نوزدهمین کنفرانس شیمی معدنی ایران
19th Iranian Inorganic Chemistry Conference
Chemistry & Chemical Engineering Research Center of Iran
www.IICC19.ccerci.ac.ir
5-7 September 2017
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Synthesis, Characterization and Antibacterial activity of Co(III) and Cu(II) Schiff-base complexes containing homopiperazine moiety

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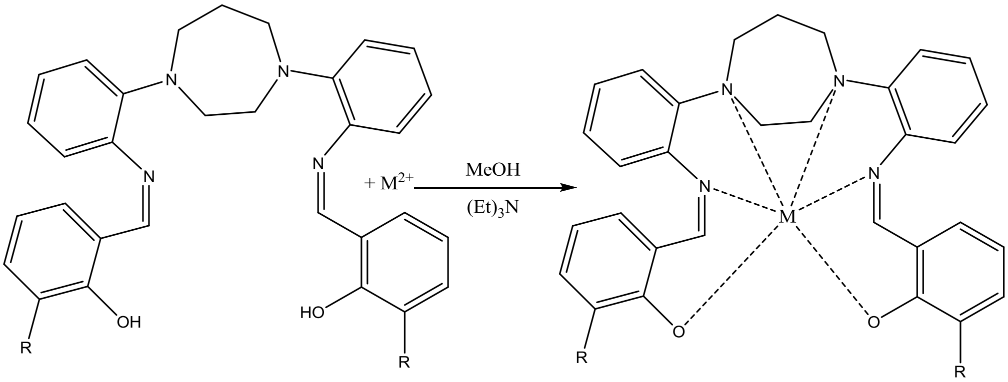
The new diamine 2,2'-(1,4-diazepane-1,4-diyl) dianiline (A^1) was synthesized by reaction of 1-Fluoro-2-nitrobenzene and homopiperazine. Two new Schiff base ligands, H_2L^1 and H_2L^2 were synthesized from the condensation of 2-hydroxybenzaldehyde (H_2L^1) and 2-hydroxy-3-methoxybenzaldehyde (H_2L^2) with A^1. In the presence of appropriate metal ions, Co(III) and Cu(II) macroacyclic Schiff-base complexes were obtained. All resultant products were characterized by elemental analysis, mass spectrometry and spectroscopic methods such as:FT-IR, ^{1}H and ^{13}C NMR. In addition the molar conductivity (Λ_M) data was measured at 25 °C using 10^{-3} M solutions of the complexes in CH_3CN solvent. The antibacterial activity of free amine and complexes has been studied against some Gram-positive and Gram-negative bacteria.



R=H, H_2L^1 , R=OCH_3, H_2L^2

M = Co^{3+}, Cu^{2+}

Keywords: Schiff-base complexes, Homopiperazine, Antibacterial activity

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Properties and application of Dimethyl carbonate

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Dimethyl carbonate (DMC) is an established solvent and a green reagent which continues to attract attention. DMC is classified in the greenest “recommended” bracket according to the solvent selection guide, and can be a potential replacement for methyl ethyl ketone, ethyl acetate, methyl isobutyl ketone, and most other ketones. Currently, the most prevalent commercial pathway for the production of DMC is through oxidative carbonylation of methanol using O_2; in addition, new alternative processes for DMC from CO_2 are being developed. DMC has found several applications such as the electrolyte in lithium rechargeable batteries and as a solvent in several reactions including pharmaceutically relevant synthesis and in biocatalysis. This report provides a brief overview of physical- thermodynamic-, toxicological- and ecotoxicological properties, production methods, reactivity, and applications of DMC as an environmentally benign chemical in chemical processes.

Keywords: Dimethyl carbonate, green solvent , production, electrolyte

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Copper supported on modified magnetic nanoparticles as efficient and reusable nanocatalyst for the synthesis of 5-substituted 1H-tetrazoles

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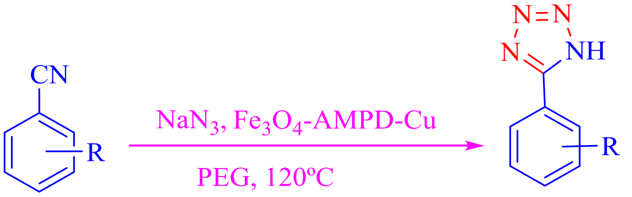
Separation nanoparticulate catalysts from the reaction mixture is often difficult, due to the need for conventional techniques such as filtration or centrifugation. In recent years, magnetite (Fe_3O_4) has been the focus of much attention as an interesting alternative to allow separation of the nanocatalyst from the reaction mixture by means of an external magnetic field [1–2].In this regard, a new magnetically reusable nanosolid (Fe_3O_4-AMPD-Cu) as a versatile and highly effective catalyst was fabricated and characterized using by FT-IR, XRD, VSM, TGA, TEM, SEM, EDX and ICP-OES techniques. This nanosolid shows great catalytic activity for the synthesis of 5-substituted tetrazoles in short reaction times and with high yields (Table 1).



Scheme 1. Fe_3O_4-AMPD-Cu catalyzed the one-pot synthesis of 5-substituted tetrazoles.

Table 1. Synthesis of 5-substituted 1H-tetrazole derivatives in the presence of Fe_3O_4-AMPD-Cu.

Entry	Substrate	Time (min)	Yield (%)^a	M.p. (°C)
1	Phthalonitrile	55	86	214-215
2	3-Nitrobenzonitrile	80	93	152-154
3	2-Chlorobenzonitrile	10	89	177-180
4	4-Nitrobenzonitrile	60	94	222-224
5	Malononitrile	8	87	115-117

^{a}Isolated yields

Keywords: Fe_3O_4 nanoparticles, Coppper(II), tetrazoles

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Preparation of nickel oxide photoelectrode in order to investigate its performance in nanostructure solar cells

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Considering the increasing global demand for energy and the harmful ecological impact of conventional energy sources, it is obvious that development of clean and renewable energy is a necessity. Since the Sun is our only external energy source, harnessing its energy, which is clean, non-hazardous and infinite, satisfies the main objectives of all alternative energy strategies [1]. Nanoscale objects provide opportunities to revolutionize the conversion of solar energy by enabling highly efficient and low-cost devices. Challenges associated with demonstrating high efficiency and stability are now being addressed in the research community. To date, significant efforts have been made to explore nanostructure's ability to improve the conversion efficiency of solar cells. Nanostructure solar cells show great potential for new-generation photovoltaics due to their ability to approach ideal light-trapping [2]. In this study, we have reported the preparation of nanostructur nickel oxide photoelectrode in order to investigate its performance in nanostructur solar cells. Firstly, nickel oxide (NiO) nanostructures were synthesized using a sol-gel method. Nickel oxide film was deposited on FTO (Fig.1) and then this photoelectrod was identified by XRD, SEM, UV-vis. In the future we plan to investigate its performance for use in nanostructure solar cells.

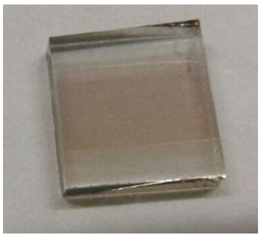

Fig. 1

Keywords: Renewable energy, Nanostructure solar cells, Nanostructure nickel oxide photoelectrode.

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Mean reverting stochastic differential equation application in mixing problems

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The main focus of this paper is to obtain mean reverting stochastic differential equation MrSDE for simple chemical mixing problems. The stochastic differential equation type is mean reverting. In realistic problem we have always some kind of noise. In this paper we work on a container full of salt solution of a certain concentration. In this paper we assume the concentration of the saline solution is corrupted by the Gaussian noise. The mathematical model will be introduced. The deterministic model is transferred to a stochastic differential equation. Then we solve it analytically, find expected value and variance to compare with ODE model. Numerical simulations via MATLAB programming are carried out in order to show efficiency and accuracy of the present model.

Keywords: Mean reverting equation, Stochastic differential equation, SDE Applications, Mixing problems

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Synthesis and characterization of nano sheet $Bi_2O_2CO_3$ structure

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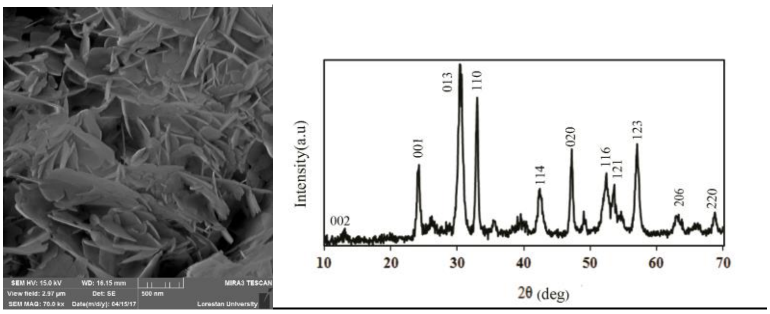
Among semiconductors, Bismuth subcarbonate $Bi_2O_2CO_3$, which is structurally close to the aurivillius family, is composed of alternate $Bi_2O_2^{2+}$ and CO_3^{2-} layers, with the plane of the CO_3^{2-} group orthogonal to the plane of the $Bi_2O_2^{2+}$ layer. $Bi_2O_2CO_3$ has long and widely been used for various medical and healthcare purposes [1]. The work aims to synthesize and characterization of $Bi_2O_2CO_3$ to obtain with flower morphologiy by hydrothermal process. To obtain $Bi_2O_2CO_3$ powders, bismuth nitrate pentahydrate was dissolved in of HNO_3, and then of citric acid was added under magnetic stirring. The pH of the solution was controlled with the addition of 2M NaOH aqueous solution. Finally the white-colored precursor suspension formed was transferred into a Teflon-lined stainless steel autoclave. The autoclave was sealed and maintained at 180°C for 24 h. The nanoparticle was characterized with FT-IR, XRD, UV-Vis, SEM and EDX analysis. The FI-IR, XRD and EDX results confirm the successful synthesis of nano sheet $Bi_2O_2CO_3$ structure.



Keywords: $Bi_2O_2CO_3$, Nanosheet

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The effect of synthesis conditions on the morphology, size and purity of Ni-Al-LDH nanoparticles

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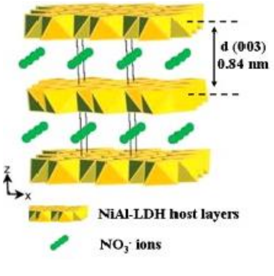
The morphology and size control of inorganic solids is an important topic in the material science [1]. Layered double hydroxides (LDHs), also known as hydrotalcite -like compounds, are a class of synthetic anionic layered clays [2]. Attempts have been made to control the morphology and size of LDHs. Because of the high rigidity and lack in tenacity of LDHs layers, only flat layers in a-axis direction were always obtained [3]. Ni-Al-CO3-LDH was synthesized by conventional coprecipitation method which produced nanoparticles with hexagonal platelet morphology. The optimal parameters were chosen pH=9, T=80°c and t=24h. The prepared LDH was characterized by X-ray diffraction (XRD), fourier transform infrared spectrometer (FT-IR), thermal gravimetry analysis (TGA) and scaning electron microscopy (SEM). The XRD patterns exhibit the characteristic reflections of LDH which are sharp and symmetric at low 2θ angle, but broad and asymetric at high 2θ angle. In the IR spectra, an intense and broad adsorption band located at 3400cm^{-1} was observed, which was attributed to the OH stretching due to the presence of hydroxyl groups and interlayer water molecule of LDH. In the low frequency region(630 and 420 cm^{-1}), the adsorption peaks correspond to the lattice vibration modes (Al-O, Ni-O, Ni-O-Al). The thermal behavior of LDH is investigated by using the TGA analysis. SEM was shown that particles size was nano and flat platelike morphology for LDH.



Schematic of Ni-Al-LDH

Keywords: Ni, Al, LDH, Nanoparticles

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The effect of synthesis conditions on the morphology, size and purity of Ni-Al-LDH nanoparticles

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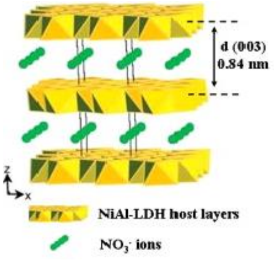

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Synthesis and characterization of some water soluble metal Schiff base complexes functinalized Fe_3O_4 magnetic nano-particles

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Schiff base transition metal complexes have been extensively studied because of their potential use as catalysts[1]. Recently, magnetic core–shell nano-structures have attracted more attention due to their unique magnetic properties. Therefore, reparation of functionalized magnetic nano-particles, $Fe_3O_4@SiO_2$, with Schiff base complexes have attracted interest to provide magnetically reusable heterogeneous catalysts[2]. In this work, firstly the magnetite nano-particles synthesized by co-precipitation method from iron(II) chloride tetrahydrate and iron(III) chloride hexa-hydrate in alkaline condition. Then the surfaces of the nano-particles were coated with SiO_2. The surface of core-shell structures functionalized with NH_2 groups by reacting with 3-amino propyl triethoxy silane. In the next step, a water-soluble aldehyde (sodium salicylaldehyde-5-sulfonate) was synthesized and characterized. Condensation reaction between the NH_2 group and carbonyl group leads to a water-soluble Schiff base that is supported on the coated magnetite. Thus the Schiff base is the result of condensation reaction between sodium salicylaldehyde-5-sulfonate and $–NH_2$ groups on the MNPs and is a water soluble Schiff base. Then the supported water-soluble Schiff base converted to the corresponding metal Schiff base complexes of Cu(II), Co(II) and Mn(II) by reaction with acetate salts of these metals. In this way three water-soluble metal Schiff-base complexes supported on core-shell magnetite silica nano-particles were synthesized and characterized by FT-IR, XRD, SEM, EDX, TEM and TG analysis.

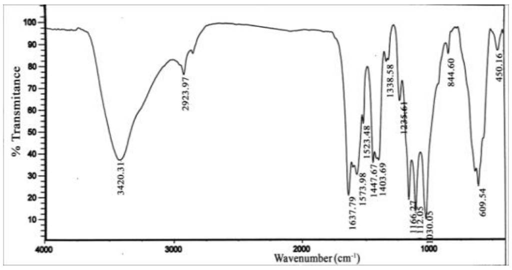

Fig.1 FT–IR spectrum for $Fe_3O_4@SiO_2$/Schiff base of Mn(II)

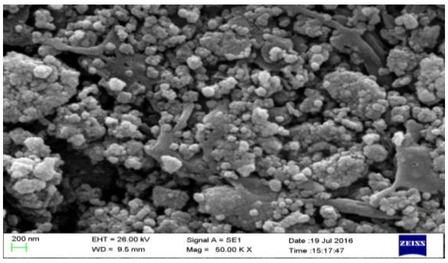

Fig.2 SEM image for $Fe_3O_4@SiO_2$/Schiff base of Mn(II)

Keywords: Core shell, Nano-Composite, Schiff base, Magnetite.

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Synthesis and characterization of a new Schiff base ligand

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Over decades, Schiff bases have played a paramount role as chelating ligands for a large variety of metal ions. Schiff bases are formed by the condensation of an amine or diamine and an aldehyde/ketone; while these compounds carry imine or azomethine (–C=N–) functional group. In general, tetradentate schiff base groups form stable complexes with transition metals known as antitumors, catalysts and etc. In addition, these compounds are employed in electrochemical and optical sensors [1,2].

In the current study, a new asymmetric tetradentate Schiff base ligand (2-((Furan 2yl)methyleneamino)-3-(2-hydroxynaphthalen-1-yl) maleonitrile), was synthesized by two-step reaction of Diaminomaleonitrile, Furfural and 2-Hydroxy-1-naphthaldehyde with 1:1:1 mole ratio. The ligand was characterized by IR in which azomethine functional group was found. Furthermore, UV-Vis, elemental analysis and ^{1}H NMR of this ligand were also investigated. The metals Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) then reacted with the ligand to synthesize the desired complexes. The complexes were characterized by some methods like IR, UV-Vis spectroscopic techniques, elemental analysis, magnetic and conductivity measurement. The results of the study show metal ions coordinate through the nitrogen and the oxygen atoms.

Keywords: Schiff-base, Ligand, Aldehyde, Amine.

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Synthesis and characterization of a new Schiff base ligand

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Schiff bases are versatile ligands which are synthesized from the condensation of amines or diamines with carbonyl/aldehyde groups were first reported by Hugo Schiff. Schiff bases played a substantial role in development of coordination chemistry and were involved as key point in the development of inorganic biochemistry and optical materials [1].These compounds are significant in medicinal and pharmaceutical fields because of their broad spectrum of biological activities [2].

In this project a new tetradentate Schiff base ligand (2-(1(2hydroxyphenyl)ethylideneamino)-3-(1-(pyridin-2-yl)ethylideneamino)maleonitrile) was synthesized by the reaction of Diamino- maleonitrile, 2-Acetylpyridine and 2’Hydroxyacetophenon in 1:1:1 mole ratio in two steps. IR, UV-Vis, elemental analysis and ^1H NMR of this ligand were investigated. Then the transition metal ions such as Mn(II), Co(II), Ni(II), Cu(II) and Zn(II) were reacted with this ligand to synthesis stable complexes. The new synthesized complexes were characterized by elemental analysis, IR, UV-VIS spectroscopic techniques, conductivity and magnetic properties. Due to our study, metal ions coordinated through the oxygen and the three nitrogens atoms.

Keywords: Ligand, Ketone, Schiff base

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Synthesis, nano-synthesis and characterization of a series of group 12 coordination compounds containing chelating Schiff base ligand

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Investigations on the synthesis, structures, and properties of new coordination compounds are still an active field in coordination chemistry [1]. The major goal in this area includes the development of strategies for a more rational synthesis of compounds with definite structure, morphology and desired physical and chemical properties [2]. In this regard, a series of coordination compounds containing *N*-(4-substituted)-1-(pyridin-2-yl)methanimine ligand were synthesized by conventional methods, characterized by spectroscopic techniques (FT-IR (Figure a) and elemental analysis) and their X-ray crystallographic (Figure b) structures were determined. The crystal structures of these coordination compounds were analyzed and studied using theoretical techniques. These compounds were also synthesized by sonochemical method and their morphologies were investigated using FE-SEM (Figure c).The results presented here provide some support for the approach taken by our group to find the relationship between molecular aggregation and morphological features.

(a) (b) (c)

Keywords: Chelating ligand, Schiff base ligand, Coordination complexes, Group 12 complexes

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Synthesis and crystal structure determination of a series of Hg(II) nano coordination compounds containing a Schiff base ligand

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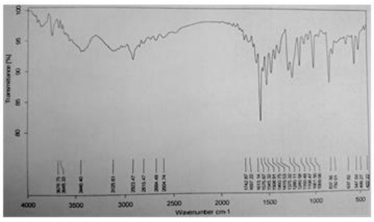
In the last two decades, crystal engineering of metal-containing compounds has received considerable attention due to their versatile structural diversity and widespread applications in diverse fields. The ultimate aim of inorganic crystal engineering is the rational choice of intermolecular interactions to predict and design the assembly of metal-containing species [1].The role of hydrogen bonding in coordination compounds is ligand-based hydrogen-bond functionalities as “supramolecular glue”, a useful addition to the field of crystal engineering [2]. In this regard, a series of Hg(II) coordination compounds containing (4-substitued-*N*-pyridin-4-ylmethylene)aniline ligands were synthesized by conventional and ultrasonic methods, characterized by spectroscopic techniques such as (FT-IR (Figure a) and elemental analysis) , and their X-ray crystallographic structures (Figure b) were determined. The crystal packing of these coordination compounds was analyzed and studied using different geometrical and theoretical techniques. The morphology of sonochemically synthesized compounds was investigated using FE-SEM (Figure c). The results presented here provide some support for the approach taken by our group to find out the missing ring between supramolecular chemistry and nanotechnology and to clarify the design of molecular materials with favorite morphology, size distribution and shape.



(a)

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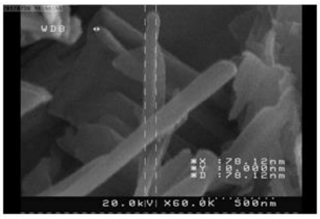

(b)

Keywords: Schiff base ligand, Hg(II) coordination polymers, hydrogen bonding

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Synthesis of MOF MIL-100(Fe), Release and Control of Drug

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Metal organic frameworks (MOFs) represent a class of porous material which is formed by strong bonds between metal ions and organic linkers. By careful selection of constituents, MOFs can exhibit very high surface area, large pore volume, and excellent chemical stability. Research on synthesis, structures and properties of various MOFs has shown that they are promising materials for many applications, such as energy storage, gas storage heterogeneous catalysis, drug delivery and sensing. In this study, MIL-100(Fe) was used for the first time to absorb the pharmaceutical products of several drug. We reported the design and synthesis of ligands Fe-metal organic frameworks (MOF) and their application as the transport vehicles for the delivery of several important drug. we have 1,3,5-benzene tricarboxylate (BTC) as linker, easily prepared by hydrothermal method. The synthesis was characterized by X-ray diffraction (XRD). The experimental incorporation was accomplished and analyzed by Fourier transform infrared spectroscopy (FTIR) and UV–Vis (ultraviolet–visible) spectrophotometry.

Keywords: Metal Organic Framework, Drug Delivery, MIL-100(Fe)

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Chemistry & Chemical Engineering Research Center of Iran
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Magnetic Ceria/Polyoxometalate Nanocomposites and use as a Photocatalysts

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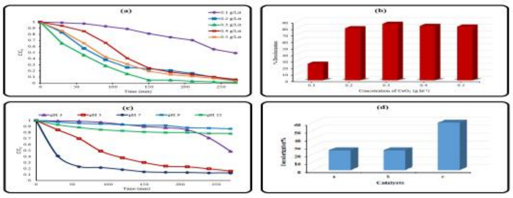
In these days, effluent of dyes recommends a challenge for environmental safety and daily operations of the industry. Dyes are constituted nearly 70% of their synthetic [1]. There are many methods to remove the effects of pollutants which are included absorption techniques, reverse osmosis, electrochemical and photocatalytic [2]. Over the past decade, Metal oxides have wide range of applications in catalysis, environmental science and material science [3]. Ceria (CeO_2) is one of the most significant rare earth metal oxide that has different applications in some fields [4]. Hetropoly anions are a kind of metal clusters, because of their various structures and unique properties. Newly, one of the most significant current discussions are easier separating and recycling of catalysts. Hence, the magnetic nanoparticles (NPs) have been attracting a lot of attention in chemical process (e.g., catalysis, photocatalysis, energy storage and etc.) [5]. Therefore, the Fe_3O_4 NPs can play an important role for recycling and separating of magnetized catalysts by an external magnetic field. The aim of this research has been attempted to synthesis of magnetic of ceria /Polyoxometalate composites in order to investigation the efficiency of as-synthesis toward improving photocatalytic activities. The prepared $Fe_3O_4@CeO_2/Cs\text{-}PMo_6W_6O_{40}$ sample displayed significantly enhanced photocatalytic activity toward CR degradation under 210 min visible light irradiation than CeO_2. Thus, the $Fe_3O_4@CeO_2/Cs\text{-}PMo_6W_6O_{40}$ sample is a promising candidate for the removal of organic materials from wastewater.



Keywords: Photocatalyst, Polyoxometalate, Ceria, Congo red, Azo dyes, Magnetic.

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Systematic, structural and computational studies of new rhenium(I)-tricarbonyl complexes bearing 1,4-diazabutadiene ligands

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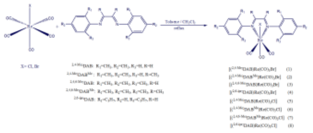
Rhenium(I) tricarbonyl complexes with NN-donor ligands display promising properties for potential applications as molecular catalysts for the reduction of carbon dioxide [1] and as biocompatible pro-drugs for the controlled release of carbon monoxide [2]. In this context the diimine type ligands are one of the most widely used bidentate chelating moieties [3]. Several $[Re(CO)_3(DAB)X]$ complexes were prepared in the standard manner by replacement of two *cis* CO groups in the starting bromo- or chloro-pentacarbonylrhenium complexes with 1,4-diazabutadiene (DAB) ligands. Their pseudo-octahedral *facial* structures were established using FT-IR, ^{13}C-NMR and ^{1}H-NMR and confirmed by X-ray crystallography. Our interest in 1,4-diazabutadiene ligands arose from the ease of manipulating their steric and electronic properties. Density functional theory (DFT) was used for geometry optimization of the singlet states in gas phase and the electronic structure calculations. The analysis of the molecular orbital compositions in terms of occupied and unoccupied fragment orbitals in each complex was performed by AOMix6.88 program. Charge decomposition analysis revealed that in all complexes the electron donation of the DAB ligands is significantly greater than the back-donation which is in good agreement to the positive charge carrying on the DAB ligands based on the Mulliken and NPA population analyses. Details of the singlet excited state character are revealed by TD-DFT calculations, calculated changes of electron density distribution using electron density difference map and confirmed the MLCT, XLCT and IL character of the electronic transitions.



Keywords: Re(I) tricarbonyl complexes, DAB, X-ray diffraction, DFT/TD-DFT.

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Ultrasound-Assisted Synthesis and Characterization of ZrO_2 Nanoparticles

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Nano-ZrO_2 was synthesized by sol-gel method under ultrasonic irradiation. Precursor of nano-ZrO_2 was prepared by direct precipitation from $ZrCl_4$ and H_2O_2. Zirconium (IV) chloride was dissolved in DI water .The white gel of peroxozirconic acid was formed after adding drop by drop hydrogen peroxide. The mixture was placed under probe of ultrasonic then precursor of nano-ZrO_2 was stirred for 5 h as aging time. Zirconium (IV) dioxide NPs was synthesized by calcination of the dried gel in furnace at 500ºC for 3 hours. The structure of Nano-Zirconia was characterized by furrier transfer infrared spectroscopy (FT-IR), x-ray diffraction (XRD) and its morphology was determined by field emission scanning electron microscopy (FESEM). The magnitude of ultrasonic irradiation and time of radiation were affected on size and morphology of nanoparticles ZrO_2. In this research, the optimum time is 30 min. Zirconia NPs can be obtained by controlling the preparation conditions and parameters, such as the concentration ratio of H_2O_2 solution and $ZrCl_4$, magnitude of ultrasonic irradiation and the processing temperature. The average size of ZrO_2 NPs is 37 nm [1-3].

