Ag, for the surface adsorption of vitamin B12 through a one-pot multicomponent reaction. [1]. Nanoparticles are of great importance because they can transfuse different components at the right time, which is important for drug carriers. [2]. The biodegradable biocompatible polymer chitosan has attracted considerable interest in drug delivery. In this study, a Chitosan nanocomposite based hydrogel was first created and then prepared and investigated with Fe3 o4 @ SiO2 Ag magnetic nanoparticles for studies of vitamin B12 adsorption. TGA, VSM, XRD, FTIR, TEM and SEM studies were carried out to determine the method for sample identification [3].



Keywords: Hydrogel, nanocomposite, chitosan, magnetic nanoparticles, surface absorption of vitamin B12

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