Keywords: Ultrasonic Irradiation, Nanoparticles, sol- gel, ZrO_2

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Preparation and characterization of a new nanocomposite of copper oxide with Nafion

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Copper oxide is an intrinsic *p*-type semi-conductor with a narrow band gap of 1.2-2.1 eV, which can be applied in electronic and electrical industries. On the other hand, Nafion is a polymer of sulfonated tetrafluoroethylene. It is the first of a class of synthetic polymers which are called ionomers. Nafion's unique ionic properties are the result of incorporating perfluorovinyl ether groups terminated with sulfonate groups onto a tetrafluoroethylene (Teflon) backbone. In this project, with the aim of examining the composite properties, a composite of nafion with nano copper oxide (CuO) was prepared and characterized by IR, XRD and SEM methods. $CuCl_2$ as a metal source and oxalic acid as a carboxylate ligand were used as starting materials to synthesize an inorganic complex. Then, CuO nanostructures were prepared *via* calcination of the complex. For the nanocomposite prepration, a nominal amount of copper oxide was added to 25 Wt% of nafion solution with the molar ratio of 1:40. After the dispersion, the solution was then slowly reconcentrated until a suitable viscosity was reached. The obtained film was dried at 100° C for 3h to eliminate the solvent. All the analyses, for example XRD pattern shown in Figure 1 confirm the synthesis of nafion/CuO nanocomposite.

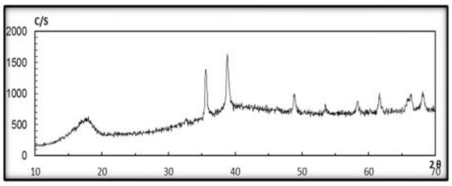

Figure 1. XRD pattern of nafion/CuO nanocomposite

Keywords: Copper oxide, Nafion, nanoparticles

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Complexes of $HgCl_2$ with tolanophanes and their application in the synthesis of the related cyclic tosylates

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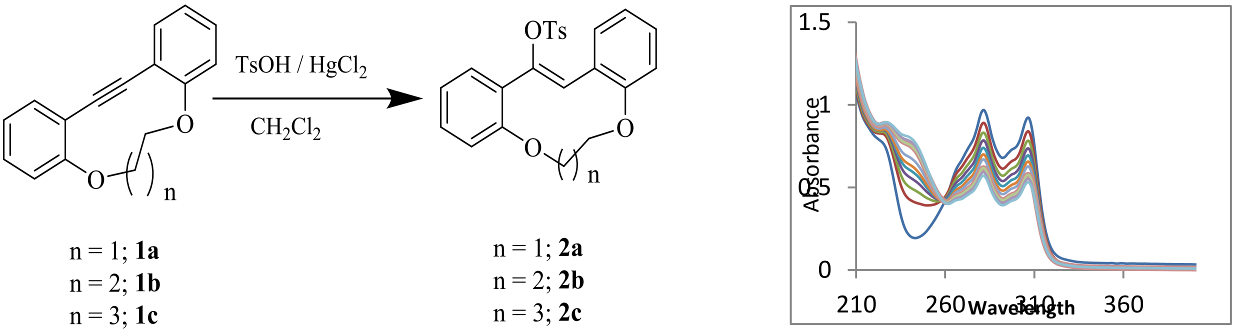
The basic principles of organometallic chemistry are the basis of the discovery of catalysts and catalytic processes.[1] The unsaturated alkyne triple bond can undergo a variety of metal-catalysed reactions, including the inter- or intramolecular addition of carbon or heteroatom nucleophiles; This reactivity is associated with a diverse coordination chemistry of organometallic alkyne species.[2,3] In continuous of our work on tolanopahnes **1**,[4] herein, we report their selective response towards $HgCl_2$ among various metal chloride ions by UV-Vis spectroscopy titration.(Scheme1) In order to evaluate the complex performance, the stoichiometric reactions of **1a-c** with p-toluenesulfonic acid in the presence and absence of $HgCl_2$ in CH_2Cl_2 were carried out which gave the corresponding cyclic tosylates **2a-c**. (Scheme1) The results revealed that *ortho* position of methoxy groups on the ring has a definite role on the tosylation. Despite the poor effect of $HgCl_2$ on acyclic tolans, a cooperative effect between $HgCl_2$ and cyclic **1a-c** was observed leading to significant increase of the yields of **2a-c**. The products are new which well characterized.



n = 1; **1a**
n = 2; **1b**
n = 3; **1c**

n = 1; **2a**
n = 2; **2b**
n = 3; **2c**

Scheme1. Synthesis of **2a-c** (left) UV-Vis spectrum of 1b with $HgCl_2$(right)

Keywords: Organometallic, $HgCl_2$, Tolanophane , tosylate

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Theoretical study of electric field effect on the reactivity in Iridabenzene

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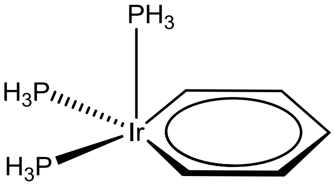
Metallacyclic aromatic compounds including transition metals are a subject of great attention, because they exhibit a behavior that includes properties from both aromatic organic and organometallic compounds [1-3]. In this work, the electric field effect on the reactivity in $C_5H_5Ir(PPh_3)_3$, a Iridabenzene complex, was investigated with MPW1PW91 method. The calculations of systems contain main group elements described by the standard 6-311G(d,p) basis set. For Ir element standard Def2-TZVPPD basis set was used and Ir described by effective core potential (ECP) of Wadt and Hay pseudo-potential with using the Def2-TZVPPD basis set. The electric field effect on frontier orbitals energies (E_{HOMO} and E_{LUMO}), HOMO-LUMO gap, hardness, electrophilicity and chemical potential were studied. We also estimate the percentage composition in terms of the specified groups of frontier orbitals for this complex to investigate the feature in the metal–ligand bonds in various external electric fields.



Keywords: Electric field, Iridabenzene, Frontier orbitals, Reactivity.

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Highly efficient removal Methylene blue from waste water by Magnetic Nanoparticle Fe-Ce-Mn-O adsorption

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In recent years, many industries give rise to dye-bearing effluents in their production processes. It noted be mentioned that textile industries are major consumers of water and release a fair amount of color in their effluents [1]. Dyes usually have a synthetic origin and complex aromatic molecular structures which make them more stable and more difficult to biodegrade [2]. In this regard, we investigated the removal of Methylene blue (MB) in waste water by the prepared magnetic nanoparticles Fe–Ce–Mn–O by co-precipitation method. As shown in Fig. 1, the majority of MB was removed in the first 15 min. Also, the adsorbent curve showed good ability of removing the cationic dyes from waste water.

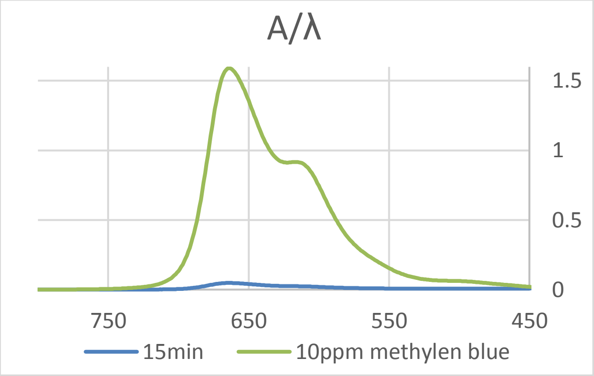

Fig. 1. UV-Vis spectra of Fe-Ce-Mn-O

Keyword: Nanoparticles, Adsorption, Methylene blue, Water treatment

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Synthesis and characterization of magnetic ferrite nanocomposite modified with porphyrin

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Magnetic materials are those materials that show a response to an applied magnetic field. Because of the widespread applications of magnetic nanoparticles, in biomedical, biotechnology, engineering, material science and environmental areas, much attention has been paid to the preparation of different kinds of magnetic nanoparticles [1, 2]. On the other hand, porphyrins are the most promising sensitizers known so far. The extensive p-conjugated framework of porphyrins makes them attractive candidates as electron donors and light harvesting [3, 4]. Considering these properties, synthesis of nanocomposites based on magnetic nanoparticles that modify with porphyrin are one of the interesting research subjects.In the present investigation, the magnetic nanoparticle of zinc ferrite was prepared by combustion method using zinc (II) and iron (III) nitrates with glycine, as a fuel. Then these magnetic nanoparticles were coated with polythiophene through polymerization of thiophene monomers. In the next stage, zinc ferrite which coated with polythiophene was also sensitized by tetrakis (4- carboxyphenyl) porphyrin. The synthesized nanocomposite has been characterized by various techniques.The as-fabricated nanocomposite, which contains central magnetic core with a strong response to external field can be readily removed from solution by externally applied magnetic field.

Keywords: Magnetic nanocomposite, Ferrite, Porphyrin

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Removal of methylene blue from aqueous solutions using magnetic nanocomposite as absorbent

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Dye contamination in wastewater can lead to a variety of environmental problems. Therefore, it is necessary to find simple, highly efficient, and economical methods to treat dye wastewater [1]. Methylene blue, is one of the typical toxic dyes with known harmful effects on humans, which has been widely used in industrial practices such as textile and printing. Because of its complex aromatic ring structure it is difficult to remove methylene blue from the environment [2, 3]. Various methods have been investigated to treat wastewater, such as photocatalytic degradation, electrochemistry, biodegradation, and adsorption. Among these methods, dye adsorption based on magnetic separation technique has been receiving considerable attention owing to its low-cost, high efficiency and easy operation process [4].

In this study, zinc ferrite nanoparticles as a magnetic core of this nanocomposite was coated with polythiophene and then modified with tetrakis (4-carboxyphenyl) porphyrin. Modification with porphyrin greatly enhances the adsorption properties of ferrite nanoparticles for absorption of methylene blue dye. This nanocomposite which contains central magnetic core with a strong response to external field, can be readily removed from solution by externally applied magnetic field. This research indicates that the as-synthesized nanocomposites, exhibit excellent magnetic properties and can be taken as adsorbent for removal of methylene blue dye from wastewater.

Keywords*:* Magnetic nanocomposite, Absorbent, Porphyrin, Methylene blue

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Synthesis of MoS_2 nanoparticles by a facile and cost-effective method

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Molybdenum sulfide is one of the widely used materials in various industrial applications. Because it has layered structure and its layers connect together by weak van der Waals force. Recently scientists found that MoS_2 nanoparticles have many applications such as electrode in lithium batteries, hydrodesulfurization and hydrodenitrogenation catalysts, wear resistance, Solar cells and solid lubricants. Easy synthesis of these nanoparticles in small size was challenging for inorganic chemistry scientists during past decade. In this work a facile and low-cost method has been introduced for synthesis of MoS_2 nanoparticles, Under 100 nm scales. This method is a sedimination bottom-up method for synthesis nanoparticles and based on using water as solvent and it has two steps. First step consist of solving ammonium-heptamolybdate as Mo source in water and second step consist of forming MoS_2 sediment in presence Sulfur salt as S source in acidic media. Final product at first was annealed in 400°C for 3 hours and then characterized by XRD and SEM analysis. The results shows that prepared nanoparticles have no impurities and they are in under 100nm size.

Keywords: molybdenum sulfide, nanoparticles, facile synthesis

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The effect of anaerobic reaction kinetics by comparing the removal of BOD and the production of biogas in the EGSB anaerobic reactor

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Expanded Granular Sludge Bed Anaerobic digesters convert Zarnam grain refinery waste (Effluent from High fructose corn syrup) into energy in the form of biogas. Most reactions that take place in EGSB reactor are slow and the consideration of the kinetics is important. EGSB reactor is a process of degradation of a organic matter in the absence of oxygen. There are four basic steps of EGSB reactor such as Hydrolysis, Acidogenesis, Acetogenesis and Methanogenesis. Important Parameters that Influence biogas Production is Temperature, pH, residence time, BOD loading and internal Circulation flow rate. The reaction rate r is the term used to represent between the reaction rate, concentration of the reagent and the order of reaction is given by the expression: $r=kC^n$ .In this paper, we study the reaction kinetics of anaerobic reactor and compare the production of biogas with removal BOD was investigated.

Keywords: Anaerobic treatment, Kinetics, EGSB reactor, Removal BOD

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The effect of removal of phosphate by polyaluminumchloride in the quality of effluent the Zarnam grain refinery

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Different types of phosphorus compounds in wastewater are available in three forms of orthophosphate, polyphosphate and organic phosphorus. 60 to 80% is polyphosphate and organic phosphate and remaining is orthophosphate. Removal Phosphate is possible in both chemical and biological treatments. Under normal conditions in the wastewater treatment plant, 5 to 10 percent of phosphate in the initial clarifier basin is eliminated due to the removal of suspended solids. In this paper, using the poly aluminum chloride and optimizing the pH value and the amounts of coagulants (100, 150, 200, 250, 300 and 400 ppm) the phosphate removal conditions during the jar test increased to 60 Percent. The reaction of phosphate ions with Al^{3+} ions causes $AlPO_4$ sedimentation, which results in a significant reduction in the phosphate content by removing the $AlPO_4$ complex in the initial clarifier basin. The polyaluminumchloride reduces turbidity, sewage pumping material and sewage paint. Also, while reducing TCOD, there is not much change in the SCOD value. Outflow waste from the initial clarifier basin by adding anionic polyelectrolyte in the DAF system, the amount of suspended solids is significantly reduced, which reduces the color and turbidity and improves the quality of the sewage, which optimizes the consumption of polyelectrolyte in the DAF system as well as efficiency Sewage treatment is anaerobic and aerobic during biological processes

Keywords: Industrial wastewater treatment, Phosphate, Chemical sedimentation, Polyaluminumchloride

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Investigation of the HSA interaction with immobilized cisplatin and carboplatin on the inorganic nano carrier

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Studies on the interactions between anticancer drugs and human serum albumin (HSA) are extremely important for drug discovery, since HSA behaves as a carrier for external drugs and internal biological molecules [1]. In this project carboplatin and cisplatin have been synthesized following the literature [2-3]. Also, for drug delivery improving cisplatin and carboplatin compounds were encapsulated in the silica hallow spheres as carrier, separately, and the characterized by using XRD, BET, TGA, FT-IR, SEM and ICP techniques. In the following, the interaction HSA and two mentioned immobilized drugs were investigated in Tris-HCl buffer of pH 7.4 at room temperature. These two complexes can denature HSA at low concentrations. Results show cisplatin-sba has more activity on protein denaturation (~0.17mM) than carboplatin –sba (~1.5mM).

Keywords: Cisplatin, Carboplatin, Sba-15, Anticancer, Drug Delivery, HSA, Denaturation

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Immobilization of anticancer cisplatin and carboplatin drugs on the inorganic nan carrier (sba-15) and the comparison of their release with HSA-drug

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To reduce the toxicities of platinum drugs, drug delivery system was developed with a capacity of passive tumor targeting [1-2]. Then, nano hallow sphere silica was synthesized and characterized by using XRD, BET, TGA, FT-IR, SEM and ICP techniques. Also, for improving of drug delivery, cisplatin and carboplatin drugs were encapsulated on the silica hallow spheres as carrier, separately. These drugs were loaded on the inner surface of hallow sphere by wetness method. Results, icp data show that mentioned drugs were loaded on silica hallow spheres. Release of both Pt-drugs from the surface of sba-15 were investigated in tris-buffer medium by using dialysis membrane. Result show two immobilized drugs release slower than HSA-drugs. This effect could be more controlled for cisplatin system.

Keywords: Anticancer, Drug Delivery, HSA, Cisplatin, Carboplatin, Sba-15

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Interaction of metal cations with specific G-rich DNA sequences

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Toxical effects of metals on living organisms are well known. Critical toxicity of metals especially on structure and function of chromatin has been considered. G-rich sequences may adopt various quadruplex structures and play very important roles in gene regulation. Therefore any alteration in their conformation may strongly affect their function. Grich sequences have been considered very important target sites in several diseases. Potential interaction between metal ions with G-rich sequences has been studies here using synthetic double-labled probes and flourescenceresonance energy transfer (FRET) method. Melting temperature of the probes was measured by recording fluorescence intensity of the probe in presence of various concentrations of metal ions when is gradually heated from 30 to 99°C. Any changes in G-quadruplex conformation may result in shift in melting temperature. Metal ions made various extents of changes in melting temperature of the probes. Most of the changes were observed as increasing melting temperature normally in concentration dependent manner, while rarely reduced that. In general metal ions showed significant impact on G-quadruplex structure and thermal stability. The direction and amount of such impact may greatly depend on special characteristics of metal ions and the conformational propertied of target.

Keywords: Metal ion, G-quadruplex DNA, interaction, FRET, stability

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Investigation of interaction of metal cations with sequence specific double strand DNA

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Metallic compounds are among the critically important pollutants in our environment. Humans are in contact with several toxic metals such as Ni, Cd, Co, Pb, Hg and several other which are normally play important roles in healthy organisms, but get toxic in high concentration by accident contaminations or supplementary diets. Cytotoxicity and severe impacts of metallic contaminations on living organisms have been more attended recently in epigenetic and molecular biology studies. Here we examined the potential interaction of about 20 different metal ions with specific double strand DNA sequences using double-labled probes and thermal fluorescence resonance energy transfer method. Double stand DNA was prepared and incubated in presence of various concentrations of each metal. Flourescence intensity of the solutions was recorded while heated from 30 to 99°C. Any changes in DNA conformation may shift its melting temperature. Most of the changes were observed as increasing melting temperature normally in concentration dependent manner, while rarely reduced that. In general metal ions showed significant impact on G-quadruplex structure and thermal stability. The direction and amount of such impact may greatly depend on special characteristics of metal ions and the conformational properties of target

Keywords: Metal ion, sequence specific DNA, Interaction, FRET, Stability

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Synthesis, characterization and biological activities of a novel orthopalladated complex; interactions with DNA and BSA

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Phosphorus ylides can be used as the chiral auxiliary reagents, reaction intermediates or starting materials in a wide variety of processes due to their nucleophilic character, particular bonding properties and diverse coordination modes [1, 2]. The phosphorus ylides can coordinate to Pd as the bidentate ligands and undergo the orthopalladation that has already been reported [3]. A new orthopalladated complex [Pd(L_1)(py)Cl] (L_1 = C_6H_4-$PPh_2C(H)C(O)CH_2Cl$ is synthesized by the reaction of palladacyclic dimer with pyridine . It has been characterized by IR, NMR and elemental analysis. The binding of the complex with native calf thymus DNA (CT-DNA) was monitored by UV-Vis absorption spectrophotometry and fluorescence spectroscopy. Our experiments indicated that the complex could strongly bind to CT-DNA via partial intercalative mode. In addition, fluorescence spectrometry of the bovine serum albumin (BSA) with the complex, showed that the fluorescence quenching mechanisms of BSA were static process. The results of site-competitive replacement experiments with specific site markers clearly helped us to conclude that the complex bind to BSA. Finally, the molecular docking experiment effectively proved the binding of Pd (II) complex to DNA and BSA.

Keywords: Phosphorus ylide, CT-DNA binding; BSA binding; Anticancer activity; Molecular docking

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Synthesis and characterization of a new palladium(II) complex. Its antitumor activity and partial interaction with DNA and BSA.

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Anti-cancer properties of cisplatin and its commercially successful analogues, carboplatin and oxaliplatin, have been known for some time, leading to an unprecedented upsurge in the synthesis and application of platinum-based potential anti-cancer agents [1]. It has been reported that many active complexes being carried by BSA and could react with DNA and inhibit its synthesis [2].Therefore, new palladium(II) complex of formula [Pd(en)(2-py)]NO_3 (Where en= ethylenediamine and 2-py is 2-pyridinecarboxylate) have been synthesized and characterized by elemental analysis, conductivity measurement, and by UV-Visible, IR, and ^{1}H-NMR spectroscopic techniques.This complex has been interacted with bovine serum albumin(BSA) and calf thymus DNA using UV-Visible spectroscopy in 30 mmol/L Tris-HCl buffer of pH=7.0 at two temperatures of 300 and 310 K. In these studies, K_{app}, the apparent equilibrium constant are 2.1×10^4 M^{-1}, 1.5×10^4 M^{-1}, 2.6×10^4 M^{-1} and 1.1×10^4 M^{-1} at 300 K and 310 K for BSA and DNA respectively. The above compound can interact with BSA as well as DNA and the concentration of the complex in the midpoint of transition, $[L]_{1/2}$, is increased by increasing the temperatures from 0.027 mmol/L to 0.031 mmol/L for BSA and from 0.028 mmol/L to 0.034 mmol/L for DNA at 300 K and 310 K, respectively. The *in vitro* antitumor properties of the Pd(II) complex were carried out with human tumor cell line K562 [3]. The 50% cytotoxic concentration(Cc_{50}) of the complex was determined 32 µM.

Keywords: Pd(II) complex, Cytotoxicity, DNA/BSA-binding

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Performance of M-ZSM-5 (M: Ag, Fe, Cr, Mn and Ni) nanocatalysts for degradation of VOC

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Volatile organic compounds are considered as one of the main air pollutants. Catalytic combustion for controlling volatile organic compounds (VOCs) emissions is a competitive method to solve the environmental problems [1]. In recent years, supported transition metal oxides were extensively used in controlling VOCs emissions, and special attention has been paid to these systems as a substitute for noble metal containing catalysts. On other hand, the materials with high thermal stability, resistance to humidity, high specific surface area and ability to stabilize the metal particles in the porous structure are desired to use as catalyst supports [2]. In this study, the catalytic oxidation of ethyl acetate has been investigated in a series of M (M: Ag, Fe, Cr, Mn and Ni)-HZSM-5 zeolites. Catalytic studies were carried out inside a U-shaped fixed bed reactor under atmospheric pressure and different temperatures, between 150 and 450°C and ethyl acetate inlet concentration of 1000 ppm. The objective was to find a catalyst with high superior activity, selectivity towards deep oxidation product and stability. Besides the higher the inlet concentration of ethyl acetate, the lower the conversion yield, and oxygen concentration in catalytic oxidation conditions has not so large influence on conversion The sequences of catalytic activity and catalytic stability were as follows: Ag–ZSM-5 > Fe–ZSM-5 > Cr–ZSM-5 > Ni–ZSM-5 > Mn–ZSM-5 > HZSM-5. The catalysts were characterized by inductively coupled plasma atomic emission spectroscopy, X-ray diffraction, scanning electron microscopy.

Keywords: Catalytic combustion; VOC; Nano catalysts, zeolite, HZSM-5.

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Oxidation of sulfides with hydrogen peroxide catalyzed by silica gel-bound Mo(VI) Schiff base complex

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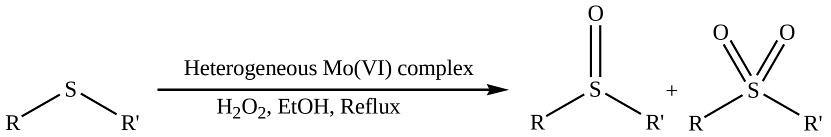
The oxidation of organic substrates by transition metal complexes has become an important research area in both organic synthesis and bioinorganic modeling of oxygen transfer metalloenzymes. Molybdenum complexes played a critical role in homogeneous industrial catalysis in the Arco and Halcon processes, involving the typical example of the industrial production of propylene oxide using alkyl hydroperoxides as oxidants, catalyzed by a homogeneous Mo (VI) [1]. Sulfoxides and sulfones have found many applications in pharmacy [2,3] and other fields such as engineering plastics and polymers [4]. Oxidation of sulfides is the most direct approach for the synthesis of sulfoxides and sulfones [5].

Herein, the hydrazone Schiff base (H_2L) was readily synthesized by condensation of 3-ethoxysalicyaldehyde with isonicotinhydrazide in methanol. The dioxomolybdenum(VI) complex of the synthesized ligand was prepared by reaction of $Mo(O)_2(acac)_2$ with H_2L in methanol and demonstrated its high catalytic activity in the oxidation of sulfides under heterogeneous conditions using hydrogen peroxide as the terminal oxidant (Scheme 1). In IR Spectrum, the two prominent bands at 935 and 910 cm^{-1} attributed to the symmetric and asymmetric stretch of *cis*-$Mo(O)_2$ are consistent with previously reported complexes. The reaction parameters such as catalyst amount, kind of solvent; oxidant amount and temperature were optimized in the oxidation of diphenyl sulfide.



(Scheme 1)

Keywords*:* dioxomolybdenum (VI), Catalytic activity, Sulfideoxidation.

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DNA binding study of antibiotic drug cephalexin by molecular docking technique

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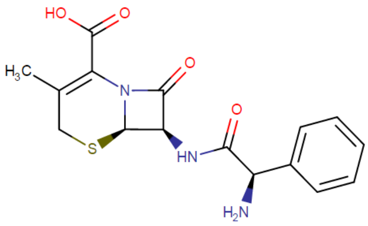
The present study purposes at exploring an accurate characterization of the binding interaction of antibiotic drug cephalexin with calf thymus DNA (ct-DNA) as a relevant biological target by means of molecular modeling study which it shaded more light on the groove binding mode of cephalexin into the DNA helix. MGL tools 1.5.4 with AutoGrid4 and AutoDock4 were used to set up and carry out blind docking calculations between the drug and DNA sequence. Determination of the binding mode and affinity between the constituent molecules in molecular diagnosis is strict to understand the interaction mechanisms and to design therapeutic interventions. Due to the hardness and economic cost of the experimental methods to characterize the structures of complexes, computational methods such as molecular docking are favorable for predicting putative binding modes and affinities. From the docking simulation the observed free energy change of binding (ΔG^o) for the complex-DNA is calculated to be (-22.97 $kJmol^{-1}$). The development of cancer drugs is slow and expensive hence one approach to accelerate the availability of new drugs is to reposition drugs approved for other indications as anticancer agents. As, cephalexin causing bacterial cell death, therefore, it may be used as anticancer drug, which locates cell walls and can interact with DNA.



Keywords: Cephalexin, DNA binding, Groove binding, Molecular docking technique

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DLLME and determination of Imidacloprid in apple using HPLC

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In modern agriculture, pesticides have been broadly employed in order to protect agricultural products against harmful insects and weeds, to improve their quality and increase their yields. Neonicotinoids are a class of neuro-active insecticides chemically related to nicotine. These compounds are the first new class of insecticides introduced in the last 50 years, and the Imidacloprid is currently widely used insecticide in the world. Many methods for analysis of pesticide in fruits and vegetables are based on chromatographic. In this research, a simple and sensitive method based on dispersive liquid-liquid micro-extraction (DLLME) for extraction and preconcentration of Imidacloprid pesticide in agricultural products such as apple,before analysis by high performance liquid chromatography was provided.In this case about 20gr of hemogenaized apple weighed and diluted with 20ml distilled water. Then it was sentrifuged by 3500prm in10 minute.5ml of upper solution mixed with 0.8ml acetonitrile (dispersive solution) and 100µl of chloroform (extractive solution) while the cloudy drop is composed. At last 25µl of cloudy drop inject in HPLC-UV .The micro-extraction optimal conditions, such as the type and volume of extraction and dispersive solvents, salt concentration and extraction time were obtained. Accordingly the salt concentration was obtained 10% and time have not influence to extraction ability. Then under optimal conditions, the pesticide in the linear range 320-5 $ng.g^{-1}$ was analyzed and the limit of detection (LOD) for apple calculated to be 0.7 $ng.g^{-1}$ .In this method evaluated recovery rates are 92.0 percent. So method was evaluated statistically and real sample were tested according the optimum conditions. Method was easy,fast and green than before method.

Keywords: DLLME, IMIDACLOPRID ,HPLC

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Preparation and Characterization of Fe-Ni oxide Nanoparticles based on Nano Alumina prepared by Co-precipitation method and the study of the effect of Aging condition on the structures

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Ferrit- nickel is one of attracting materials due to their properties such as low melting point, high specific heating, large expansion coefficient and low saturation magnetic moment [1,2]. It has many technical applications such as in photoelectric devices, catalysis, sensors, nano devices, microwave devices and biomedical applications like drug delivery and hyperthermia [3,4]. In this research nan crystalline ferrit-nickel was prepared via co-precipitation method.0.16M solution of sodium carbonate (as precipitating agent)was slowly added to salt solution of 0.02M ferric nitrate and 0.017M nickel nitrate and 0.02M nano alumina as substrate. Consider aging condition at different times (2, 4, 6, 8, 10, 12 hours), dried at 120^{0}c for 4 hours and calcinated at 550^{0}c for 4 hours. X-ray diffraction (XRD) indicated that Fe_3O_4 (cubic), Fe_2O_3 (cubic), NiO (monoclinic), $NiFe_2O_4$ (cubic) and Al2O3(Rhombohedral) have grown respectively in the pages (311), (110), (111$^-$), (311) and (104). The particles size in the SEM were between 27.51-45.76nm.The result of (EDX) analysis showed the present of Fe, Al, O, Ni in the samples. All of the products were superpara magnetic. The result showed that the 4 hours aging is the best time.

EDX analysis	**FE-SEM information**		**XRD information**		**Aging conditions**	**samples**
Elements	**morphology**	**Average nano particles size**	**Average crystal size**	**Phases**		
O,Fe,Ni,Al	spherical	41.3	35.38	NiO,Fe_3O_4,$NiFe_2O_4$,Al_2O_3, Al_2FeO_4,Fe_2O_3	2	S1
O,Fe,Ni,Al	spherical	31.41	7.26	NiO,Fe_3O_4,$NiFe_2O_4$,Al_2O_3, Al_2FeO_4,Fe_2O_3	4	S2
O,Fe,Ni,Al	spherical	40.54	8.2	NiO,Fe_3O_4,Al_2O_3,$Al_3Fe_5O_{12}$	6	S3
O,Fe,Ni,Al	Layer-layer	27.51	9.85	NiO,$NiFe_2O_4$,Fe_3O_4,Al_2O_3, Al_2FeO_4	8	S4
O,Fe,Ni,Al	spherical	45.76	43.67	NiO,Fe_3O_4,Al_2O_3,FeO,$FeNi_2O_4$,Fe_2O_3	10	S5
O,Fe,Ni,Al	spherical	34.97	34.5	NiO,$NiFe_2O_4$,Fe_3O_4,Fe_2O_3,Al_2O_3	12	S6

Keyword: Co-precipitation, Nanoparticles, X-ray diffraction

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Unsymmetrical Palladium(II) N,N,O,O-Schiff Base Complexes: Efficient Catalysts for Suzuki Coupling Reactions

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One of the strongest and best tools for preparation of biaryl compounds which play a significant role in structural formation of pharmaceutical intermediates, natural products and many polymer agrochemicals is the Suzuki-Miyaura cross-coupling reaction of aryl halides with aryl boronic acids [1]. Manipulating the ligand environment around the palladium center, results in the change of efficiency of catalytic system which are composed of Pd(0) or Pd(II) derivatives associated with suitable ligands [2]. Lately, various nitrogen containing ligands which are involved in Suzuki reaction attract a great amount of attention among researchers [3]. In This study, the reaction between palladium(II) acetate and Schiff base ligands, in a molar ratio 1:1, resulted in the formation of palladium(II) Schiff base complexes **PdL^1** and **PdL^2** (**L^1** = N-2-hydroxyacetophenon-N´-2, 4-dihydroxbenzaldehyde-1,2 phenylenediimine and **L^2** = N-2-hydroxyacetophenon-N´-2-hydroxynaphthaldehyde-1,2 phenylenediimine) which could be identified by elemental analysis, FT-IR, UV-Vis, ^{1}H NMR spectroscopies. The X-ray analysis of **PdL^2** showed that the Schiff base acts as a tetradentate ligand which through both the phenolic O atoms and the azomethine N atoms coordinated to the Pd atom with square planar geometry. Using GC, the catalytic activity of the Pd(II) complexes for Suzuki coupling reaction were studied. After 8 hours of reaction time at 80 ^{o}C in ethanol it was concluded that both Pd(II) complexes are good catalysts for this reaction by more than 90% conversion of the starting materials to the biphenyl product.

Keywords: Schiff base, Palladium(II), Suzuki reaction, X-Ray crystallography

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Synthesis and Characterization of a Schiff base ligand Derived from p–toluene sulfonyl hydrazide and 2- hydroxy 3- methoxy benzaldehyde

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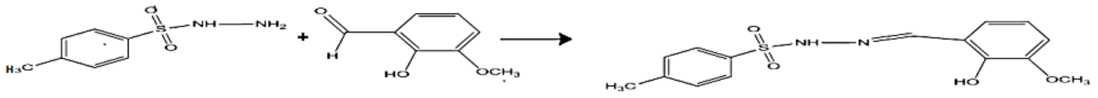
Sulfonamide base Schiffs are the important ligand for synthesis of metal complexes. These ligands as a chelating agent can be used in extraction and separation of metals in solution [1]. In this study, the sulfonamide Schiff base was synthesized from reaction of p-toluene sulfonyl hydrazide and 2- hydroxyl- 3- methoxy benzaldehyde (1:1 molar ratio) in ethanol under reflux condition. (Scheme 1)



Scheme 1. Preparation N-(2- hydroxyl -3- methoxybenzylidene) -4- methlbenenesulfonohydrazide

The crystal structure of the compound was determined by X- ray crystallography (Stoe IPDS-II) [2][3]. The crystal structure study of single crystal shown that crystalline system is monoclinic by C/2c space group with: a= 15.807(1) Å, b= 10.457(1) Å, c= 20.779(1) Å, в= 109.68º, and each cell made of 8 molecules (Figures 1 and 2). A molecule of methanol was seen in structure. There is hydrogen bond between the NH group from one molecule with the OH group of the side molecule (Figure 3). These hydrogen bond converts the molecules into an infinite chain along [010].

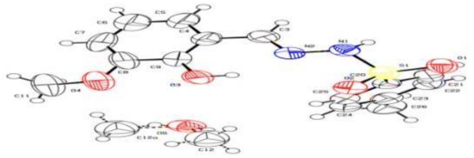


Fig 1. The molecular structure of synthesized compound

and representation of methanol in structure

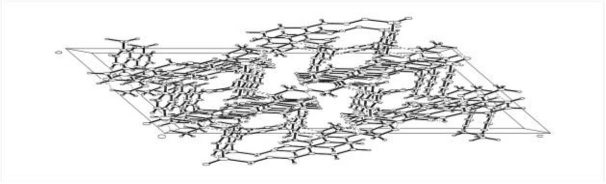


Fig 2. Crystal packing of synthesized compound

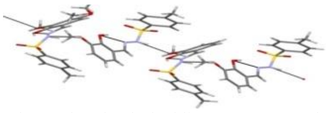


Fig 3. N-H….O hydrogen bonds (dashed lines) were caused chains along [010]

Keywords: Sulfonamide base Schiff, Crystal structure, p-Toluene sulfonyl hydrazied

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A new water-soluble thiosemicarbazone ligand and it's Copper, nickel and zinc complexes: Synthesis, characterization, stability and antioxidant properties

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New water soluble Schiff base thiosemicarbazone ligand, namely (sodium 4-hydroxy-3-{[(methylaminocarbonothioyl)hydrazono]methyl}-benzene sulfonate) (**NaH$_2$L**) was obtained by the reaction of methylthiosemicarbazide with sulfonate salicylaldehyde and characterized by elemental analysis, spectroscopic methods (UV-Vis, FTIR, ^{1}HNMR, and ^{13}CNMR) and electrospray ionization mass spectrometry. The X-ray structure of **NaH$_2$L** ($NaH_2L{\bullet}CH_3OH{\bullet}0.5H_2O$) shows that sodium atoms are interconnected through sulfonate groups of the ligands into one-dimensional coordination polymer network. Reaction of the ligand with metal acetates produced following complexes: **CuHL**, **NiHL** and **ZnHL**. All complexes were characterized by means of elemental analyses, IR spectroscopy, and ESI-Mass measurements. The dinuclear structure of the copper complex was determined by single-crystal X-ray crystallography and showed the square pyramidal geometry for each metal center. **NaH$_2$L**, **CuHL**, and **NiHL** showed high solubility in water (50, 25 and 25 g/L, respectively, at 25 °C), while solubility of **ZnHL** was very low. **NiHL** was stable at all pH ranges for 4 days while stability of **NaH$_2$L** and **CuHL** was decreasing at acidic and basic pHs. Antioxidant activity of the compounds for scavenging activity of DPPH$^{\bullet}$ and ferric reducing antioxidant power (FRAP) was evaluated and the ligand indicated the strongest radical scavenging relative to the complexes and L-ascorbic acid as standard.

Keywords: Thiosemicarbazone; Water-soluble Schiff base; Stability; Antioxidant

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Synthesis of phosphoramidate and it's graphene oxide composite, anticholinesterase activity and study fluorescence spectra

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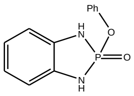
Phosphoramidates are best known for their highly toxic effect as agricultural chemicals. Phosphoramidates with the general structure of X–$(NH)_2$ P(O) skeleton are important class of compounds that exhibit the insecticide properties to inhibit the acetylcholinesterase (AChE) enzymes [1, 2].little attention has been given on the interaction mechanism of the ChE enzymes and phosphoramidate. Spectrophotometric studies of the interaction of Acetylcholinesterase and phosphoramide ligands have shown that it can binds to Acetylcholinesterase. If two partial composites of this compounds by GO synthesized, this compounds have highly exceed AChE properties than phosphoramide. That this matter recognized by Fluorescence spectrum. This analyze shown times that phosphoramide (PA) without synthesize GO/PA composite has approximately 1/1000 AChE properties into GO/PA composite and this matter very important due to very little pollutant materials enter the nature. The chart and table of this analysis IC50 for GO, PA and GO/PA composite exhibit in the following. [3]



L1-ligand

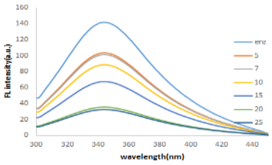


Figure 1: Fluorescence spectrum of AChE in presence GO in 5,7,10,15,20,25 µl

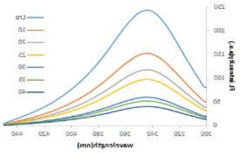


Figure 2: : Fluorescence spectrum of AChE in presence L1 in 10,20,25,30,35,40 µl (4Mm)

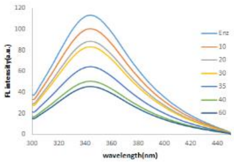


Figure 3: Fluorescence spectrum of AChE in presence GO/L1 composite in 10,20 ,30,35,40,60 µl
3µM L1 in 0.01_{gr} GO/$5cc_{solvent}$

sample	L1 ligand	GO	GO/L1 composite
IC50	84mM	0.027gr/lit	0.013mM

Keywords: AChE, Fluorescence, Phosphoramidates , GO composite

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Development of gas sensors based on modified nano metal oxides to measure volatile organic compounds (VOCs)

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Sensor technology is one of the most significant technology for the future with a constantly growing number of applications, ranging from toxic gas detection, manufacturing process monitoring to medical diagnosis and health monitoring [1]. Semiconductors are used as gas sensors based on the principle of the variability of electrical conductivity of metal oxides when exposed to these gases. These properties can be utilized to detect Volatile Organic Compounds (VOCs), SO_X, CO_2 and O_2, etc. Metal Oxide Semiconductor (MOS) sensor technology is based on the change in resistance of a sensitive metal oxide layer which is induced by the interaction between a surface and ambient gases. MOSs demonstrate good detection sensitivity. A voltage detecting method was used to calculate the sensitivity of the sensor, which was defined as:

$$(R_{air} - R_{gas}) / R_{air} * 100\ (\%)$$

Where R_{air} and R_{gas} were the electrical resistances in VOCs and clear air, respectively [2]. The n-type metal oxides like ZnO, SnO_2, Fe_2O_3, WO_3 are generally used as sensing material for semiconductor sensors [1]. In this research, different types of nano metal oxides such as ZnO, SnO_2, Fe_2O_3 or combination of them have been synthesized with sol gel methods and compared for sensing the concentration of VOC. The composition and surface morphologies of nano metal oxides films were studied with FT-IR, XRD and scanning electron microscopy (SEM).

Keywords: Gas Sensor, VOC, Metal Oxide.

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Theoretical study of Scandium and Titanium (central metal) effects on the verdoheme ring opening reaction

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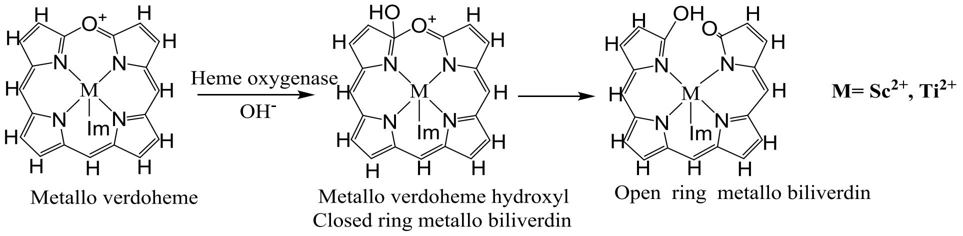
Heme catabolism is an important physiological process that converts heme to the biliverdin in the presence of heme oxygenase which has essential role in destroying unwanted heme[1].These reactions occur by nucleophilic attack at one of the carbon atoms adjacent to the oxygen of the verdoheme ring(Fig. 1).The roles of the metals in the course of heme degradation are not yet known completely. Previously,conversion of iron (II) verdoheme to iron (II) biliverdin in the presence of hydroxyl ion as a nucleophile and imidazole as axial ligand was studied using the B3LYP method and the 6-31G basis set [2].In this research conversion of scandium or titanium verdoheme (II) to scandium or titanium biliverdin (II) was studied with the same pathway and same basis set as iron ones.Conversion of scandium verdoheme (II) to scandium verdoheme hydroxyl (II) is more endothermic than iron analogues (145.78 with regard to 153.41 kcal/mol for scandium and 148.87 in regard to 153.41 kcal/mol for titanium), the Scandium verdoheme hydroxyl changes to more stable scandium biliverdin (25.41 to 14.15 kcal/mol) with a low barrier energy (2.5 to 5.66 kcal/mol) (Fig. 1).



For titanium step one is more endothermic than iron analogues (148.87 in regard to 153.41 kcal/mol), the titanium verdoheme hydroxyl changes titanium biliverdin (24.55 to 14.15 kcal/mol) with very low barrier energy (0.74 to 5.66 kcal/mol) in comparison with iron ones. Verdoheme ring opening process in the presence of titanium is much faster than that reaction in the presence of iron.

Keywords: Verdoheme, verdoheme hydroxyl, biliverdin,Hemoxygenase, DFT

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Synthesis, Characterization, Density Functional Theory Calculation and Antibacterial Activities of Five-Coordinate Complexes of iron (II) and cobalt (II) Transition Metals Containing a Benzoyl Thiourea Derivative

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In recent years, many research has been focused on the development of efficient antimicrobial agents to inhibit the growth of various drug-resistant strains [1]. Two compounds of first-row transition metals, i.e. $[M(L^{'})(H_2O)_2]$ (M = Fe (C1) and Co (C2)), of benzoyl thiourea ligand which have been extracted from the condensation of 2-chlorobenzoyl-isothiocyanate with 2,6-diaminopyridine, called 1,1'-(pyridine-2,6-diyl)bis(3-(2-chlorobenzoyl) thiourea) (L), were synthesized and specified through analysis of elements, Fourier Transform Infrared (FTIR) and UV-visible spectroscopies, as well as conductivity measurements. The structures proposed for two complexes were confirmed through the application of conformational analysis and geometry optimization by utilization of Gaussian 09 suite of programs and Beck's 3-parameter hybrid method at the B3LYP level with the 6-31G(d,p) basis set as a supplementary tool due to inaccessibility to suitable crystals from pure solid thiourea compounds for X-ray measurements. These compounds were studied *in vitro* in terms of antibacterial properties against Staphylococcus aureus and Enterococcus faecalis as 2 standard gram-positive and Escherichia coli and Pseudomonas aeruginosa as 2 standard gram-negative bacterial strains, through minimum inhibitory concentration by using the broth macrodilution procedure and inhibition zone via the disk diffusion method [2]. The superior antibacterial activities of two complexes compared to those of the new thiourea derivative were proven through the experiments.

Keywords: Density Functional Theory; Antibacterial Activity; Benzoyl Thiourea; 2,6-Diaminopyridine

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Synthesis and characterization of novel metal based infinite coordination polymer nanoparticles

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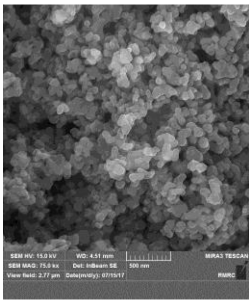
Coordination polymers have attracted high interest in materials science and modern chemistry which are based on metal ions coordinated with organic ligands and can be used in multitude forms, like metal organic frameworks (MOFs) and infinite coordination polymers (ICPs). The properties of these compounds depend on their microscopic structures and therefore lead to different applications as catalysts [1,2], drug delivery [3,4], separation [5] and antisense gene regulation [6].

In this paper, we have succeeded to report the constitution of novel ICP nanoparticles by various metals and bicarboxylic acid functionalized organic linker by precipitation and hydrothermal methods.

The results of ^{1}HNMR show that the ligand was synthesized purely. The prepared coordination polymers were characterized by CHN, ICP-OES, TGA, SEM techniques. This study provides a new insight into the formation of nanosized infinite coordination polymers.

Keywords: Infinite coordination polymer, nanoparticles, metal oxide



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Preparation of Titanium oxide nanocomposites using Ni-Cr LDH

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Layered double hydroxides (LDH) known as anionic or hydrotalcite-like clays, have growing interest for using in the wide fields. The main properties of LDH arise from their wide layer and interlayer chemical compositions. Titanium oxide is one of the most promising candidate materials for fabrication of sensing devices such as chemical sensors. In TiO2/Ni-Cr LDH nanocomposites probably exhibit improved structural and functional properties of great interest for different applications. The current research in the preparation of nanocomposite materials containing TiO_2 reports the use anionic clays (type layered double hydroxides) [1,2,3]. We report the synthesis of composite nanostructures comprising LDH and TiO_2 by different methods [4]. TiO_2/ Ni-Cr LDH nanocomposite was synthesized by the co-precipitation method in constant pH .The chemical compositions and morphology of the synthesized materials were investigated by the FT-IR and XRD. For examples Ti–O and Ni-Cr-OH vibration were observed in the FTIR spectrum. The average crystallite size of the nanoparticles has been estimated from the XRD patterns.

Keywords: LDH, Layered double hydroxide, Coprecipitation, Nanocomposite , Titanium oxide

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Hydrophobic and hydrophilic effects in different heterogeneous acid catalysts for the esterification of acetic acid with butanol

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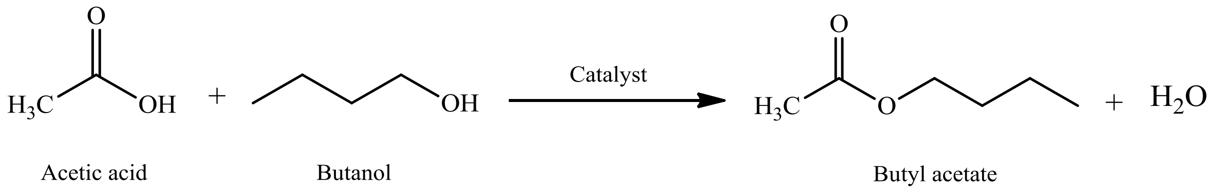
The catalysts used for the esterification reactions require hydrophobicity to avoid strong adsorption of water. Since the reaction involves highly polar reactants (or products) such as acids, alcohols, and water, leaching of the active components to the liquid phase is an important factor for designing the proper catalysts. For this aim, we used three kinds of supports with different surface characteristics such as silica coated magnetite nanoparticles (SCMNPs), MCM-41 and activated carbon (AC) for immobilizing sulfonic acid groups. These solid acid catalysts were characterized by various physicochemical methods such as FT-IR spectroscopy, SEM analysis and CHNS elemental analysis which showed that the sulfonic acid groups have been attached successfully to the surface of these supports. Then, they were utilized in the esterification reaction between acetic acid and butanol in order to investigate the hydrophobicity and hydrophilicity effects on their efficiency. It has been found that among these solid acid catalysts, the catalyst with hydrophobic support (AC) exhibits more than 99 percent of butyl acetate production whereas the other two hydrophilic catalysts show less efficiency. The reusability of these catalysts was also investigated and showed three cycle stability for acetic acid esterification without significant loss of activity.



Keywords: Solid acid catalyst, Sulfonic acid, Hydrophobicity, Hydrophilicity, Esterification.

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Enhancing acidic properties of supported solid acid catalysts: A new method for anchoring two acidic sites on the surface of $Fe_3O_4@SiO_2$

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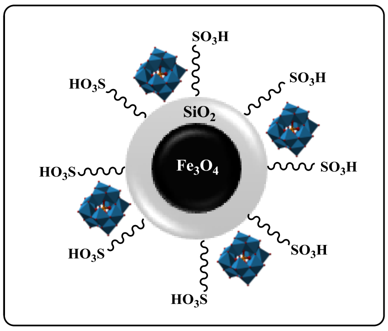
In recent years, different types of solid acid catalysts have been developed, and each type of these catalysts exhibited their unique catalytic activity. Among these synthesized catalysts, a catalyst with two distinct acidic sites which could be separated easily from the reaction mixture is promising. In order to reach this purpose, we prepared a solid acid catalyst based on silica coated magnetite nanoparticles with two kinds of bronsted acidic sites, sulfonic acid groups and phosphotungestic acid species. These functional groups were characterized by FT-IR spectroscopy and CHNS elemental analysis. Vibrating sample magnetometry (VSM) and X-ray diffraction (XRD) analyses were used to identify its magnetic properties and crystal phase, respectively. Also shape and size determination of these nanoparticles were performed by transmission electron microscopy (TEM). The prepared catalyst showed very good activity in the esterification of acetic acid with butanol. Conversions up to 70% of butanol and 100% selectivity toward the ester were reached after 8 h. The results exhibited that this catalyst with double acidic groups is promising solid acid catalyst to be used in the esterification of carboxylic acids with alcohols.



Keywords: Magnetite nanoparticles, Sulfonic acid, Phosphotungestic acid, Esterification.

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Synthesis, Spectral and Luminescence Study of Pd(II) complexes with Mixed-Ligand of 4-methyl-4H-1,2,4-triazole-3-thiol and Ethylene Diamine

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As a polyazaheteroaromatic compound, triazole and its derivatives are widely used as ligands in the neutral and anionic forms and well-known for the importance in industry. The 1,2,4-triazoles present antibacterial activities and are being widely used as agricultural chemicals. In this study, Complexes $[Pd_2(\mu\text{-mptrz})_2(mptrz)_2(en)].CH_3OH$ (**1**), $[Pd_2(\mu\text{-mptrz})_2(mptrz)_2(en)]$ (**2**) (where mptrz is 4-methyl-4H-1,2,4-triazole-3-thiolato and en is ethylene diamine) were synthesized by reaction of (Hmptrz) and ethylene diamine with $PdCl_2$ (**1**) and $Pd(OAc)_2$(**2**) The two complexes were thoroughly characterized by elemental analysis, IR, UV–Vis, 1H NMR, luminescence spectroscopy.

Complex (**1**):Anal. Calcd for $C_5H_7Cl_2N_4PdS$(%): C, 18.06; H, 2.11; N, 16.84; S, 9.62. Found: C, 17.93; H, 2.09; N, 16.72; S, 9.55. IR (CsI, cm^{-1}): 3134w, 3095w, 2994m, 2864m, 2741s, 1695m, 1555s, 1492s, 1389m, 1343s, 1292w, 1221s, 1154s, 1050s, 949s, 867m, 686w, 640w, 518w, 427w, 392w, 333w, 261w. UV-Vis: λ_{max} (DMSO) 231 and 284nm.^{1}H NMR (DMSO-d_6, ppm): 3.38 (s, $-CH_3$), 4.33 (s, $-CH_3$), 4.97 (s, 1H) and 8.56 (s, 1H).

Complex (**2**): Anal. Calcd for $C_{15}H_{28}N_{14}OPd_2S_4$(%): C, 23.65; H, 3.68; N, 25.74; S, 16.81. Found: C, 23.51; H, 3.65; N, 25.59; S, 16.69. IR (CsI, cm^{-1}): 3201w, 3120w, 3080w, 2950w, 2900w, 2400w, 1606m, 1519s, 1470m, 1416s, 1358s, 1210m, 1158m, 1097m, 1063m, 988w, 834w, 708m, 648m, 613w, 574w, 522w, 467w, 419w, 353w, 325w, 278w, 258w. UV-Vis: λ_{max} (DMSO) :325, 259, 425nm.^{1}H NMR (DMSO-d_6, ppm): 2.71 (s,$-CH_2$, ethylene diamine), 3.29 (s, $-CH_3$, methanol), 3.41 (s, $-CH_3$, triazole), 3.47 (s, $-CH_3$, triazole), 4.08(s, -OH, methanol), 4.90 (s, NH_2, ethylene diamine), 8.18(s,-CH, triazole), 8.25 (s,-CH, triazole).

Keywords: 1,2,4-triazoles, IR; UV-Vis, Luminescence

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Green synthesis of copper oxide nanoparticles using extracts of Garlic

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In recently, researchers have been interested to find a safe and environment friendly method to reduce metal ions into metallic nanoparticles (NPs) due to the damaging effects of the chemicals on human health and the environment. The preparation of NPs is using extracts of various parts of plants such as roots, peels, leaves and fruit is a clear and nontoxic method [1]. Garlic is composed of carbohydrates, sulfur and phenolic compounds, and amino acids. Garlic also has antibacterial properties and high biocompatibility. Copper oxide Nps are very good catalysts. They also have electrical properties, nano-fluid, and anti-bacterial activities [2].

In this work, dried powder of garlic was soaked in ethanol-water (50%) with ratio 5:1 for two days in absent of sunlight. After separation of the extract solution by centrifuge is stored at 4ºC in refrigerator.

The CuO NPs were obtained from the reaction of $CuSO_4.5H_2O$ and garlic extract at 80ºC for 3h. These NPs were characterized by common methods such as FT-IR spectra, XRD patterns, UV-Visible spectroscopy.

A band observed at 383 nm in UV-Vis. spectra of solution is due to surface plasma resonance of CuO NPs [3]. The XRD patterns of CuO NPs showed ten peaks at 32.6, 35.6, 38.7, 48.4, 58.3, 61.5, 65.2, 67.8 72.4 and 75.1 º that were corresponded with JCPDS: 80-1916 [4]. The average size of CuO nanoparticles were calculated 40-50 nm by Deby-Scherrer equation from XRD patterns. The FT-IR spectra as-synthesized CuO NPs showed a band at 525 cm^{-1} is due to stretching vibration of Cu-O bond [5].

Keywords: metallic nanoparticles, Garlic extract

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Acid-functionalized infinite coordination polymer nanoparticles as precursor of metal oxides

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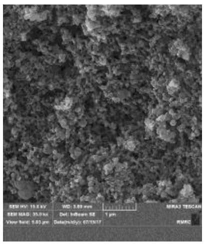
Fabrication of novel coordination polymers (CPs) is very attractive due to their interesting topologies and theirs application. It is well known that preparation of CPs is a complicated self-assembly process which is influenced by many factors such as temperature, PH value, metal-to-ligand ratio, organic ligands and coordination geometry of central metal. Metal-Organic Frameworks (MOF) are subclass of coordination polymer with the special feature that they are often porous. MOFs are compounds consisting of metal ions or cluster which coordinated by organic ligands. Infinite coordination polymers (ICPs), as another subclass of coordination polymers, have attracted many concern in chemistry and material science for variety of application such as catalysis, optic, separation and gas storage. ICP compounds have two parts in which metal ions or metal cluster used as nodes to attach organic or metal-organic linkers. Despite metal-organic framework (MOF), ICPs illustrate structural scale, containing of size and morphology properties. There are three different strategies for synthesizing ICP particles: (i) precipitation method, (ii) micro emulsion techniques and (iii) solvothermal synthesis.

In this article, metal-organic compounds containing bicarboxylic acid groups were used as linker to attach metal ions via precipitation method. The prepared coordination polymers were characterized by CHN, ICP-OES, TGA and SEM techniques. Subsequently, these infinite coordination polymers were used as precursors for the preparation of crystalline metal oxide particles by calcination route.



Keywords: Infinite Coordination Polymer (ICP), precipitation method, metal oxide.

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Synthesis of copper oxide nanoparticles for supercapacitor applications

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Copper (II) oxide is a p-type semiconductor oxide with wide industrial applications as electrode material for lithium ion batteries [1], gas sensors [2] and catalysts [3]. It also has an emerging application as a charge storage material in supercapacitors [4]. In this work, we synthesized CuO nanoparticles (Fig.1) by utilizing mechanochemical reaction and then calcination procedure. Copper (II) acetate monohydrate and diammonium oxalate monohydrate were used as reagents and the resulting precursor was calcinated at 400 ℃ for 2h in air. The product was characterized using FT–IR, XRD and TEM techniques. The charge storage ability and cycle stability of the obtained CuO nanoparticles were investigated by means of cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) cycling in 6.0M KOH. The electrode with nanoparticle morphology showed the specific capacitance of 112F/g at the scan rate of 1 mV/s.

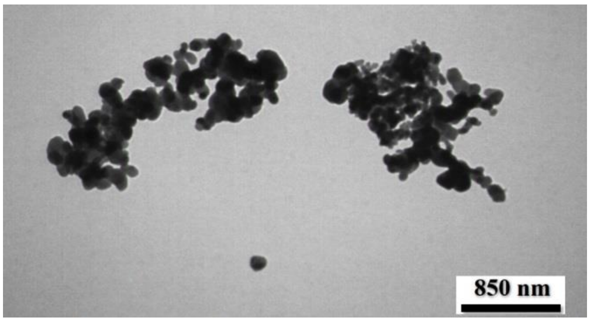

Fig. 1. TEM image of CuO nanoparticle.

Keywords: Copper (II) oxide, Mechanochemical method, Nanoparticle, supercapacitor

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Electronic Structure and Properties Studies of [2,2ˈbipyridine]Ni[4,5-dichloropyridazine] Complex by Hybrid Density Functional Theory

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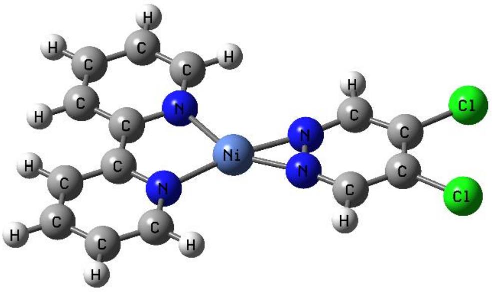
The electrostatic potential is widely used in studies on biological systems to predict the reactivity of numerous chemical systems in electro- and nucleophilic reactions [1]. The structure parameters and ionization energies of [2,2ˈbipyridine]Ni[4,5-dichloropyridazine] Complex were calculated by Density Functional Theories (DFT) using Becke's three-parameter hybrid functional with 6-31+G* basis set and LANL2DZ effecitive core potential using Gaussian 03 software [2]. Vibration frequencies were also calculated to the structure with optimized geometry and no imaginary frequency were obtained, so the stationary point correspond to the minima of the potential energy surface. Electronic structure studies were carried out in a DFT method with a B3LYP potential, which is the most complete potential actively used in modern research and showing the best agreement to experiment in the sequence of levels. Also, the restricted Hartree–Fock method was employed for electronic structure calculations of closed-shell complexes, and the unrestricted approximation was used for open-shell complexes. The contributions of atomic orbitals were evaluated from the squares of the diagonal elements of the density matrix. Also, the bond orders and the electronic properties of the complex were calculated. The relationship between the stability constants of the complexes and the electronic properties of the complex were examined. It was found that the stability constants of the complexes correlate with the calculated bond orders between metal and ligand, and also geometry of [2,2ˈbipyridine]Ni[4,5-dichloropyridazine] Complex.



Keywords: [2,2ˈbipyridine]Ni[4,5-dichloropyridazine] Complex, Electronic Properties, DFT

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Theoretical Investigation of Geometric Configurations and Vibrational Spectra in [3-(pyridine-2-yl)pyridazine]Ni[4,5-difluoropyridazine] Complex

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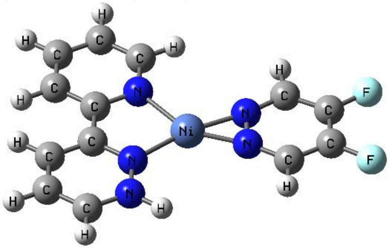
Studies of the chemistry of organometallic complexes [1] consisting of metal atoms, metal clusters, and metal surfaces interacting with organic molecules have been carried out for a long time using conventional chemical synthesis procedure. A fundamental understanding of this interaction, however, is hampered by the fact that one must incorporate the effects of the solvent [2]. The electrostatic potential is widely used in studies on biological systems to predict the reactivity of numerous chemical systems in electro- and nucleophilic reactions [3]. The quantum chemical calculations of [3-(pyridine-2-yl)pyridazine]Ni[4,5-difluoropyridazine] complex were made by Hartree-Fock (HF) and Density Functional Theories (DFT) using Becke's three-parameter hybrid functional with 6-31+G* and 6-311+G basis sets and LANL2DZ effecitive core potential [4]. Vibration frequencies were also calculated to the structure with optimized geometry and no imaginary frequency were obtained, so the stationary point correspond to the minima of the potential energy surface. Electronic structure studies were carried out in a DFT method with a B3LYP potential, which is the most complete potential actively used in modern research and showing the best agreement to experiment in the sequence of levels. The restricted Hartree–Fock (RHF) method was employed for electronic structure calculations of closed-shell complexes, and the unrestricted (UHF) approximation was used for open-shell complexes. The contributions of atomic orbitals were evaluated from the squares of the diagonal elements of the density matrix. Also, the bond orders and the electronic properties of the [3-(pyridine-2-yl)pyridazine]Ni[4,5-difluoropyridazine] complex were calculated.



Keywords: [3-(pyridine-2-yl)pyridazine]Ni[4,5-difluoropyridazine] Complex, Quantum Chemical Calculations

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Manufacturing and characterization of dye-sensitized solar cells based on organized and nonorganized porous titania nanostructures and investigation of their performance

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In this study, organized porous titanium dioxide photoelectrodes known as mesoporous templated films were prepared and their performance was investigated in dye-sensitized solar cells (DSSCs). The mesostructured films were compared with nonorganized porous photoelectrodes containing spherical particles of nanocrystalline titanium dioxide (NC-TiO2) which are commonly used in DSSCs. In the first section, ordered and disordered mesoporous templated films were prepared by using dip and spin coating methods. To obtain these types of films with high thickness and without any cracking, a stabilization step after each coating and a calcination step after every five layers were used and finally their performance in solar cells was investigated. A maximum efficiency of 8.33% was achieved for the solar cells made of the ordered mesoporous films prepared by dip coating method. In the second step, solar cells based on mesoporous films with four different morphologies of hexagonal, cubic, wormlike and gridlike were prepared and maximum efficiency of 8.73%, open circuit voltage of 743 mV, short circuit photocurrent density of 16.35 mA/cm2, and fill factor of 0.72 was recorded for the cell made of photoelectrode with cubic morphology. It should be noted that, for characterization of the films TEM, SEM, XRD, BET, Ellipsometry and UV-vis techniques and for characterization of the prepared solar cells I-V measurement, IPCE and electrochemical impedance were used.

Keywords: Dye-sensitized solar cells, Nonorganized porous nanostructures, Templated mesoporous, Evaporation-induced self-assembly.

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Synthesis of $Ni_{0.5}Zn_{0.5}Fe_2O_4/ZnO$ composite as a magnetically separable photocatalyst for removal of dye pollutant in aqueous solution

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The removal of dye pollutants in waste water *via* adsorption and photocatalytic destruction is most popular method. Until now, efforts have been made to develop efficient magnetically separable photocatalyst. Ferrites as a stable spinel-type material, has potential applications in field of gas sensors, biomedicine, pigments and photocatalyst. In recent years, ferrites as a magnetically photocatalyst for pollutant removal has received increasing attention [1-3]. In this work the $Ni_{0.5}Zn_{0.5}Fe_2O_4/ZnO$ composite as an efficient magnetically separable photocatalyst were synthesized. The prepared samples were characterized by X-ray diffraction (XRD), fourier transform infrared (FT-IR) spectroscopy, field emission scanning electron microscopy (FE-SEM) and energy dispersive X-ray analysis (EDX). The adsorption and photocatalytic efficiency of the sample for removal of methylene blue, congo red, methyle orange dyes and two dye mixture- methylen blue and methyl orange in aqueous solutions were examined. The results indicated that the $Ni_{0.5}Zn_{0.5}Fe_2O_4/ZnO$ sample is a promising candidate for effective photodecolorization of dyes in aqueous solution. For the $Ni_{0.5}Zn_{0.5}Fe_2O_4/ZnO$ show high removal capacity for the congo red *via* adsorption. Morever results indicated that 31% and 85% of two dye mixture- methylen blue and methyl orange in aqueous solutions were removed *via* photocatalytic decolorization after 180 min respectively. The prepared sample demonstrated the good removal ability after five repeated utilizations.

Keywords: Magnetically separable, Photocatalyst, Adsorption, Dye removal, $Ni_{0.5}Zn_{0.5}Fe_2O_4/ZnO$

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Synthesis and characterization of a new vanadium containing polyoxomolybdate as an efficient heterogeneous sulfoxidation catalyst

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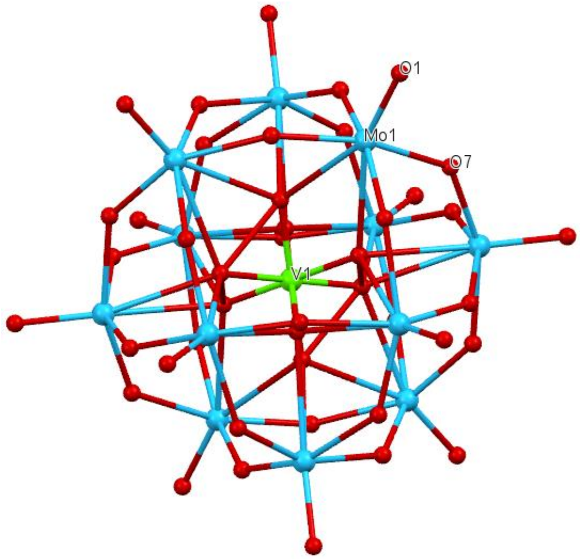
Metal–oxygen clusters, namely polyoxometalates (POMs), are anionic clusters of oxygen-bridged early transition metal cations in their highest oxidation states (configuration d^0 or d^1) with (heteropolyoxometalates) or without (isopolyoxometalates) heteroatoms (such as B, Al, Ge, Si, P and many more) [1-2]. Tetraethylammonium salt of a new Keggin-type 12-molybdovanadate nanocluster, $[(C_2H_5)_4N]_4[VMo_{12}O_{40}]$ (**1**) was synthesized via reaction between sodium tungstate, ammonium vanadate and tetraethylammonium bromide in acidic medium. Compound **1** was characterized by X-ray crystallography and FT-IR and then applied as an efficient heterogeneous catalyst to oxidation of various organosulfides to sulfoxides with H_2O_2 at room temperature with 81–100% conversion and 60–99% selectivity. Nanocluster **1** was also shown to display excellent recyclability – it can be reused more than 10 times.



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Keywords: 12-molybdovanadate, Nanocluster, Sulfoxidation

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Synthesis of highly porous alumina mediated by CTAB and its use as a Carrier for Designing sustained Release of Mefenamic Acid

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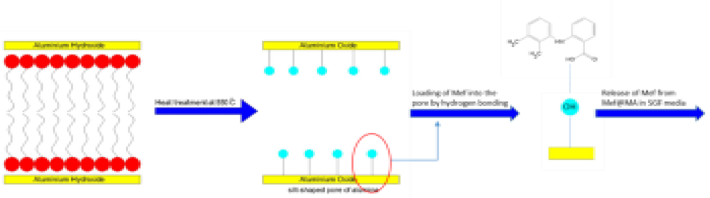
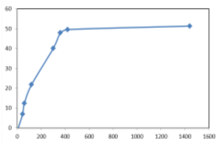
Lately, synthesis of mesoporous alumina with appropriate textural properties such as high surface area, large pore volume and narrow pore size distribution has been the subject of academic and industrial research[1]. In current study, mesoporous alumina (MA) was successfully synthesizedvia Sol-Gel-EISA combination method (SG-EISA). Aluminum isopropoxide and CTAB were used as aluminum source and structure directing agent (SDA) respectively. The synthesized MA was characterized using FT-IR, XRD, FE-SEM and N_2physiosorption. N_2 adsorption-desorption results showed that mesoporous alumina with high surface area (402 m^2/g), narrow pore size distribution centered at 3.53 nm and largest pore volume among the CTAB-assisted aluminas[3,4] (1.71 cm^3/g) was obtained. The drug loading efficiency of the low density alumina was investigated using mefenamic acid (Mef) as a model drug to evaluate its potential as a carrier system. Mef was loaded into the pores of MA with the ratio of 1:3 (Mef@MA). According to the result of FT-IR, XRD, BET and BJH methods, it can be concluded that the drug is well-dispersed into the slit-shaped pores of MA. The *in-vitro* release of mef from mef@MA was examined in simulated gastric fluid (SGF) during 24 hours via UV analysis. It was observed that about 13% of mef was released from carrier in the initial sixty minutes and this value reached to about 50% after passing 24 hours. It can be emphasized that MA can be used for design of sustained release preparation of Mef.





Keywords: Low density, Mesoporous alumina, SG-EISA, CTAB, Sustained release

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Tuning the acidity of H-ZSM-5 zeolite with boron

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Acidity is very important factor for performance of H-ZSM-5 zeolite. Modification with varieties of elements is one of simple methods for tuning the acidity of this zeolite [1]. Boron with three valence can substitute with framework aluminums and increases weak acid sites. Therefore, zeolites are prepared via hydrothermal method and boron incorporation. These zeolites characterized with XRD, FE-SEM, BET, FTIR and NH_3-TPD techniques. The catalytic performance of the zeolites can be studied in the MTP reaction.

NH_3-TPD profiles of zeolites exhibit a low temperature peak at 100-250 ºC (weak acid sites) and a high temperature peak at 300-450 ºC (strong acid sites). The peak positions for both strong and weak acidity only slightly shift after boron incorporation, indicating the acid strength maintains. For H-[Al-B]-ZSM-5 samples the intensity of low temperature peak is higher and high temperature peak almost is constant. Consequencely, density of weak acid sites increase with adding boron. These results emphasize the effective interaction of boron atoms with the zeolite framework.

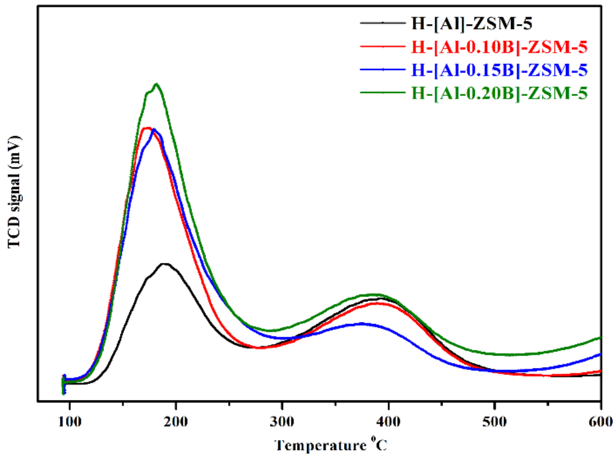

Fig. 1. NH_3-TPD profiles of zeolites

Keywords: ZSM-5, Boron, Incorporation

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Seed-induced method for synthesis of Nano-sized ZSM-5 zeolite

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ZSM-5 is a medium pore zeolite having a 10-membered ring structure with two types of channels, straight and zigzag. It has attracted considerable attention in area of catalysis, due to its unique channel structure, thermal stability, and acidity. Seed-induced crystallization is a method for synthesis of nanocrystals in zeolites. The ZSM-5 zeolite with nanocrystals was synthesis with seed-induced method and characterized with XRD, FE-SEM, BET, FTIR and NH_3-TPD techniques. The catalytic performance of the zeolites can be studied in the MTP reaction.

The FE-SEM results indicate reduction in crystal size from microstructure to nanostructure in the ZSM-5 zeolite synthesized with seed-induced method. The external surface area provide by the seeds play a vital role in accelerating the nucleation rate by offering specific sites for the formation of nuclei. Decreasing crystal sizes can decrease the diffusion path length and increase the external surface area. Therefore, catalytic stability increases [1].

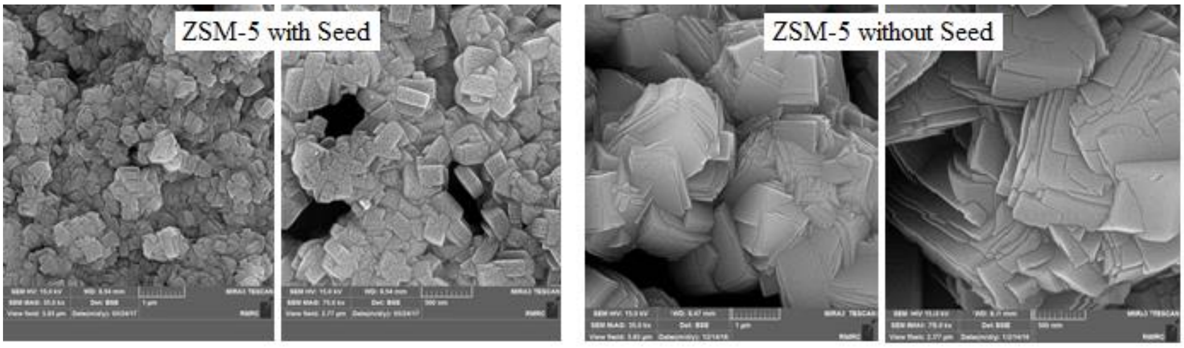

Fig. 1. FE-SEM images of ZSM-5 zeolites synthesized with/without Seed

Keywords: ZSM-5, Seed, Nanocrystal

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Phosphonate Calix[4]arene as a new ligand for selective recognition of Pd^{2+} and Ni^{2+} in aqueous media

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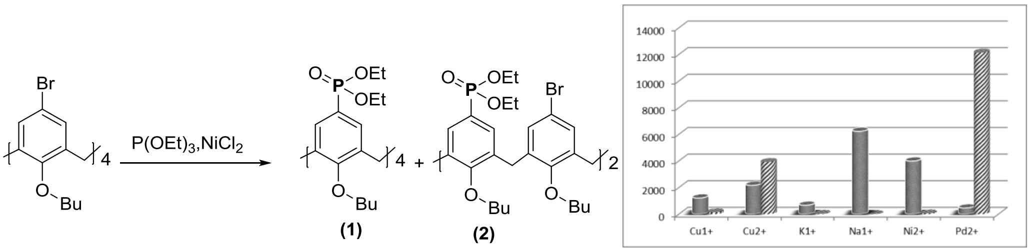
Therefore the separation of Pd^{2+} from Ni^{2+} is one of the most important topics in the automobile catalytic converter industry and medicinal chemistry.

In this work, two novel receptors based on Calix[4]arene bearing Phosphonate groups (**1** and **2**) were synthesized, and their structures were characterized by HRMS, NMR and FTIR. Furthermore, their binding properties towards various biologically relevant metal ions were studied by UV-Vis spectrophotometric technique [1,2]. The receptor **1** displayed excellent binding affinity and selectivity toward Pd^{2+}, which was characterized using UV-Vis spectroscopy. On the other hand, **2** exhibited very remarkable UV-Vis changes, in presence of Ni^{2+} ions. Finally, Job's plot method revealed 1:1 binding stoichiometry for both **1**: Pd^{2+} complex and **2**: Ni^{2+} complex [3,4].



Scheme1: left: Synthetic route of **1** and **2;** right**:** Comparison of binding constant (K_a) between **1** or **2** and different metal ions.

Keywords: Phosphonate Calix[4]arene, UV-Vis Spectroscopy, Palladium, Nickel, Titration

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Co-Precipitation method for synthesis of Fe-Ni oxide Nanoparticles supported by Nano Alumina and Investigation of the Calcination conditions on their Structures

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In this study, Nano particles Fe-Ni oxide was synthesized with Co-precipitation method. The nanoparticles synthesis in various time and different temperatures of calcination conditions. The synthesized particles were characterized by X-ray Diffraction (XRD), Field Emission Scanning Electron Spectroscopy (FESEM), Energy-dispersive X-ray Spectroscopy (EDS). According to the XRD pattern, products were crystallized and structure was cubic. The crystal size ranged from 10-30 nm. Because of the obtained Fe_3O_4, NiO and $NiFe_2O_4$ compounds and the smaller particles the best time and temperature of calcination was 6 hours and $550C^0$.

Keywords: Co-precipitation; Calcination; Alumina; Fe-Ni Nanoparticles

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Study of structural and catalytic properties of Co-Zn catalyst prepared from inorganic complex precursor for Fischer-Tropsch synthesis

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In recent years, the Fischere Tropsch synthesis (FTS) has received considerable attention from academic institutions and governments alike, due to environmental contamination, rapidly rising price of crude oil and subtractive oil reserves [1-3]. The FTS is a viable route for the production of clean fuels from biomass-derived syngas, natural gas, or coal. In this process, highly important factor is a catalyst, which is selected based on the key role in product distribution [4,5]. The Co-Zn/TiO_2 catalyst synthesized by thermal decomposition of inorganic precursor was evaluated for Fischer–Tropsch synthesis (FTS); the structural properties and performance of the catalyst was compared to those of sample constructed via impregnation method. The results revealed that the synthesized catalyst have higher catalytic activity comparison to it prepared via the conventional impregnation method. The effect of the preparation method on the structural properties shows that synthesizing the catalyst through inorganic precursor route is more appropriate. The SEM micrographs of samples display that synthesized catalyst have lower particle sizes and agglomeration in comparison with reference catalyst. These results are in good agreement with the BET outcomes; it means that the catalyst prepared by thermal decomposition of inorganic precursor have higher surface area than reference catalyst. Activity of the catalyst in FTS was investigated at 280-400°C with H_2/CO ratio of 2 and specified that the fabricated catalysts are more active than impregnation reference sample. Furthermore, it can be concluded that preparing catalyst by inorganic precursor is more suitable procedure toward impregnation method. Characterization of catalysts is carried out using powder X-ray diffraction (XRD), scanning electron microscopy (SEM), and BET specific surface area.

Keywords: Fischer–Tropsch synthesis, Inorganic precursor, Impregnation.

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Cyclometalated platinum(II) complexes comprising O,S-heterocyclic ligand: searching for anticancer drugs

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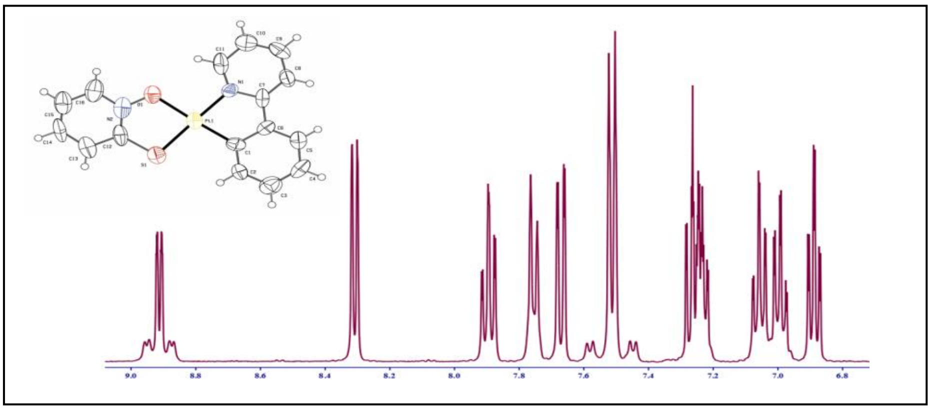
Cancer remains a leading cause of death worldwide. Conventional cancer therapies, while highly efficacious, are generally non-specific for cancer cells over healthy cells resulting in dose-limiting toxic side effects. Drug resistance is also a major drawback associated with many therapies. Of the chemotherapeutics in clinical use, platinum drugs, namely cisplatin, carboplatin and oxaliplatin, are amongst the most widely employed [1]. Pt drugs exert their cytotoxic effect by binding irreversibly to DNA nucleobases leading ultimately to induction of apoptosis [1]. In this direction, Cyclometalated platinum(II) complexes have shown very promising results for the development of anticancer drugs and several of them have been successfully considered as drug candidates with higher activities than that of *cis*-platin [2]. In this work, we describe the synthesis, characterization, reactivity and stability of related cyclometalated platinum(II) complexes containing the aromatic amine N-oxide, pyridine-2-thiol-1-oxide. We also report their cytotoxic activities against various cancer cell lines together with preliminary biological studies.



Keywords: Pyridine-2-thiol-1-oxide ligand, Cyclometalated platinum(II) complexes, Biological study.

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Synthesis of ZnO incorporated magnetically recoverable KIT-6: Efficient catalyst in the preparation of 2-aminothiophenes

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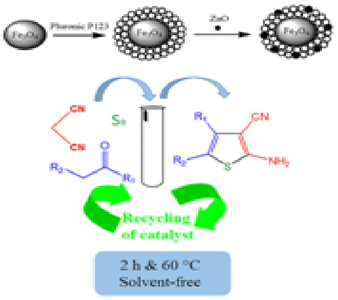
In recent years, mesoporous silica modified with transition metal oxides has received considerable attention as suitable catalyst and photocatalyst for a variety of organic reactions [1]. Kit-6 is one of the most prominent examples of ordered mesoporous silica; KIT-6 exhibits a three-dimensional cubic Ia3d symmetric structure with an interpenetrating bi-continuous network of channels [2]. Up to now, several papers are reported on the use of modified KIT-6 as catalysts for the synthesis of different organic compounds [3]. In this work, a magnetically recoverable nanocomposite (Fe_3O_4@KIT-6) was prepared by utilization of chemically synthesized magnetite nanoparticles (Fe_3O_4) as a core and mesoporous silica (KIT-6) as a shell. Then zinc oxide modified magnetically recoverable nanocomposite (Fe_3O_4@KIT-6@ZnO) was prepared by a conventional wet impregnation method and was used an efficient heterogeneous nanocatalyst in the synthesis of 2-aminotiophene derivatives by Gewald reaction. The synthesized nanocomposite was characterized by XRD, FT-IR, ICP, FESEM, VSM, and nitrogen adsorption/desorption isotherm. Moreover, the prepared nanocomposite showed very high activity and reusability in the synthesis of 2-aminotiophenes under solvent free conditions.



Keywords: Nanocomposite, KIT-6, Mesoporous silica, Magnetite nanoparticles, 2-aminothiophenes.

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Synthesis, Characterization, Crystal Structure, Thermal Property and Anti-Fungal Activity of Zn(II) Complex of 4′-Hydroxy- 2,2′:6′,2″-Terpyridine

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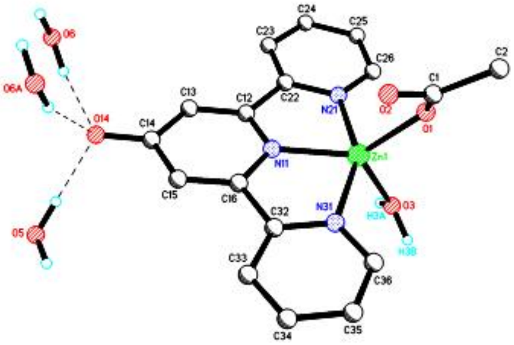
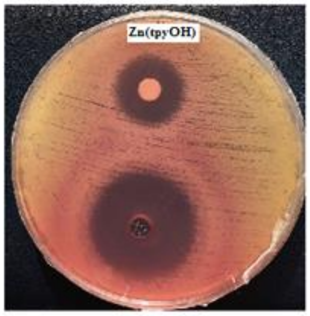
2,2′:6′,2″-terpyridine (tpy) and its derivatives are versatile building blocks for the synthesis of supramolecular structures [1]. 4′-hydroxy-2,2′:6′,2″-terpyridine (tpyOH) is well studied among terpyridine derivatives since the hydroxy moiety in this fragment can act as a potential hydrogen bond donor. The terpyridine complexes of transition metals also have antiproliferative agents which make them attractive as the chemotherapeutic agents for cancer and infectious diseases [2]. The reaction of tpyOH with zinc(II) acetate resulted in the formation of the new complex of [Zn(tpyO)(CH_3COO)(H_2O)]. The Zn^{2+} is penta-coordinated by three nitrogen atoms of tpyOH, an acetate ion, and a water molecule in the form of distorted square pyramid [ZnN_3O_2]. According to potential pharmacophores of 2,2′:6′,2″-terpyridine agents, the anti-fungal activities of product was also tested *in vitro* for their growth inhibitory activities against Candida-albicans pathogenic fungus.





Keywords: Terpyridine, Zinc, Hydrogen bonding, Thermal analysis, Anti-fungal

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Enhancement of dye sensitized solar cells using plasmonic nanoparticles

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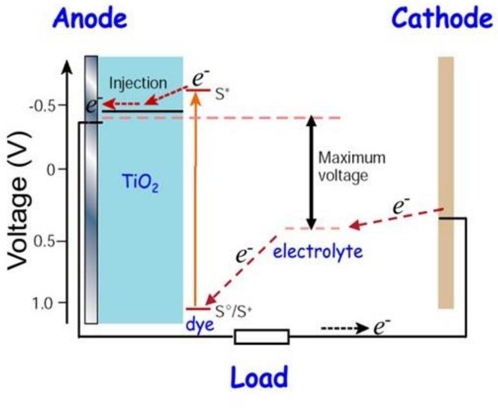
Parallel to present p-n junction solar cells, dye-sensitized solar (DSS) cells provide a technically and economically reliable alternative source of clean and cheap energy. In a DSS cell, light is absorbed by a synthetic or a natural sensitizer. The sensitizer is anchored to the surface of a wide band semiconductor such as titanium dioxide [1]. After charge separation, which occurs via photo-induced electron injection from the dye into the conduction band of the solid, carriers are transported in the conduction band of the semiconductor to the charge collector. DSS cells have upsides and downsides. A great feature of a DSS cell is its near 100 percent conversion of incident photon into electric current from UV to the near IR region of the electromagnetic radiation. Despite great achievements during past 30 years, there is still a lot of room for the improvement of this generation of photovoltaic devices. For example, these cells are not stable and also their outdoor overall efficiency is still lower than that of commercial amorphous silicon based solar cells. Herein, we report re-construction of a photovoltaic cell based on titanium dioxide nanoparticles and a ruthenium dye. In order to improve the efficiency of these cells, we have implemented surface plasmons of gold nanoparticles. Collective motions of surface electrons in a plasmonic metal nanoparticle, can in theory be excited and the generated electric currents directed toward a fluorophore. Initial results from our experiments regarding this phenomenon will also be presented.



Keywords: p-n junction, Dye sensitized cell, Photovoltaic, Plasmon

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Magnetic Nanoparticles Modified with Novel Ferrocene-Triazine Schiff-base; An Adsorbent for Dye Removal from Aqueous Solution

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A new Schiff-base based on ferrocenyltriazine (fts) has been synthesized and fully characterized by different techniques. The electrochemical study of the fts compound exhibit redox behavior which is responsible for different reactions. The recoverable covalently attached fts on Fe_3O_4 nanomagnetite (Fe_3O_4@fts) was also prepared by silanation method and its morphology and structure were explored using X-ray powder diffraction (XRD), N_2 adsorption-desorption isotherm, BET, FT-IR, EDS, SEM and vibrating sample magnetometry (VSM). In addition, dye adsorption activity of the prepared Fe_3O_4@fts was evaluated for methyl orange (MO) removal from aqueous solution. The effect of operational parameters (pH, initial dye concentration, adsorbent dosage and oxidant) on dye removal was also investigated. The prepared Fe_3O_4@fts exhibited an excellent adsorption capability of 90% in acidic medium; which reached to 100% in shorter time, in the presence of an oxidant. In order to study different light wavelengths on MO adsorption, all the experiments were repeated in darkness, under UV as well as visible light. No remarkable change in removal efficiency was observed indicating that light irradiation has almost no effect on adsorption efficiency of Fe_3O_4@fts.

Keywords: Ferrocene Schiff base, Nanomagnetite, Surface modification, Dye removal

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

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During the past decade, a great deal of attention has been paid to developing greener chemical processes and synthetic methods [1]. Catalysts bound to inorganic solids are widely used for organic transformations due to environmental and economical considerations [2]. Nanoparticles supported on a metal oxide as an inorganic solid, in particular magnetic nanoparticles (MNPs), have been extensively studied in the field of chemical catalysis, environmental protection, sensors, magnetic storage media, and clinical diagnosis treatments [3]. MNPs have great potential in view of the their recovery, since the magnetic separation of MNPs from the reaction mixture with an external magnet is simpler and more efficient than conventional separation with filtration or centrifugation. On the other hand, MNPs are accessible from inexpensive materials and can be easily supported by organic and inorganic materials [4]. Recently, MNP-supported-copper ions have been used extensively in organic transformations.[5].

In this work, a new magnetically recoverable nanocatalyst was developed by covalent binding of a ligand, 2-amino banzhydrazide and 2-hydroxy naphtaldehyde on the surface of silica coated magnetite nanoparticles (SCMNPs) and followed complexation with $CuCl_2.4H_2O$. Characterization of the prepared nanocatalyst was performed with different physicochemical methods such as FT-IR, TCP-AES, VSM, SEM EDS and TGA analyses. Finally, catalytic activity of the prepared nanocatalyst was examined in the preparation of 2-amino-4*H*-benzo[*h*]chromene derivetives through a one-pot, three component reactions of 1-naphthol, various aldehydes and malononitrile.

Keywords: Heterogeneous catalysts, Magnetic nanoparticles, Three component reactions

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Preparation of two different FCC catalyst binders and their influence on catalyst size and morphology

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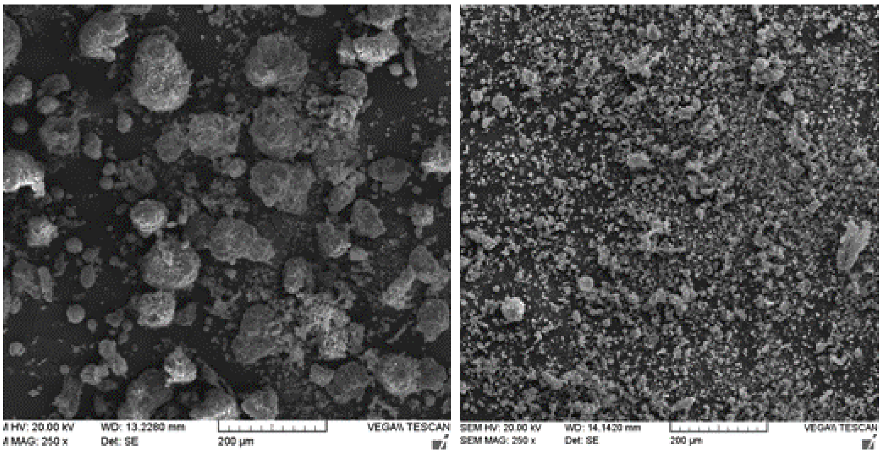
Fluid catalytic cracking (FCC) is one of the major conversion technologies in the oil refinery industry and produces the majority of the world's gasoline [1]. It uses heat and catalyst to convert a variety of high molecular weight feed types such as gas oils into lighter and more valuable products such as gasoline and petrochemical feedstocks including ethylene and propylene. Catalysts are the heart of the fluid catalytic cracking process and transfers heat between the regenerator and riser [2]. The main parts of a FCC catalyst are zeolite, matrix, binder and filler. Filler and binder are key factors in preparation of a FCC catalyst with proper attrition resistance, size and morphology. Binder is usually inactive material such as alumina or silica [3]. It acts as ''glue'' that holds all catalyst components together and provides particle physical integrity. In the present study, two kinds of binders including silica sol and alumina-silica sol were prepared using aluminum sulfate and sodium silicate along with an acid as peptizing agent. The prepared binders were utilized to prepare FCC catalyst by mixing with other catalyst components comprising zeolite Y, kaolin and alumina. The scanning electron microscopy images of two catalysts showed that binder have significant influence on morphology and structure of the FCC catalyst.



Keywords: Fluid catalytic cracking, Catalyst, FCC, Binder, Silica sol, Alumina-silica sol

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Dioxo-molybdenum Schiff base complex immobilized on surface modified magnetite as a nanocatalyst for the oxidation of organic compound

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Nanoscale materials have been a subject of particular interest due to properties, which differ from their bulk counterparts [1]. They have been used extensively in chemistry [2], physics [3], biology and catalysis [4]. Recently, magnetic core–shell nano-structures have attracted more attention due to their unique magnetic properties. In contrast to the difficulty observed in recovering and reusing most solid catalysts, core–shell nanostructure magnetic catalysts can be easily retrieved under the influence of a magnetic field and used in subsequent reactions. Due to this property, using magnetic core–shell structure composites as catalysts has been recommended in literature. Schiff base transition metal complexes have been extensively studied because of their potential use as catalysts in a wide range of reactions. These complexes have been extensively used for hydrogenation of organic substrates, epoxidation of olefins, conversion of epoxides into halohydrines, asymmetric ring opening of terminal epoxides and oxidation reactions [5].

In this work, a new magnetically recoverable nanocatalyst was developed by covalent binding of a ligand, 2-amino banzhydrazide and 2-hydroxy naphtaldehyde on the surface of silica coated magnetite nanoparticles (SCMNPs) and followed complexation with $MoO_2(acac)_2$. Characterization of the prepared nanocatalyst was performed with different physicochemical methods such as FT-IR,TCP-AES, VSM, SEM, EDS and TGA analysies. Finally, catalytic activity of the prepared complexes was examined in the oxidation of sulfids and epoxidation of olefins.

Keywords: Nanoscale ,materials Schiff base , Nanocatalyst.

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Synthesis, characterization and biological evaluation of some mono and bis-acephate derivatives.

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In this work, mono and bis-acephate derivatives we synthesized (as shown in the figure 1) and characterized by ^{31}P, ^{13}C, ^{1}H NMR and IR spectroscopy. The biological inhibitory of acephate derivatives were evaluated using the modified UV/Visible absorption, fluorescence spectral data on human acetylecholinesterase (AChE) and urease enzymes. In this study, quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR) by means of multiple linear regressions (MLR), principal component analysis (PCA) and genetic algorithm (GA) were performed to investigate the relationship between acephate derivatives and their bioactivities against AChE and urease.

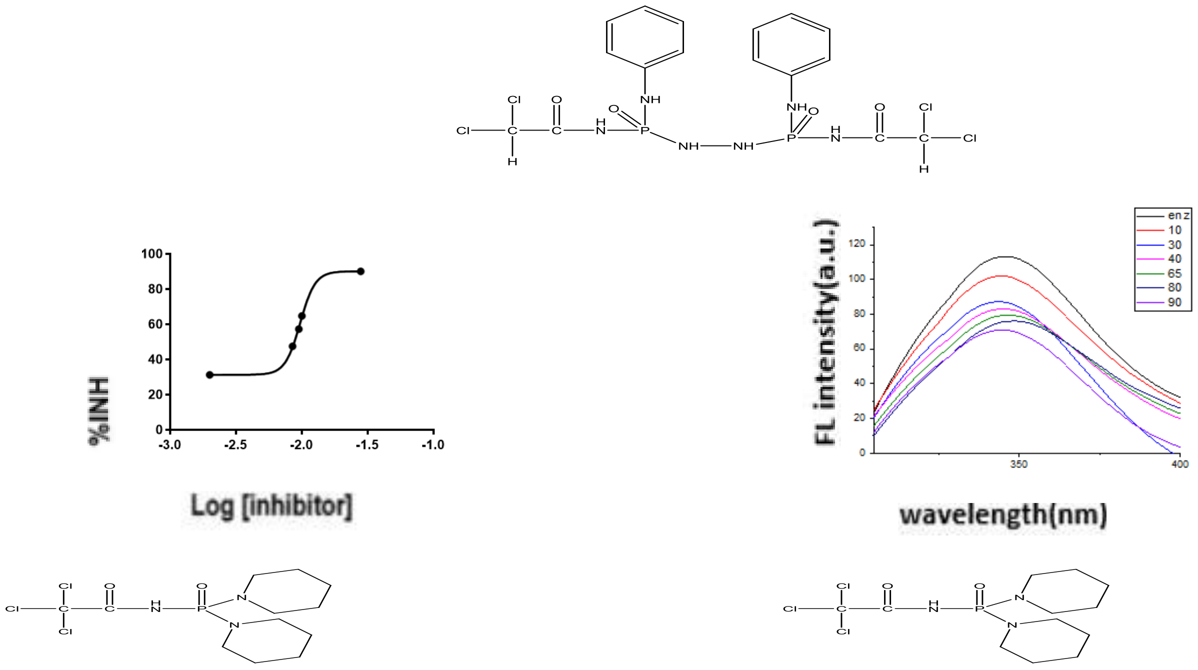

Figure 1

Keywords: Acephate,spectroscopy, Biological

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The Investigation of the Reactivity of a Platinum Complex Precursor with a Borate Based Ligand

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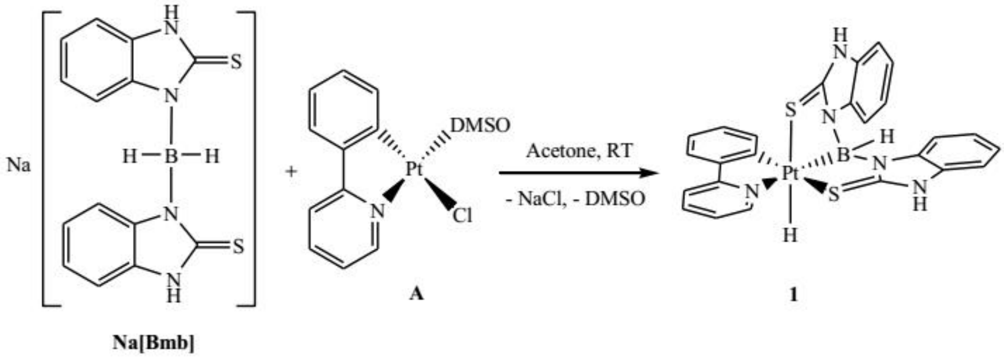
Trofimenko’s poly(pyrazolyl)borates recognized as "Scorpionate ligands" have undergone numerous modifications since their discovery decades ago [1]. Notable among these changes have been the addition of an extra atom or atoms between boron bridgehead and scorpionate's donor atom as well as changes in the nature of the donor atom such as the use of softer sulfur or phosphorous electron donors in place of nitrogen. These structural alterations have introduced more flexible scorpionates, thus allowing closer proximity of B–H or BH_2 units of the scorpionate ligand to the metal center with an increased likelihood of an intramolecular metal–boron interaction [2]. Recently, we discovered the unexpected and facile formation of a platinum hydride complex {[(κ^3-S,B,S-HB(mb)$_2$]Pt(ppy)H}, **1**, ppy = 2-phenylpyridine and mb = 2-mercapto-benzimidazole, from the acetone mediated reaction of [Pt(ppy)(DMSO)Cl], **A**, with sodium dihydrobis(2-mercapto-benzimidazolyl)borate Na[H_2B(mb)$_2$]. The aerobic hydrolysis of complex **1** led to the formation of a dimeric half-lantern platinum(II,II) complex [{Pt(ppy)(μ_2-mb)}$_2$], with simultaneous release of 2-mercaptobenzimidazole boronic acid.



Keywords: Hydride complex; Platinum; Borate ligand; Structural analysis; Metallaboratrane.

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Coordination chemistry of some new Ni(II), Cu(II) and Co(II) macroacyclic Schiff base complexes; Synthesis, Characterization and theoretical studies

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The research field dealing with Schiff base metal complexes is very broad due in part to their potential interest for a number of interdisciplinary areas that include bioinorganic chemistry, catalysis, and magnetochemistry[1-3]. These complexes were prepared by reaction of two N_2O_4 Schiff base ligands, H_2L^1 and H_2L^2 and Cu (II), Ni(II) and Co(II) metal ions (Fig. 1). Computational calculations of relevant complexes are done by using one of the hybrid density functional theories which is B3LYP method with 6-31G(d) basis set in vacuum. NLO properties of $[M(H_2L^1)]^{2+}$ and $[M(H_2L^2)]^{2+}$ type complexes are predicted by using some quantum chemical descriptors which are total static dipole moment (μ), the average linear polarizability (α), the anisotropy of polarizability (Δα), the first hyper polarizability (β), energy of HOMO (E_{HOMO}), energy of LUMO (E_{LUMO}) and energy gap between LUMO and HOMO (E_{GAP}). According to these rankings, Co(II) complexes are is the best candidate for NLO properties in each type complexes.

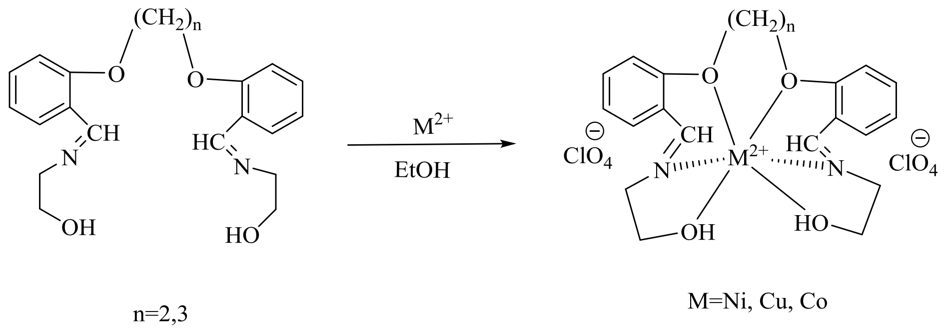

Fig. 1

Keywords: Schiff base ligands, Macroacyclic complexes, NLO properties, Theoretical studies.

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A novel Graphene/polyoxometalate Nanocomposites as an efficient and eco-friendly catalyst for the one-pot synthesis of 3,4-dihydropyrimidin-2(1H)-ones

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Catalytic reaction by polyoxometallates is an expanding field of active research being perused world wide. Due to the super acidic properties of solid heteropolyacids (HPAs), they have found numerous applications as useful and versatile acid catalysts under homogeneous as well as heterogeneous conditions for some acid-catalyzed reactions, for example biginelli reaction for synthesis of 3,4 -dihydropyrimidin-2(1H)-ones(DHPMs). DHPMs and their synthetic analogues are of considerable importance because of their promising biological activities such as antibacterial, antiviral, anti-inflammatory and antitumor. In this research descibed Keggin-type phosphotungstic acid on modified graphene substra was synthesised as an active acidic heterogeneous catalyst for three component Biginelli condensation reaction, Between aryl aldehyde, b-diketones compound and urea or thiourea to afford the coresponding 3,4-dihydropyrimidin-2(1H)-ones with excellent yields and high purity.The synthesized catalyst was characterized by employing various spectroscopic techniques as well as different analytical methods,such as X-ray diffraction (XRD) powder patterns of the synthesized catalyst was recorded on a X-ray diffractometer Morphology has been studied by scanning electron microscope (SEM), and FTIR spectra recorded and studied. The product obtained from multicomponent reaction characterized by FTIR, ^{1}H NMR and ^{13}C NMR spectroscopic data and its melting point is compared with reported values. Moreover, the catalyst could easily be recovered and recycled without any significant loss of its catalytic activity.

Keywords: Polyoxometalate, Multicomponent reaction (MRCs), Graphene, 3, 4-Dihydropyrimidin-2(1H)-ones, Characterization, Heterogeneous catalyst

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Manganese porphyrin immobilized on Fe_3O_4@MCM-41 as efficient and selective catalyst for oxidation of alkenes with $NaIO_4$

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The oxidation of olefins is one of the most important and attractive process in chemistry, since epoxides are valuable intermediates in both biological and industrial systems [1]. Synthetic metalloporphyrins, as models for cytochrome P-450 monooxygenation enzyme, in presence of single oxygen donors such as PhIO, H_2O_2, ROOH and IO_4^- have been found as catalysts for homogeneous selective oxidation of organic compounds [2]. Despite high yields obtained with metalloporphyrins, deactivation due to the formation of inactive dimeric μ–oxo species in reaction media and non-recovery are two serious problems of these expensive catalysts [3]. One strategy to overcome these problems is immobilization on a solid matrix. During the past two decades, the manganese porphyrins supported on inorganic and organic materials have been extensively studied for their ability in oxidation reactions. Over the last two decades, several manganese porphyrins have been successfully immobilized on MCM-41 and studied for catalytic performance in organic reactions [4]. Fe_3O_4 magnetite nanoparticles have been investigated due to easy functionalized and superparamagnetic properties. In this work, magnetic nanoparticles of Fe_3O_4 was prepared. Fe_3O_4@MCM-41 was synthesized and functionalized with imidazole. The inorganic-organic hybrid materials were used for immobilization of manganese porphyrin. The synthesized Fe_3O_4@MCM-41@MnTPPCl catalyst was characterized by FT-IR, ICP, XRD, SEM, TG, BET and DRUV-Vis analysis. Effect of various parameters such as solvent, oxidant and the amounts of catalyst on oxidation of cycloocten was investigated. The result showed that the manganese porphyrin on functionalized magnetic nanoparticles is an efficient and reusable catalyst for oxidation of olefins.

Keywords: Epoxidation, Heterogeneous catalyst, Manganese porphyrin, Magnetic nanoparticles, $NaIO_4$

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Synthesis and Study of Metal-Organic-Framework Uio-66-NH_2 as a Drug Delivery

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Metal-organic frameworks (MOFs) are crystalline materials constructed from metal ions or clusters and organic ligands bridging between metal centers to form one-, two-, or three dimensional structures[1]. What makes MOF materials outstanding are their exceptionally large surface areas and excessively high porosities which were attributed to the absence of dead volume in the structure. These characteristics have placed them in the realm of materials with diverse applications such as stationary phase in chromatography, as bioreactor for trypsin immobilization, as sensor, as gas storage, as catalyst, etc. Moreover, MOFs emerging potential in the field of biomedicine include storage, delivery of gasotransmitter gases. Drug delivery is becoming an extremely demanding science.Over the past few decades, drug delivery systems (DDS) have been developed as the most advancing area of science[2].

In the present study, MOF [Uio-66-NH_2] was synthesized and characterized by IR spectroscopy and x-ray powder diffraction (XRD), then ibuprofen, etc was loaded in synthesized MOF and drug release in PBS buffer was measured at 37 ^{0}C.

Keywords: Drug Delivery, Uio-66-NH_2, Metal Organic Framework

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Mechanosynthesis of azine-functionalized Zn(II) metal–organic frameworks for improved drug delivery

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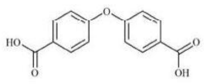
We have witnessed a rapid growth in the field of a new nanoporous material group, metal organic frameworks (MOFs), over the past decade. MOFs possess a wide array of potential applications in chemical engineering, chemistry, and materials science, including gas storage, gas separation, and catalysis[1,2]. One of the areas MOFs started to appear recently is biomedical applications. The unique physical and chemical characteristics of MOFs make them promising candidates for drug storage and drug delivery, nitric oxide storage and delivery, imaging, and sensing[3,4]. In this work, Three 3D, porous Zn(II)-based metal–organic frameworks, TMU-4**,** TMU-5 and TMU-6, containing azine-functionalized pores, were synthesized as potential drug carriers to evaluate the effect of pore size and functional group on the amount of drug loading in a MOF. An anti-cancer drug is used for colon cancer, esophageal cancer, stomach cancer, pancreatic cancer, breast cancer, and cervical cancer, Fluorouracil (5-FU), was laden into pores of the three structures**.** These MOFs respectively could adsorb up to 1.56 g, 2.1 g and 7.5 g of 5-FU per gram of composites. The results showed that pore size has a special effect on the amount of drug loading.



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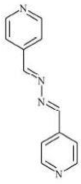
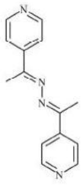
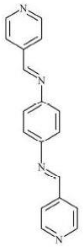


4-bpdb



4-bpdh



4-bpmb

Keywords: Metal organic frameworks (MOFs), Drug delivery, Fluorouracil (5-FU).

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Adsorption of H_2 molecules on vanadium oxide nanotube

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In this research, vanadium oxide nanotube (VONT) was considered as an absorbent in hydrogen storage system. Monte Carlo simulation was applied to investigate adsorption behavior of hydrogen in VONT[1,2]. All calculations were performed at experimental pressures of H_2 in the range of 0.5-70 MPa and temperatures of 250, 275 and 300 K. The effects of temperature and pressure on the adsorption capacity of VONT were also studied. Over investigated temperatures and pressures, the maximum gravimetric adsorption was occurred at 250 K and 50MPa.

Keywords: Monte Carlo simulation, Vanadium oxide nanotube, Adsorption, Hydrogen

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Synthesis and characterization of Zr doped vanadium oxide nanotubes

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Vanadium oxide nanotubes (VONTs) have recently attracted attention because they offer a large active surface area and numerous channels for ionic transport owing to their multiwall tubular structures. The ends of these nanotubes are open. So, different cations can be introduced into the inner cavity of the nanotubes[1]. In this research, for the first time, zirconium doped vanadium oxide nanotubes were synthesized. Zr is widely in biomedical applications as orthopedic, and dental implant materials but pur zr metal cannot bond directly with bone [2,3]. The obtained results showed that Zr doping level was 2 wt %. The samples were found to have a tubular morphology. XRD patterns of the samples indicated that the interlayer distances of the Zr doped nanotubes are more than that of VONTs.

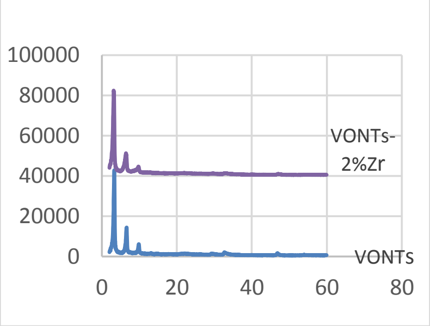

Figure1: XRD patterns of VONTs ,VONTs-2%Zr

Keywords: Vanadium oxide nanotubes, X-ray diffraction

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Copper(II) complexes containing hemilabile tridentate ligand as Chromotropic probes

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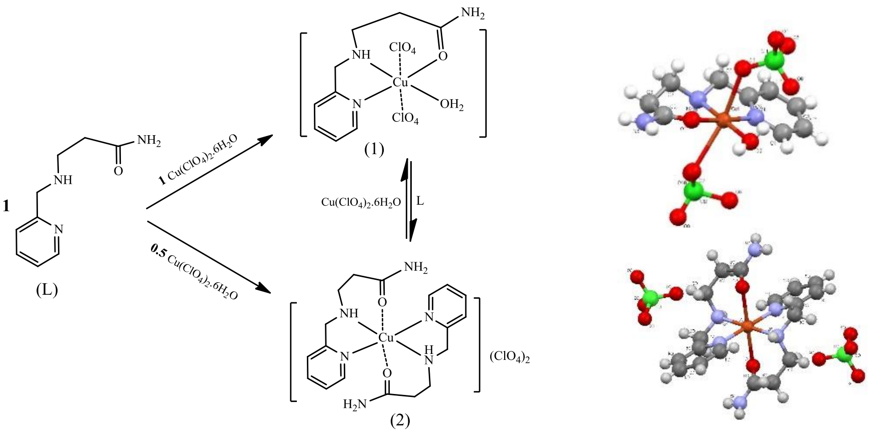
Molecules responding to external motivation have received considerable attention in recent years that are potentially suitable in the preparation of molecular switches [1]. Generally, a molecular switch is based on a molecule, which can reversibly alter distinct states (on and off) given an external motivation (solvent, temperature, pH, metal ions, light and so on). The sum total of the behavior of complexes is called chromotropism [2]. In this work we prepared two copper(II) complexes with the general formula of $[Cu(L)(H_2O)](ClO_4)_2$, **1**, and $[Cu(L)_2](ClO_4)_2$, **2**, where L =3-((pyridin-2-ylmethyl)amino)propanamide were synthesized and characterized by elemental analyses, IR, UV-Vis spectroscopy techniques, molar conductance measurements and X-ray crystal analysis (Scheme 1). The chromotropism (halo-, solvato- and ionochromism) of both complexes were studied using visible absorption spectroscopy. The complexes are found to be soluble in water and organic solvents and displayed reversible halochromism due to the flexible and sensitive nature of the amide group with changing pH values. The solvatochromism property is due to structural change followed by solvation of the vacant sites of the complexes. The complexes demonstrated obvious ionochromism and exhibited high-sensitive and selective towards CN^- and N_3^- anions in presence of other halide and pseudo-halide ions.



Scheme 1. Synthetic outline for preparation of complexes

Keywords: copper (II); Chromotropism; hemilabile ligand; tridentate ligand

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Preparation of mesoporous titania–silica binary metal oxides with crystalline framework in the presence mixed directing agents

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In a new approach, titania–silica binary metal oxide material with a mesostructured feature has been synthesized by one step hydrothermal method using TEOS and (Titanium isopropoxide) TIP as silica and titania source, respectively, as well as nonionic block copolymer P123 ($EO_{20}PO_{70}EO_{20}$) and anionic sodium dodecyl sulfate (SDS) as structure directing agents in acidic condition. Fourier transformed infrared spectroscopy (FT-IR), Wide angle X–ray diffraction (WAXRD), scanning electron microscopy (SEM), BET surface area and BJH pore size distribution have been used to determine the mesostructure properties of the sample. The resultant nanocomposite showed high surface area of 237 m^2/g, pore diameter of 11.4 nm and the pore wall framework with anatase and rutile phases. FT-IR spectra showed the formation of a Ti-O-Si bond at 940 cm^{-1} suggesting that silica was incorporated in to the lattice of titania to form a composite. The results from all the techniques clearly suggested that the binary oxide as-prepared by hydrothermal method will have potential impact on the photocatalyst performance of TiO_2.

Keywords: Titania-silica binary oxide, Mesostructure, Structure directing agents

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Synthesis, X-ray studies and hydrogen bonding analysis in solid state of a new Phosphoramide counter ion

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It is well known that physicochemical properties of compounds (boiling and melting points, density, dipole moment ...) depend on the presence of non-covalent interactions and intermolecular hydrogen bonds [1]. Therefore, the analysis of hydrogen bonds is helpful to rationalize the structural and physicochemical properties of compounds.

In the present study, we report the structure of one new phosphoramidate counter ion. The single crystal X-ray analysis revealed that C_{18} H_{18} N_3 O_4 P_1, consists of discrete $[C_{18}$ H_{18} N_2 O $P]^+$ cation and NO_3^- anion that crystallizes in space group $P\bar{1}$ and crystal system, triclinic with a=9.4935 Å, b=10.4556(4) Å, c= 11.1560(3) Å, α= 63.951(3)°., β= 67.039(3)º, γ= 66.017(3)° (Fig. 1).

The interaction between cation and anion has occurred through hydrogen bonding.The strength of different hydrogen bonds between two counter ion has been widely studied by DFT calculations in the gas phase. We optimized the hydrogen atoms and kept all other atoms invariant in the optimization process. The H-optimized systems include one nitrate anion and one phosphoramide cation which are connected by special intermolecular interactions. The binding energies of these interactions were calculated (M062X/6-311G*) and corrected for the basis set superposition error (BSSE) using by Counterpoise (CP) procedure. Moreover, the main noncovalent intermolecular interactions were studied by Hirshfeld surface analysis and fingerprint plots for the title compound.

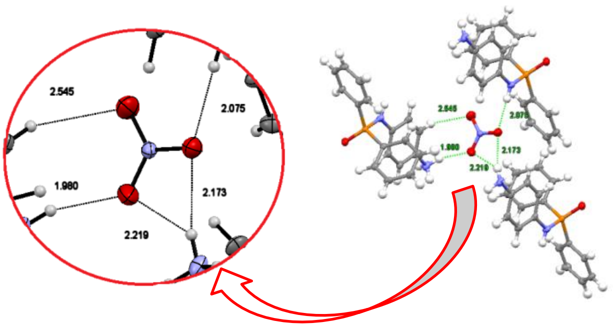

Fig. 1. ORTEP view of the crystal structure and showing the interaction between cation and anion.

Keywords: Phosphoramide, crystal structure, hydrogen bonding.

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New asymmetric azo-azomethine ligand and its Cu^{2+} complex: detection of cyanide ion in aqueous media

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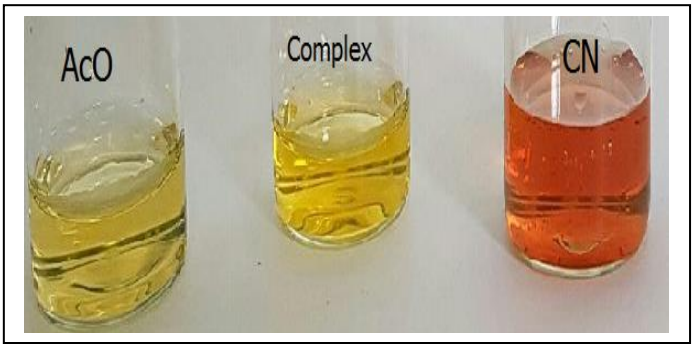
In this communication, new azo-azomethine ligand, H_2L, contains electron withdrawing groups has been design and synthesized. The prepared ligand was characterized using spectroscopic methods (IR, ^1H NMR, UV-Vis) as well as elemental analysis. Cu(II) complex of H_2L was also prepared and characterized spectroscopically. The Cu(II) complex was used as a colorimetric sensor for cyanide in DMSO/H_2O (v/v = 2: 3). An obvious change in color from pale yellow to pale orange that could be detected by naked eye. No significant color change was observed upon the addition of other anions such as F^-, Cl^-, Br^-, N_3^- ،AcO^- and NO_3^-. Job plot data showed that the binding stoichiometries of the Cu(II) complex with CN^- was 1:2. The detection limit of CN^- was also reported.



Keywords: Azo-Azomethine, Sensor, Anion sensing, Aqueous media

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Synthesis, biological evaluation, of novel N-(4-amino carbonylpiperazinyl) (thio)phosphoramide derivatives as cholinesterase inhibitors

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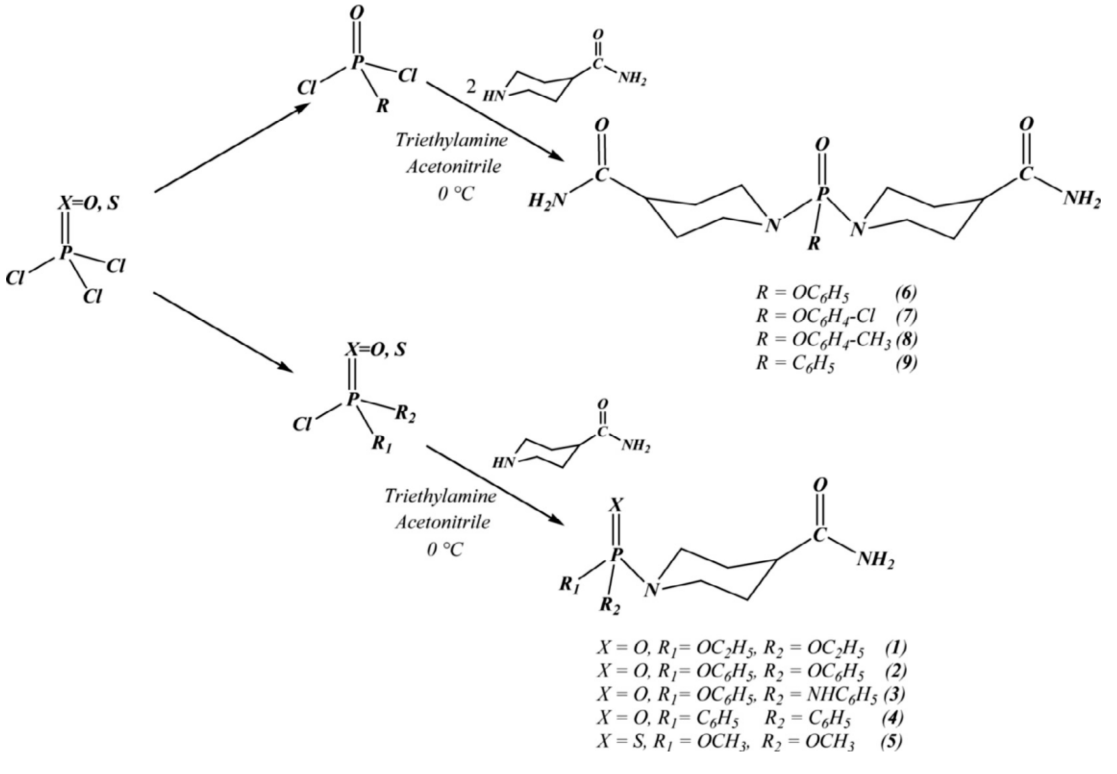
Novel (thio)phosphoramidate derivatives based on piperidincarboxamide with the general formula of $(NH_2–C(O)–C_5H_9N)–P(X = O,S)R1R2$ (1–5) and $(NH_2–C(O)–C_5H_9N)_2–P(O)R$ (6–9) were synthesized and characterized by ^{31}P, ^{13}C, ^{1}H NMR, IR spectroscopy. Furthermore, the crystal structure of compound $(NH_2–C(O)–C_5H_9N)_2–P(O)(OC_6H_5)$ (6) was investigated. The activities of derivatives on cholinesterases (ChE) were determined using a modified Ellman's method. Also the mixed-type mechanisms of these compounds were evaluated by Lineweaver–Burk plots.



Keywords: Cholinesterase,nhibitors

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Synthesis of CuS and $CuS_{1-x}M_x$(M=Zn and Mg) by hydrothermal method and study of their electrical , magnetic and optical properties

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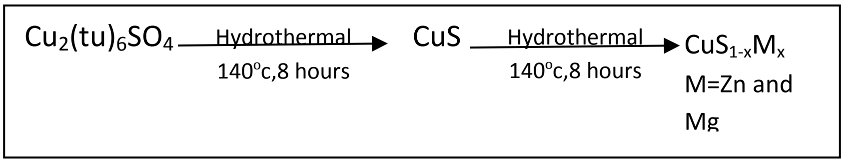
Recently CuS were synthesized from reagent such as copper nitrate or copper sulfate or copper acetate or sodium thiosulfate with ethylene glycol. But $CuS_{1-x}M_x$(M=Zn and Mg) complex weren't synthesized or not reported yet [1]. Generally materials include copper have broad application in electronics, catalysts, solar energy conversion, antibiotics, tissue imaging and photo thermal cancer therapy and the other hand we can use copper, zinc, magnesium and sulfide ions properties and features[2,3].

In this work, initially $Cu_2(tu)_6SO_4$ complex was obtained . Then this product at 140ºC for 8 hours via hydrothermal method. Indeed CuS produce from other method but it was tried to use green chemistry then it was prepared in two forms of thin film and nanoparticles powder then Zn and Mg doped CuS with different molar raitas(X=0.1 till 10). All the products X-ray diffraction were examined by to showing that they have signal phase and no impurities. The FT-IR spectra of as prepared products were taken. Also further investigations were doing with EDS, VSM or magnetization measurements and electrical conductivity and UV –Vis diffuses reflection spectrum shown the multiband structure and the band gap of nanoparticles are confirmed. The morphologies of the synthesized materials were studied by field emission scanning election microscope (SEM) and analyzed the size of nanoparticles.



$$Cu_2(tu)_6SO_4 \xrightarrow[\text{140ºc,8 hours}]{\text{Hydrothermal}} CuS \xrightarrow[\text{140ºc,8 hours}]{\text{Hydrothermal}} CuS_{1-x}M_x \text{ M=Zn and Mg}$$

Keywords: Copper, Zinc, Magnesium, Hydrothermal, Green chemistry

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Ultrasonically extraction of curcumin from turmeric and its formulation to enhance the solubility in simulated body fluids

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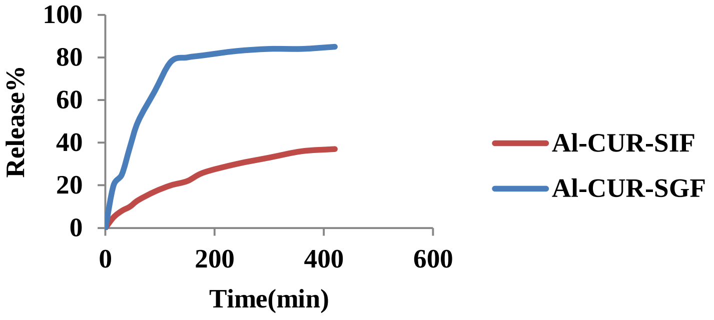
Chemically, curcumin is a diarylheptanoid, belonging to the group of curcuminoids, which is isolated from turmeric. In current research, curcumin was successfully extracted from turmeric via ultrasonic method from ethanol 70% medium. Sample characterization carried out with FT-IR and XRD. Since then curcumin is insoluble and non-absorbable in simulated body fluids SBFs, it should be in form of nano-formulation in order to reach higher solubility. For this purpose, curcumin was loaded into mesoporous gamma-alumina that was synthesized with sol-gel method in the ratio of 1:5 and the nano-drug-carrier was abbreviated as CUR@SGAL. Synthesized gamma-alumina and CUR@SGAL were characterized with FT-IR, XRD, SEM and BET. The release of CUR from SGAL was investigated in simulated gastric fluid (SGF) and simulated intestinal fluid (SIF) during 7 hours via UV analysis. It was observed that 85 and 38 percent of CUR was sustained release in SGF and SIF, respectively, after 7 hours.



Keywords: Extraction, Curcumin, Turmeric,Mesoporous alumina, Sol-gel, Sustained release

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Ultrasound Synthesis a New Nanostructure Supra-molecular Compound Of $[Cr(dipic)_2Mn(O)_2]_n$

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The nano structure polymer of $[Cr(dipic)_2Mn(O)_2]_n$ (where dipic is pyridine-2,6 dicarboxylic acid), was synthesized by sono-chemical method. Characterization of this complex was performed using Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), X-ray powder diffraction (XRD), thermal analysis method (TGA), BET specific surface area and vibrating sample magnetometer (VSM). The crystal structure of this polymer was found to be a binuclear coordination polymer. In this structure, the chrome center achieves hexa-coordination by coordinating with two deprotonated dipicolinate groups, acting as tridentate chelating ligands. Manganese center achieves tetra-coordination with four μ-carboxylate oxygen from the dipic ligand of $Cr(dipic)_2^{-2}$. The SEM images indicates that the polymer which was prepared by ultrasonic waves have nano-structure. This polymer as nanostructure shows broad absorption bonds at 3476 cm^{-1}, for symmetric and asymmetric stretching vibration of coordinated and lattice water (H_2O) and 1684, 1547 cm^{-1} for asymmetric stretching vibrations of $\upsilon_{as}(COO)$ and 1434,1384 and 1277 cm^{-1} for $\upsilon_s(COO)$ respectively.

Keywords: Sonochemical method, Nano-sized polymer, Crystal structure, Bulk polymer, Binuclear.

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Partial interaction studies of a synthesized Platinum (II) antitumor complex with BSA and DNA

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Anti-cancer properties of cisplatin have been discovered by B.Rosenberg in 1960. Its commercially successful analogues, carboplatin, oxaliplatin, nedaplatin…..etc are second generation drugs. These properties are mostly due to their interaction with cell DNA.

Present research work includes synthesis of a platinum (II) complex of formula [Pt (en) (2-py)] Cl (Where en = ethylenediamine and 2-py = 2-pyridinecarboxylate) and characterized by elemental analysis (C, H, N), conductivity measurement, and by UV-Visible, IR, and ^{1}H NMR spectroscopic techniques [1].

The interaction of the complex with calf thymus DNA (CT-DNA) and bovine serum albumin (BSA) were carried out using UV-Visible spectroscopy in 30 mmol/L Tris-HCl buffer of pH =7.0 at two temperatures of 300 and 310K. In these studies, K_{app}, the apparent equilibrium constant are 2.3×10^4 and 2.5×10^4 M^{-1} at 300K and 1.7×10^4 and 1.4×10^4 M^{-1} at 310K for BSA and DNA, respectively. The above compound can interact with BSA as well as DNA and the concentration of the complex in the midpoint of transition, $[L]_{1/2}$, is increased by increasing the temperatures from 0.028 mmol/L to 0.033 mmol/L for BSA and from 0.029 mmol/L to 0.035 mmol/L for DNA at 300K and 310K respectively. This complex can inhibit the growth of K562 [2] cancer cells and has Cc_{50} value (50% cytotoxic concentration) of 40 μM.

Keywords: Antitumor activity, Pt (II) complex, BSA/DNA-binding

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Synthesis of New Sodium Lanthanide Tungstate NaM(WO_4)$_2$ [M=Dy and Ho] Via Solid-State Method And Investigation Of Their Optical, Magnetic And Electrical Properties

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Recently, tungstate with a scheelite-type structure has been attracting attention. Because of their good photoluminescence (PL) properties optical fibers and scintillators [1].They are used as solid-state laser materials [2].They can provide properties such as negative thermal expansion (NTE),high anisotropic transport. Moreover some of them are receiving attention as laser host materials and stimulated-Raman-scattering active media .The materials exhibit high potential for a wide range of applications such as in phosphorescent materials , solar cells and luminescent diodes [3].

In this paper, we synthesized new NaRE(WO_4)$_2$ (RE=Dy and Ho) at 800 ºC for 10 hours by solid state method. The products characterized by X-Ray powder diffraction analyses that shown as a single phase and IR spectroscopy that demonstrated all bands were as we expected.The SEM and EDS analysis emphasized that compounds have almost the same morphology and also the size of nanoparticles was measured. Also the electrical conductivity was determined. The magnetization curve under the external magnetic field was measured and VSM curve shown that each of them is paramagnetism. Furthermore their spectroscopic properties i.e. absorption emission, excitation and luminescence was investigated at room temperature.

Keywords: Tungstate, Lanthanide, laser, Optical properties , Scheelite-type structure

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Synthesis and characterization of a new macrocycle based on a Schiff base ligand and preparation of their complexes by a few transition metals

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As an important class of compounds, Schiff bases have received much attention in the wide variety of fields. Schiff bases were prepared from condensation reaction between amine and carbonyl groups which can coordinate to metal ions via azomethine nitrogen [1]. Schiff bases have immense applications owing to their characteristic properties such as preparative accessibility, structural variety, diverse coordinating ability and thermal stability [2]. These compounds are used in food industry, dye industry, catalysts, fungicidal, polymers, agrochemical, pharmaceutical and biological activities [3,4].

In this project, a type of dialdehyde was synthesized according to the Mannich reaction [5]. Afterwards, the [2+2] Schiff base condensation reaction was accomplished between the synthesized dialdehyde and phenylenediamine. The prepared macrocycle used as ligand to synthesis metal complexes. The obtained products were investigated in each step by different methods like UV-Vis FT-IR, ^{1}HNMR, ^{13}CNMR spectroscopies and CHN analysis. The absence of aldehyde signal in ^{1}HNMR spectrum and appearance of imine proton were confirmed the Schiff base formation. According to mole ratio method by UV-Vis titration, the ratio of metal to ligand is 1:1.

Keywords*:* Schiff base, Mannich reaction, Macrocycle

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Study of SiO_2 shell effect on CeO_2 nanoparticles in the light alcohols identification

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Identification and measurement toxic and explosive gases or some harmful volatile organic substances always have been considered for the protection of the environment and human health. Isopropanol is a very detrimental organic colorless flammable liquid with a strong odor, from this compounds. Breathing or absorption of Isopropanol through the skin can be caused somnolence, respiratory depression, dizziness, abdominal cramps, nausea, headache and Hepatic dysfunction. There are many monitoring methods in the detection of Volatile organic compounds but high cost, complicated process and anomalous detection limit caused the researchers to think about constructing gas sensors to solve not only previous problems, but also improve selectivity and response time [1].The idea of gas sensors production was first proposed by Seiyama et al. (1962). Semiconductor metal oxide based gas sensors have been attracted widespread attention during the past decade [1,2]. Among the metal oxides, CeO_2 is a suitable candidate for this sensor due to its high oxygen storage capacity, high vacancy oxygen and the low potential for reduction between Ce^{3+} and Ce^{4+} is a good candidate for the sensor[3]. Cerium dioxide has been used as an ethanol sensor, moisture, carbon dioxide, carbon monoxide, etc. [4]. In the last few decades, extensive research has been carried out on core / shell structures and their impact on the sensitivity of gas sensors. So, in the present study, sensors of CeO_2 with SiO_2 shell have been developed and their ability to evaluate isopropanol quantitatively and qualitatively has been investigated Sensitivity sensors examined for quantitative and qualitative analysis. The results showed that cerium dioxide nanoparticles have the best answer in Iso-propanol and then core-shell composition ($CeO_2/SiO_2@CeO_2$), the lowest response was cerium dioxide nanoparticles coated with SiO_2. It seems that a number of factors be effective on performance of the sensor that including the structure morphology, particle size, surface area, pore volume and pore size.

Keywords: Cerium dioxide, Core/shell, Sensor, Iso-propanol

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Synthesis and characterization of metal oxides using metal organic frame works (MOF) by 4,4'-Diaminodiphenylsulfone

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Metal-Organic Frameworks (MOFs) are counterparty of many porous entities and are pertinent materials for future needs in almost in every sphere of life.The augmentation in the study of MOFs elicits significant information related to many potential applications.There are many systematical and facile synthetic routes such as hydro/solvothermal technique, microwave, electrochemical and mechanochemical etc.Metal-organic frameworks a class of porous materials bring great promise for a diverse array of applications ranging from gas storage and separation to heterogeneous catalysis.Synthesized reaction of ligand 4,4´-Diaminodiphenylsulfone with $Cu(CH_3COO)_2$.Structures of compound have been characterized by elemental analysis,IR spectroscopy.

Keywords: Metal-Organic Frameworks,catalysis,hydro/solvothermal

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Synthesis of nanoparticles Carbon Compounds doped with metal oxide and its use as alcohol sensor

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Carbon materials with inherent nanoscale features have potential for becoming ideal components for the next generation of autonomous sensor technology, since they combine excellent detection sensitivity with interesting transduction properties in a single layer of material [1]. Conductometric (resistive) metal oxide sensors comprise a significant part of the gas sensor component market. While many different approaches to gas detection are available, metal oxide sensors remain a widely used choice for arange of gas species. These devices offer low cost, high sensitivity, fast response and relative simplicity, especially in the field of portable devices. The working principle of a typical resistive metal oxide gas sensor is based on a shift of the state of equilibrium of the surface oxygen reaction due to the presence of the target analyte [2].

We have synthesized undoped and metal oxide-doped bamboo charcoal (BC) with a facile yet efficient sol-gel approach and investigated their nanostructures for gas sensing response to alcohol, focusing especially on the impact of Ti doping. BC powder was prepared through a carbonization treatment at 700°C. The prepared materials are characterized with FT-IR and XRD. From XRD spectrogram (Fig. 1) show of TiO_2/BC, we can see that the characteristic peak of TiO_2 is seen obviously, which indicated TiO_2 was loaded onto BC successfully.

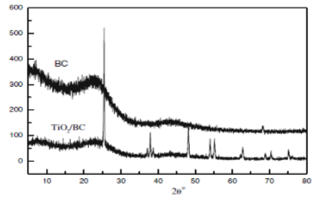

Fig. 1 XRD of BC and TiO_2/BC

Keywords: Carbon Compounds, Metal oxides, Bamboo charcoal, Sensors.

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Synthesis, characterization and interaction studies between a novel Pd(II), [(DACH)Pd(8Q)]NO_3 anti-tumor complex and calf thymus DNA

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Among transition metal complexes palladium(II) complexes are very interesting candidates for alternative metal-based drugs, because the coordination geometry and complex forming processes of palladium(II) are very similar to those of platinum(II)[1-3]. Thus our research in this area is focused on the interaction of Calf Thymus DNA (CT-DNA) with a new palladium(II) anticancer complex of [(DACH)]Pd(8Q) NO_3 (where 8Q = 8-hydroxyquinolin and DACH = 1,2-diaminocyclohexane). There is a set of 2 binding sits(g) for the complex on the DNA with positive cooperativity in binding. The Hill coefficient find out to be 3.05 at 300 K and 2.46 at 310K respectively. K_{app} are 23.54 and 25.43 mM^{-1} at 300K and 310K respectively. The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.082 at 300 to 0.050 mmol/L at 310K. The $\Delta G^0_{H_2O}$ determined to be 46.83 and 45.84 kJ/mol at 300 and 310K respectively. values for m, are 565.24 and 601.3 (kJ/mol) at 300K and 310K respectively. $\Delta H^0_{conformation}$ in the range of 300K and 310K is find out to be 76.00 kJ/mol. $\Delta S^0_{H_2O}$ of DNA denaturation by complex is 0.097 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The cytotoxicity assay of the complex has been performed on human breast adenocarcinoma MCF7 cell line, at micromolar concentration.

Keywords: Anti-tumor complex, Thermodinamic parameters, Spectroscopic techniques, Palladium (II) complex

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Crystal structure, photo-catalytic properties of PdO nanoparticles, DNA binding studies and cytotoxicity of a new hydroxyl-quinolinato-palladium complex

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The development of palladium anticancer drugs has been promising and their design has been based mainly on the structure-activity relationship used for platinum anticancer drugs as well as good models for the analogous Pt(II) complexes in solution[1-3]. Thus our research in this area is focused on the interaction of Calf Thymus DNA (CT-DNA with a new palladium(II) anticancer complex of [Pd(8Q)(Phen)]NO_3 (where 8Q = 8-hydroxyquinolin and Phen = 1,10 phenanthroline).There is a set of 4 binding sits(g) for the complex on the DNA with positive cooperativity in binding. The Hill coefficient find out to be 2.59 at 300 and 2.34 at 310 K respectively. K_{app} the apparent equilibrium constant are 76.52 and 83.03 mM^{-1} respectively. The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.057 at 300 to 0.054 mmol/L at 310K.($\Delta G^0_{H_2O}$) determined to be 47.63 and 46.68 kJ/mol at 300K and 310K respectively. values for m, are 846.8 and 881.3 at 300K and 310K respectively. $\Delta H^0_{conformation}$ in the range of 300K and 310K is find out to be 75.44 kJ/mol. $\Delta S^0_{H_2O}$ of DNA denaturation by complex is 0.092 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The cytotoxicity assay of the complex has been performed on human breast adenocarcinoma MCF7 cell line, at micromolar concentration.

Keywords: Crystal structure, Spectroscopic techniques, Anti-tumor, Palladium (II) complex

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A newly synthesized proton transfer ligand with 2, 6–pyridine dicarboxylic acid and pyridine–3–carboxamide: Characterization and DFT study

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In this work we report the synthesis, structural characterization, and theoretical studies of a new proton transfer ligands (PTLs) including Pyridine–3–carboxamide (*py–3–cm*) and 2,6–pyridine dicarboxylic acid (*2,6–pydc*). A PTL has mostly composed of anionic carboxylic acids and cationic amines parts which interact through intermolecular forces like N−H···O hydrogen bonds (HBs) [1,2,3]. First, aqueous solution of *py–3–cm* was added to the solution of *2,6–pydc*. Then, after hitting the mixture, the colorless crystals of the related PTL [*2, 6–pydc (Py–3–cm)*] (MP: 198℃) (**1**) obtained in RT. In following, its structure characterized by FTIR, UV–Vis, and CHNS elemental analysis (The proposed formula: [$C_{13}N_3H_{11}O_5$], C% (Calc.: 53.98, Exp.: 54.02), N% (Calc.: 14.53, Exp.: 14.61), and H% (Calc.: 3.90, Exp.: 3.87). Finally, the molecular and electronical structure of **1** experimentally and DFT/B3LYP/6–311+ G (*d,p*) theoretically one investigated that they confirm each other as below: FTIR: Stretching of C=O of carboxylate and carboxamide groups (Exp.: 1720; Calc.: 1745, 1777 cm^{-1}), Stretching of O–H (Exp.: 3160, 3745; Calc.:2949, 3772 cm^{-1}), the amide stretching bands of carboxamide group (Exp.: 3405, 3690; Calc.: 3772, 3596 cm^{-1}) and bending bands of carboxamide group (Exp.: 1600; Calc.: 1628, 1640 cm^{-1}). The experimental UV–Vis of **1** shows a broad band at 220-380 nm with maximum wavelength at near 305 nm that could be assigned to the major bands at 260.4 and 287.0 nm theoretical ones. The theoretical bands have $n \rightarrow \pi^*$ character that can be attributed to LLCT from carboxylic group of *2, 6–pydc* to pyridine moiety of *Py–3–cm.*

Keywords*:* [2, 6–pydc (Py–3–cm)]; Proton transfer; Pyridine–3–carboxamide; 2,6–pyridine dicarboxylic acid; DFT; Electronic bands.

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Synthesis and characterization of two macroacyclic protonated ligands that prepared in the presence of Mn(II) metal ions; X-ray crystal structure determination and antibacterial and antifungal studies

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Schiff bases have been extensively employed in the understanding of molecular processes occurring in biochemistry, antibacterial activities, DNA cleavage, science, catalysis, encapsulation, activation, transport and separation phenomena, hydrometallurgy, etc [1,2]. Herein, we report the synthesis of two new protonated ligands containing N and O donor atoms. These ligands were prepared by reaction of two N_2O_4 Schiff base ligands and Mn(II) metal ions. All compounds were characterized by microanalysis and IR spectroscopy, whereas compound **1** was also characterized by single crystal X-ray (Fig. 1). The X-ray structure of compound **1** showed that both imines are compensated by two perchlorate ions. Also the synthesized compound were screened for their antibacterial activities against nine bacterial strains and showed antibacterial effects. These compounds also showed antifungal effects on two species of Candida.

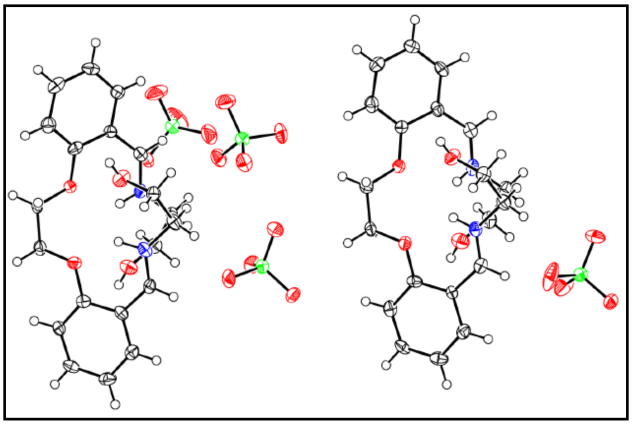

Fig. 1

Keywords: Schiff base ligands, Protonate imines,Crystal structure, Antibacterial, Antifungal studies.

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Direct Effect of Halides on Rigidity of Luminescent Double Rollover Cycloplatinated(II) Structures

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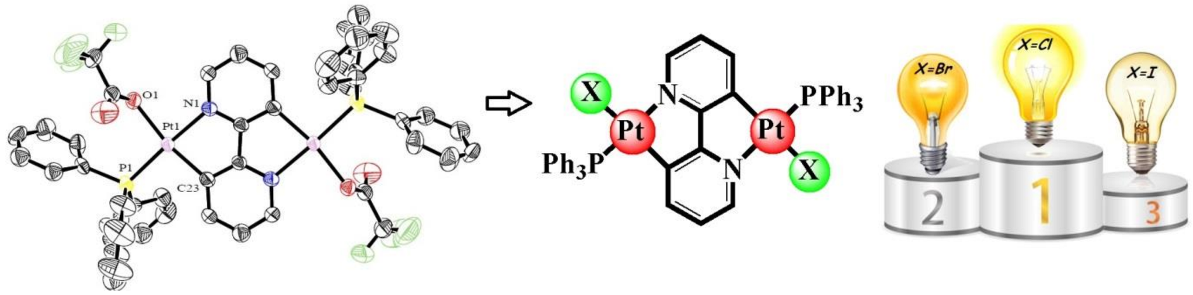
In continuation of our previous investigations [1,2], the present study highlights the effects of anionic ligands, halogen or trifluoroacetate, on the structural rigidity of a double rollover cycloplatinated(II) structure. In fact, it has been proven that the halide ligands can tune the brightness of organometallic compounds as organic light emitting diodes (OLED) emitters by affecting the structural rigidity of these complexes. As such, a serious of closely related platinum (II) complexes with general formula of $[Pt_2(\mu\text{-bpy-2H})(X)_2(PPh_3)_2]$ has been prepared, incorporating a double rollover cyclometallating ligand, two triphenylphosphine ligands and either two trifluoroacetate ligands (X = CF_3COO), **3**, or two halide ligands (X = Cl, **4a**, Br, **4b**, or I, **4c**). The complexes were characterized by multi-nuclear ^1H and ^{31}P NMR spectroscopy and structure of the complex $[Pt_2(\mu\text{-bpy-2H})(CF_3COO)_2(PPh_3)_2]$, **3**, was typically determined by single crystal X-ray crystallography. The luminescence properties of the newly synthesized complexes, supported by DFT calculations, were investigated at 298 and 77 K over the wide range of 295-505 nm for excitation wavelengths.



Keywords: Cycloplatinated(II), Halide, Structural Rigidity, Luminescence

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The comparison of reactivity and host-gust chemistry studies of two cyclophane cationic compounds; experimental and theoretical studies

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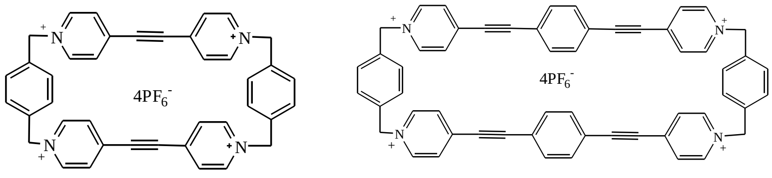
Cationic cyclophanes, referred to as Ex^{n}Box^{4+} compounds, created by reacting rigid bipyridyl-based linkers, where n is the number of p-phenylene spacers between the pyridinium rings, with 1,4-bis(bromomethyl)benzene, have been employed toward diverse chemistry on account of their highly strained and π-electron-poor nature [1-3]. Herein, we combine the principles of strain and cooperative reactivity to achieve cascade reactions. we report the synthesis of an Ex^{n}Box^{4+} (n=0.8 and 2.2) (Fig.1)(cyclophane with strained, electron deficient triple bonds inserted between pyridinium rings, resulting in the so-called Ex$^{0.8}$Box^{4+} and Ex$^{2.2}$Box^{4+} and their subsequent successive cycloadditions with (i) cyclopentadiene and (ii) 1-azidoadamantane. When compared with a bigger one analogue, Ex$^{0.8}$Box^{4+} undergoes cycloadditions much more quickly because of the release of strain inherent in the cyclophane. Furthermore, the cycloadditions proceed in the fashion of at and cascade, with no evidence observed for the formation of mono functional intermediates by ^{1}H NMR spectroscopy, pointing to a situation in which the first cycloaddition increases the reactivity of the cyclophane, rendering the second cycloaddition even faster. Molecular modeling of the energy landscape reveals a lower barrier for the kinetically favored second cycloaddition compared with the first one.



Ex$^{0.8}$Box

Ex$^{2.2}$Box

Fig. 1

Keywords: Cyclophane, Reactivity studies, Host-gust Chemistry, Theoretical studies

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Oxidation of cycloplatinated(II) complexes by iodomethane: isolation of the kinetic product

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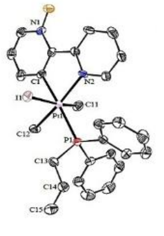
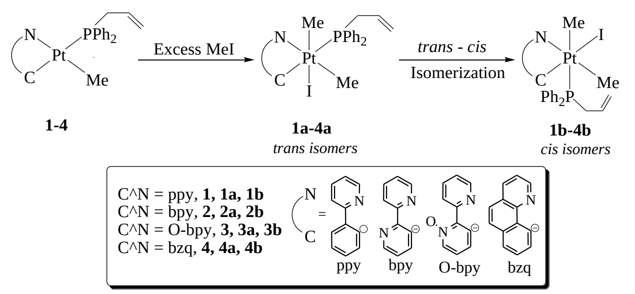
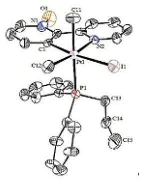
Oxidative addition reactions to unsaturated d^8 transition-metal, especially Pt(II), compounds, have always been among the most investigated dynamic processes in chemistry [1]. The kinetics and mechanism of this reaction for organoplatinum(II) complexes were investigated extensively, and these studies clearly revealed that the reaction mechanism is commonly a classical S_N2 reaction [2, 3]. In current study, the oxidative addition of iodomethane to cycloplatinated(II) complexes containing allyldiphenylphosphane (PPh_2allyl) ligands, namely, [Pt(C^N)Me(PPh_2allyl)] [**1–4**; C^N= deprotonated 2-phenylpyridyne (ppy), **1**; 2,2′-bipyridine (bpy), **2**; 2,2′-bipyridine N-oxide (O-bpy), **3**; and 7,8-benzoquinoline (bzq), **4**], occurs readily with trans stereochemistry to give the *trans*-Pt(IV) isomers **1a–4a**, which then transform slowly to the *cis*-Pt(IV) isomers **1b–4b**. All of the complexes were characterized by NMR spectroscopy, and the structures of **1b**, **3a**, and **3b** were determined by single-crystal X-ray diffraction. Kinetic studies through UV/Vis spectroscopy suggested that the oxidative addition reaction proceeded through an S_N2 reaction. The rate of the oxidative addition reaction was measured at different temperatures, and large negative $\Delta S^{\#}$ values consistent with the proposed mechanism were found for each reaction. This reaction was also monitored by NMR spectroscopy to determine a correct value for the rate of the *trans/cis* isomerization. The theoretical aspects of the mechanism for the oxidative addition reaction were also studied by density functional theory (DFT) calculations to support the claimed experimental results.



(3a)





(3b)

Keywords: Oxidative addition, Platinum, Kinetics, Reaction mechanisms, Density functional theory.

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Novel CdS-$NiFe_2O_4$/reduced graphene oxide photocatalyst with enhanced photocatalytic activity under visible-light irradiation

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In this study, a core-shell structured CdS-$NiFe_2O_4$ nanocomposite photocatalyst in order to increase the efficiency of methylene blue (MB) degradation and to enable photocatalyst separation was synthesized and characterized using different analytical tools. The synergic effect of CdS and $NiFe_2O_4$ nanoparticles can decrease the recombination of photogenerated electron-hole pairs and increase the charge separation efficiency. In the present study, we have reported a two-step hydrothermal method toward the preparation of a novel CdS-$NiFe_2O_4$ nanocomposite. It has been demonstrated that the synthesized CdS-$NiFe_2O_4$ nanocomposite perform as a good photocatalyst for degradation of methylene blue under visible-light irradiation. It is very interesting that the combination of CdS-$NiFe_2O_4$ nanocomposite with graphene oxide (GO) nanoparticles results in a conversion of the good CdS-$NiFe_2O_4$ photocatalyst into a perfect photocatalyst for the degradation of MB under exposure to visible-light. Furthermore, CdS-$NiFe_2O_4$/rGO nanocomposite have prepared by a facile method and the synergistic effect of RGO content on the photoactivity of the CdS-$NiFe_2O_4$ composite was investigated. CdS-$NiFe_2O_4$/rGO nanocomposite opens hopeful outlook for preparation of visible-light photocatalysts based on graphene oxide for degradation of organic contaminates such as organic dyes.

Keywords: Nickel ferrite; Cadmium sulfide; Reduced graphene oxide; Photocatalyst; Methylene blue.

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Solution Behaviour and Metal Substitution of a New Family of Hybrid Amino Acid-Polyoxometalates

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Comprehensive solution studies of a new family of hybrid amino acid polyoxometalates have provided key insights into the molecular and electronic structure. These compounds vary in the nuclearity, type and degree of the reduction of the metals (Mo/W and V/W) in the central core of the POM as well as amino acid ligands and organic cations which affect the solution behavior of these hetropolyanions (HPA) in aqueous solution and DMSO. Small angle X-ray scattering, electronic absorption and NMR spectroscopy have confirmed the maintenance of the polyoxometalate framework in solution. Electrochemical studies have elucidated the electronic structure and redox properties, revealing unusual stability of "heteropoly blue" reduced analogues. Density Functional Theory (DFT) calculation results are in an excellent agreement with the experimental findings. Circular dichroism measurements indicate that the incorporation of chiral amino acid ligands into the reduced analogues affords chirality in solution. An exchange was observed in amino acid buffer solution and confirmed by single x-ray diffraction technique.

Keywords: Hybrid-Polyoxometalates, Amino acid, Mixed-metal, Mixed-valence

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Highly efficient Zn(II) complexes exhibiting thermally activated delayed fluorescence for applications in OLEDs

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Harvesting of all singlet and triplet excitons for light generation in OLEDs is possible by the mechanism of thermally activated delayed fluorescence (TADF). [1] It has been demonstrated that Cu(I) and Ag(I) complexes [1-3] as well as purely organic molecules [4] can be highly attractive TADF materials and be used as efficient emitters in OLEDs. Recently, it has been reported that Zn(II) complexes can also show the TADF effect. [5] Herein, we report a novel TADF material based on Zn(II) being coordinated by one organic bidentate N̂N aromatic ligand and two halides. This material is thermally stable and shows relatively short TADF decay time at an emission quantum yield of more than 80 %.

Keywords: TADF, Zn(II) complexes, OLEDs

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Enzyme-free glucose biosensing via a glassy carbon electrode modified by zinc oxide/graphene oxide

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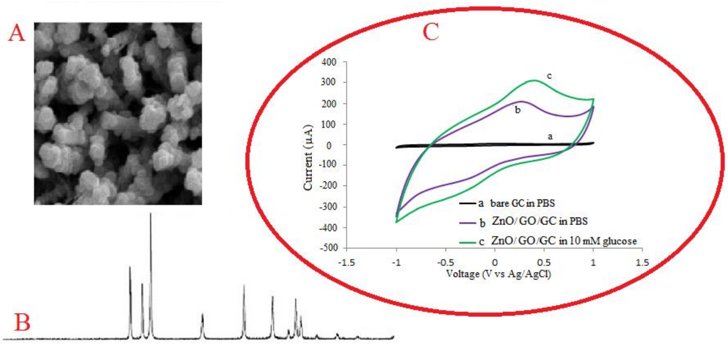
In this study, a fast and sensitive nonenzymatic glucose sensor is reported utilizing a glassy carbon electrode modified by synthesizing nanocomposites of ZnO and graphene oxide. of ZnO was synthesized via solvothermal method by using different additives (l-lysine and oxalic acid) and then characterized by scanning electron microscope (SEM) and X-Ray diffraction analysis (XRD). Based on the extraordinarily properties of graphene oxide (GO), ZnO/GO/glassy carbon (GC) modified electrode was prepared by electrodeposition of ZnO on the GC surface previously modified with GO and subjected to cyclic voltammetry (CV). Compared with ZnO/GC electrode, ZnO/GO/GC modified electrode exhibited much more sensivity 58.3 μA/cm^2 mM in electrocatalytic oxidation of glucose. The linear range for determining of glucose is from 1 to 10 mM with the detection limit of 0.73 mM. In addition, the effects of common interfering species, including ascorbic acid (AA), uric acid (UA), and fructose were investigated in detail. The result indicated that these foreign substances did not interfere significantly on the determination of glucose.



Keywords: Graphene oxide, Nonenzymatic sensing, Cyclic voltammetry, Glucose biosensor

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Chlorometal of Mo in the Neighborhood of Solvated Li-Ion

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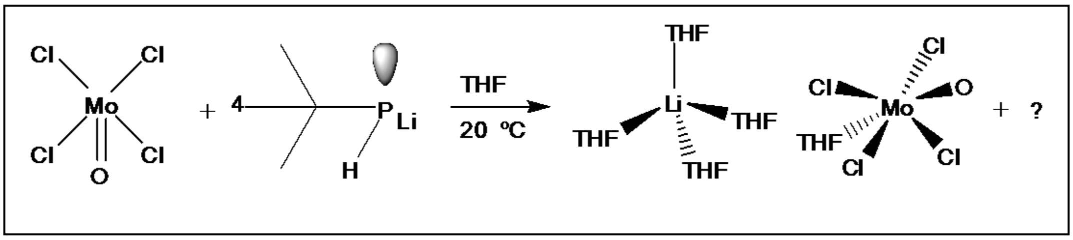
Chlorometals with solvated lithium ions are a widely known category of compounds in the coordination chemistry. Some major examples for such chlorometals include in the form of separated ion pairs $[Li(THF)_4][ClInFI_3]$ [1], two nuclear chloro bridged four membered ring system $[(THF)_2LiCl_2Cu(Ph_3P)_2]$ [2], or simple chloro bridged two nuclear complex salt $[(THF)_3LiClInCl_2\{Si(SiMe_3)_3\}]$ [3]. In this study, we present chlorometal of Molybdenum (V), synthesized in a direct way. Oxomolybdenum tetrachloride was reacted with four equivalent $^tBuP(H)Li$ in THF at 20 °C for 12 hours. The red brown mixture was filtered. Normal pentane was added to the filtrate and the mixture was kept at -30 °C. After couple of days, the big plates with a color of emerald green were crystallized. According to the crystallographic studies, the Mo-O- and Mo-Cl- bond lengths are typically in accordinated with free or just weak coordinated $[OMoCl_4]^-$ ions. The weak ligand THF is trans toward oxygen atom. The octahedral complex is distorted as the result of π-donor effect of O^{2-} ligand. So, four Cl-atoms are squeezed toward THF ligand.



Keywords: Molybdenum, Trans effect, Chlorometal

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A review of fabrication and modification of halloysite nanotubes

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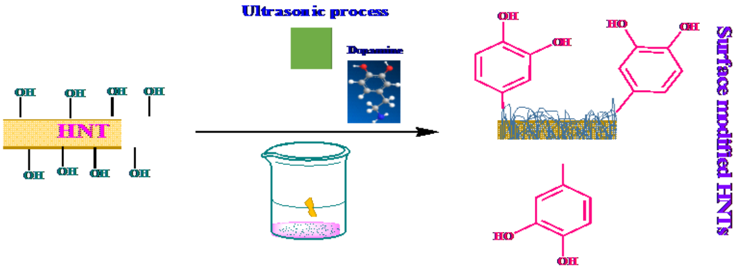
Natural nano-tubular halloysite (HNT) comprises of different proportion of aluminum, silicon, hydrogen, and oxygen atoms [1]. It has chemical formula of $Al_4Si_4O_{10}(OH)_8$ **.**$4H_2O$. Nano- tubular geometry of halloysites exhibit nanoscale dimensions. In this study different functionalization process of halloysite nanotubes will be reviewed [2]. Halloysite structure is well known as an ideal filler for fabrication of polymer nanocomposites, because this structure has high volume to surface ratio, good dispersion state, and suitable mechanical properties. The modifications of HNTs were characterized by transmission electron microscopy (TEM), fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM) and X-ray photo-electron spectroscopy analyses. Dopamine is a vital compound used in this process. The results showed that dopamine could self-polymerization to adhere to the surface of HNTs and form a thin active coating [3]. The surface coating of HNT by polydopamine as biopolymer was illustrated in scheme 1.



Scheme 1. Functionalizatioin of HNTs by biopolymers

Keywords: Halloysite, Nanotubes

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Synthesis of ZnO@alum doped with manganese nanocomposite as hydrophobic compound for separating petroleum from water

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Large quantities of oily wastewater are produced from the activities in the petroleum industry, oil transportation, distribution facilities, metal rolling workshops, paper deinking and reduction of work-pieces prior to metal finishing. Draining of these effluents not only pollutes the environment but also reduces the yield of oil and water [1-2]. On the other hand, ZnO has excellent physical properties, such as high melting point (1975 ºC) and high thermal stability [3]. When ZnO is doped with transitional metal ions such as manganese, its properties will be improved. In addition, potassium aluminum sulfate (alum) is being used in water and wastewater refinement process, as a hydrophobic agent [4-5].

In this study, 3% of manganese was doped to ZnO@alum nanocomposite that synthesized by hydrothermal method and calcinated at 800 ºC. Also nanocomposite was characterized by Fourier Transform Infrared spectroscopy (FT-IR) and X-Ray Diffraction (XRD). One of the applications of this nanocomposite is that it separates petroleum from water. 0.01 g of nanocomposite was added to the 10 ml of water and petroleum mixture (bahregansar petroleum) (0.02 M). After a little stirring, the solution was filtered using filter papers. The results showed that petroleum was completely removed from filtered solution.

Keywords: Oily wastewater, ZnO, Alum, Nanocomposite, Petroleum.

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Cubic manganese oxide/MWCNT nanocomposite as a new electrocatalyst for glucose oxidation

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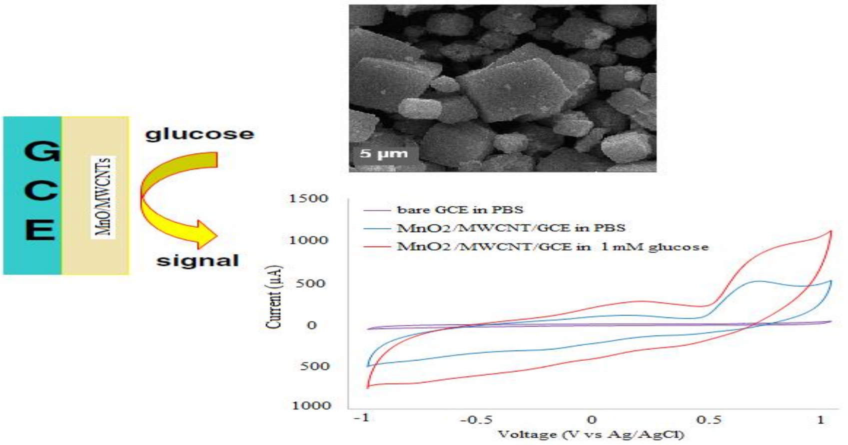
In this report, a novel type of manganese oxide (MnO_2) nanostructers modified by multi-walled carbon nanotubes (MWCNTs) array glassy carbon electrode was applied for nonenzymatic detection of glucose. The morphology of the manganese oxide was characterized by scanning electron microscope (SEM) and X-ray diffraction (XRD). The electrochemical performance of the MnO_2/MWCNTs/GCE for detection of glucose was investigated by cyclic voltammetry and chronoamperometry. The MnO_2/MWCNTs/GCE in SBF solution showed much higher electrocatalytic activity MnO_2/MWCNTs/GCE towards oxidation of glucose. The MnO_2/MWCNTs/GCE presented a high sensitivity of 61.4 μA/cm^2 mM to glucose. In addition, a linear range was obtained over a concentration up to 2 mM with a detection limit of 0.76 mM. The response time is about 3 s by the addition of 2 mM glucose. More importantly, the MnO_2/MWCNTs/GCE is also highly resistant against poisoning the interference from the oxidation of common interfering species such as ascorbic acid, dopamine, uric acid and carbohydrate compounds at working potential of +0.8V in PBS. The MnO_2/MWCNTs/GCE exhibited an enhanced electrocatalytic property, low working potential, high sensitivity, excellent selectivity, good stability and fast amperometric sensing towards oxidation of glucose, thus it is promising for the future development of nonenzymatic glucose sensors.



Keywords: Manganese oxide, Carbon nanotubes, Electroanalysis, Glucose, Sensor

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Nanosized rhodium oxide for water oxidation: An organometallic precursor for the preparation of rhodium oxide

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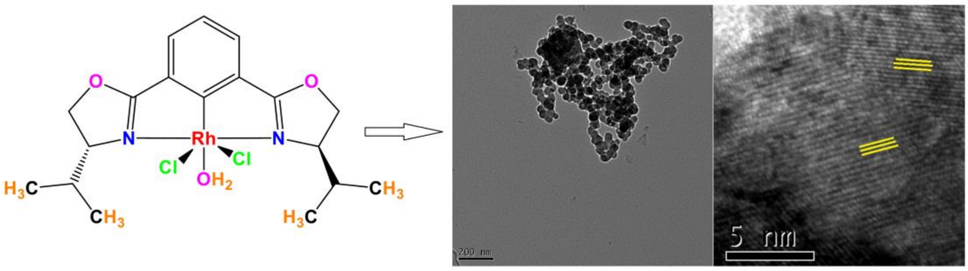
Electrochemical production of hydrogen from water splitting is a promising process to store the intermittent energies. However, the anodic water oxidation, which is a complicated four protons-four electrons transfer process, affects the efficiency of hydrogen generation due to the need to apply large overpotentials. Rhodium is a rare, hard, and chemically inert transition metal [1]. Some groups reported different applications for Rh_2O_3 [2-4]. Rh_2O_3 has been rarely studied for water oxidation. Harriman et al. reported Rh_2O_3 as efficient catalyst for water oxidation under photochemical conditions [5]. Herein, we synthesized nanosized rhodium(III) oxide by the thermal decomposition of a known rhodium organometallic precursor. The prepared samples were identified by some characterization methods such as XRD, SEM-EDAX, TEM, IR. The electrochemical results showed that the nanosized rhodium oxide is a promising catalyst toward water oxidation.



Keywords: Artificial photosynthesis, hydrogen production, nanosized rhodium oxide, organometallic precursor, water oxidation.

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Unprecedented photocatalytic degradation of MB by ZSM-5 templated with novel ethylenediammonium iodide

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ZSM-5 zeolite has been widely used in industry as catalyst in terms of unique properties e.g. high surface area, acidity, and shape selectivity [1]. The catalytic performance of ZSM-5 is controlled by different factors such as synthesis gel composition, nature of template, pH, temperature and duration of aging of the gel and hydrothermal treatment conditions [2]. It is well known that the template effect plays a prominent synthetic role in structure of zeolites. Meanwhile, there are varieties of organic substances that are applied as templator in a ZSM-5 synthesis [2,3]. Among these, Tetrapropylammonium hydroxide (TPAOH) is considered as a very effective template. Nevertheless, TPAOH is an expensive material and causes an increase in the cost of the production of the catalysts. [3] In this study, we report a novel and cost-effective method to synthesize of ZSM-5 (Si/Al=23) by employing N,N'-dipropyl-N,N,N',N' tetramethyl-1,2- ethylenediammonium diiodide (EDI) as a new templating agent. The abovementioned catalyst was denoted as EDI-ZSM-5 and compared that with a commercially available ZSM-5 templated with TPAOH (TPAOH-ZSM-5). The catalysts were characterized by using XRD, BET, N_2 adsorption-desorption, FE-SEM, FT-IR techniques. To investigate the photocatalytic activity of the ZSM-5 zeolites, the catalysts were used in degradation of methylene blue (MB), under UV irradiation (Fig. 1). The observed degradation time for MB in the presence of EDI-ZSM-5 was reduced from 135 min to 20 min which to the best of our knowledge, this the lowest MB degradation time reported for ZSM-5.

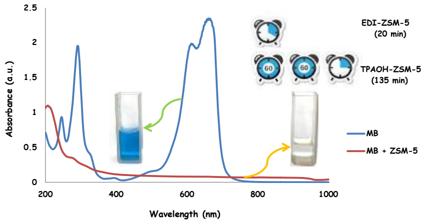

Fig. 1. Absorption spectrum changes of methylene blue solution ($5x10^{-4}$ M) in the presence of ZSM-5 powder under UV light irradiation.

Keywords: ZSM-5 zeolite, photocatalytic degradation, methylene blue, template, ethylenediammonium iodide

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Synthesis and Characterization of a New Polypyridyl Ru(II) Complex as the Electrocatalyst for CO_2 Reduction

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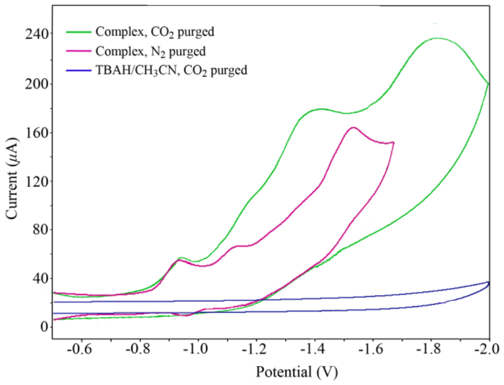
Greenhouse gases such as CO_2, CH_4, hydrofluorocarbons, and perfluorocarbons increase the Earth's atmosphere temperature. The industrialized countries promised to reduce their levels of emission of the greenhouse gases, especially CO_2. In the Earth's atmosphere, CO_2 is removed and return according to the carbon cycle [1]. Among the various transformations of CO_2, the electrochemical reduction of CO_2 has drawn much attention from researchers for the past three decades [2,3]. CO_2 can be reduced to CO by electrochemical method using pure metals, alloys, metal coordination complexes or organometallic catalysts at room temperature. In recent years, polypyridyl complexes of Ru(II) have proven to be active in electrocatalytic reduction of CO_2 to CO [4,5].

Here, we report the synthesis, characterization, crystal structure, and electrocatalytic activity of a new mononuclear polypyridyl Ru(II) complex, $[RuCl_2(tpyt)(CH_3CN)]$. The electrocatalytic activity of the complex was investigated for $2\bar{e}$ reduction of CO_2 to CO in acetonitrile by cyclic voltammetry under different reaction conditions. In addition, the electrocatalytic mechanism of reduction of CO_2 was investigated by means of DFT calculations. The obtained results are of great significance as they provide a theoretical insight into new transition metal electrocatalysts for the reduction of CO_2 to CO.



Keywords: Ru(II) complex, Electrocatalytic reduction of CO_2, Single crystal X-ray structure, DFT calculations

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Organoplatinum(II) complexes bearing various isocyanide ligands: synthesis, spectroscopic characterization, and biological activity

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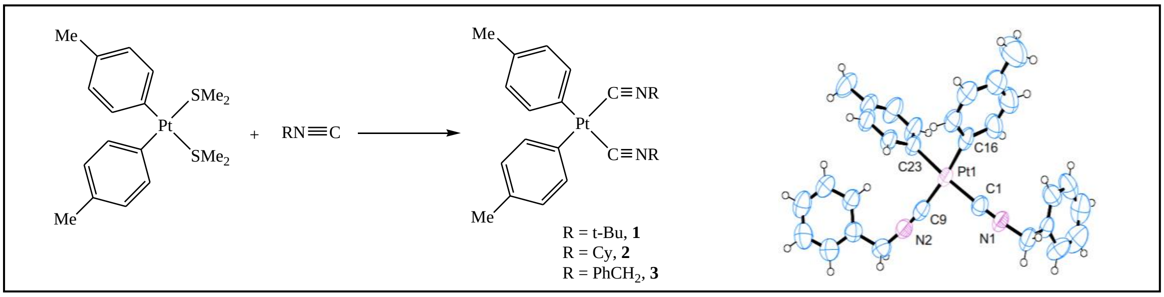
Isocyanide ligands have been attracted considerable attention by organometallic chemists as a result of their versatility in both organic synthesis and coordination chemistry[1]. Isocyanides have been long heralded in coordination chemistry for their strong σ-donor and weak π-acceptor properties [2]. There is considerable evidence in the literature that platinum complexes with isocyanide ligands should be stable and display interesting properties [2]. Pt(II)-isocyanide complexes have been explored their liquid crystal properties, their use as probes for important intermediates in platinum catalyzed reactions, and their use as vapochromic sensors [3]. In this contribution, a series of platinum complexes contain isocyanide ligands has been prepared. The Pt(II) complex with general formula of [Pt(*p*-$MeC_6H_4)_2(SMe_2)_2$] was reacted with two equivalent of CNR ligands (R = *tert*-butyl, (**1**), cyclohexyl, (**2**), benzyl, (**3**)) to give [Pt(*p*-$MeC_6H_4)_2(CNR)_2$]. All complexes were characterized by NMR spectroscopy and the structure of **3** was confirmed by single-crystal X-ray analysis. The cytotoxic activities of **1-3** containing the isocyanide ligands have also been evaluated on several cancer cell lines.



Keywords: Platinum, Isocyanide ligands, Biological activity.

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Synthesis and characterization of a new dinuclear copper complex with 2-aminopyrimidine as epoxidation catalyst

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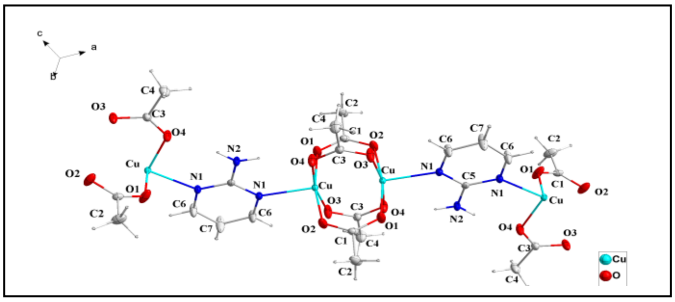
Copper is an essential metal that is capable of forming complexes with many compounds of biological importance. The coordination chemistry of copper has become a fascinating area of research in recent years because of the presence of copper in metalloenzymes. The catalytic oxidation of alkenes has been a subject of growing interest in the production of chemicals and fine chemicals [1,2]. Copper salts and copper containing coordination complexes are well-known catalysts for the selective oxidation of alkenes and quite a number of studies have been conducted. In this study bis copper (tetra μ-acetato)(2-aminopyrimidine) complex designated as$[Cu_2(\mu\text{-}OAc)_4(ampym)]$ was prepared from cooper acetate monohydrate and 1,2-dihydroxy-1,2-bis(2-pyrimidylamino)ethane under reflux condition and characterized by single crystal X-ray diffraction, FTIR, TGA,^{1}H NMR and elemental analysis techniques. In this complex, the metal ion is surrounded by 4 oxygen and 1 nitrogen atoms in a severely distorted square pyramidal 5-coordinated geometry (fig 1). Single crystal X-ray analysis revealed that the complex crystallizes in the monoclinic C 2/c with Z = 4 space group, with a =15.0998(9) Å, b = 13.5326(7) Å, c = 8.5733 (6) Å, α = 90°, β = 94.148 (5)° and γ = 90°. The catalytic activity of complex was evaluated by the epoxidation of norbornene, cyclooctene, styrene, a-methyl styrene and trans-stilbene with tert-butyl hydroperoxide (TBHP), with 30–99%conversions and 30–100% selectivity.



Keywords: Epoxidation catalyst, 2-aminopyrimidine,Cu(II) complex

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Synthesis, Spectral and Luminescence Study of Zinc (II) Bromide Coordination Polymer with 4,7-Phenanthroline

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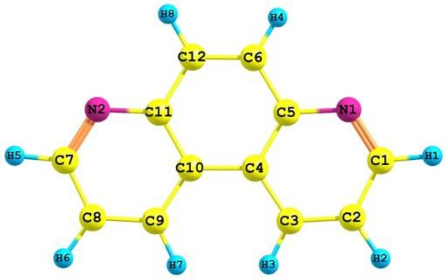
4,7-phenanthroline is a rigid N-donor ligand that favors coordination to metals in a bridging bidentate manner rather than chelation and also proved useful in the formation of supramolecular H-bonded networks containing hydrated first-row transition metal ion and π-π interaction in this structures cause to more stability. In this study, The novel coordination polymer of Zn(II) and 4,7-phenanthroline ligand, was synthesized by reaction between $ZnBr_2$ and this ligand in 1:1 mole ratio. This complex was characterized by IR ,^1H , $^{13}CNMR$,UV-Vis and Luminescence spectroscopy and elemental analysis.



Scheme1- 4,7-phenanthroline

Keywords: Phenanthroline, Coordination Polymer, Luminescence

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Urea-based Metal-Organic Framework for Carbonyl Compounds Sensing

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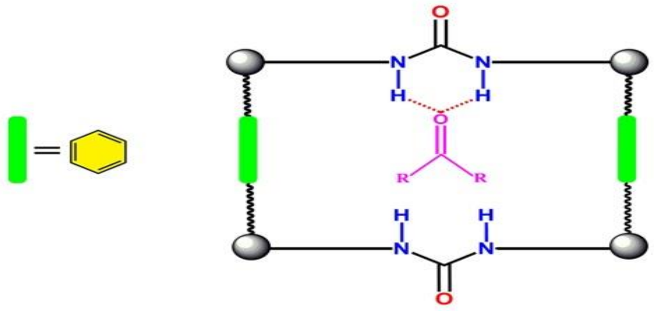
An urea-based MOF, namely TMU-35, was synthesized and characterized with X-ray crystallography and different spectroscopic techniques like PXRD, FT-IR, TGA and SEM. Since this material has urea functional group, it can interact favorably through hydrogen bonding with carbonyl compounds and thus it can be a potential candidate for carbonyl compounds sensing. Our research is focused on the pillaring linker of this MOF which containing benzene core (TMU-35), and its fluorescence sensing ability for carbonyl compounds is dramatically high for this MOF. It can be resulted that in the investigation of TMU-35 structure which has a more electron-rich and hydrophobic pore walls which can interact favorably with organic analytes. This conclusion is interesting as it indicate the first example of the application of functionalized MOFs for carbonyl compounds sensing.



Keywords: Metal-organic Framework, Sensing, Hydrogen bonding, Carbonyl compounds,

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Synthesis, characterization and biological evaluation of some phosphorus(IV) compounds

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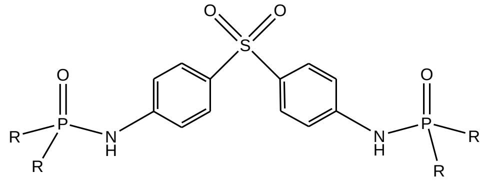
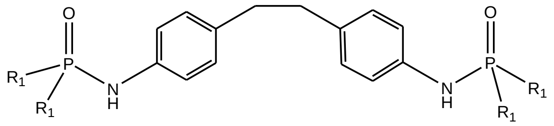
Bisphosphoramidates have been found to exhibit a wide range of biological activities. A large volume of research on their synthesis and biological activities has been reported during the last 20 years. A considerable number of bisphosphoramidate derivatives are known to be an antiviral, antibacterial and inhibitory effect. Considering the above sentence, and in connection with our current works in the biological activity of phosphorus (IV) compounds, in this work, we synthesized a series of bisphosphoramidates derivatives. All compounds were characterized by 31P, 13C, 1H NMR and IR spectroscopies.



R=N $(CH_3)_2$,, $N(C_2H_5)_2$,$(CH_2)_5N$ ....



R_1=C_6H_5, O (C_6H_5) .

Keywords: phosphoramidate, biological

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Design and syntheses of new coordination supramolecular compounds of silver with btz ligands

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The design a set of coordination supramolecular compounds with different metal ions and ligands, solvent and counter ions have led to a large variety of materials with potential applications in molecular adsorption, catalysis, magnetism, luminescence, nonlinear optics, and molecular sensing, among others, that don't seem to be found in mononuclear compounds. Many different synthetic approaches have already been explored for the preparation of coordination compounds. In the last two decades, design and syntheses of coordination supramolecular compounds, has produced appreciable progress within the field of supramolecular chemistry and crystal engineering. This article focuses on the simple synthetic preparation of a new Zn(II) bithiazole coordination supramolecular compound. New coordination supramolecular compound were produced by using Zn(II) salt and btz in an efficient and quick way. For the characterization of the products, ^{1}H-NMR, ^{13}C-NMR, and FT-IR spectroscopy were used. The thermal stability of new complex was studied by thermal gravimetric (TG) and differential thermal analyses (DTA). The compound was further characterized by UV-visible spectrophotometric measurements.

Keywords: Design, Syntheses, Coordination, Supramolecular

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Synthesis and characterization of two Aldehydes containing piperazin moeities and related schiff base complexes with some transition metal ions

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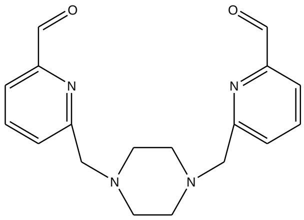
The stability of metal complexes with polydentate ligands depends on a range of factors such as the number and type of donor atoms present and their relative positions within the ligand, the nature of the ligand backbone, and the number and size of the chelate rings formed on complexation. If the ligand is a macrocycle, then the ring size is a further factor that will influence the complex stability. Consequently, macrocyclic ligands provide an excellent basis for the study of molecular recognition phenomena since their cavity size, shape and components can be varied readily [1,2]. In previous works, we have reported some macrocyclic Schiff base complexes containing N_3O_2 donor groups[3], And in another work we have reported some macrocyclic Schiff base complexes containing pyridine moieties [4, 5].

In this work Two aldehydes (Scheme 1 and 2) have prepaired by use of Mannich reaction method and their related complexes by perchlorate salts of Ni^{2+} , Cu^{2+} and Cd^{2+} were obtained by template method In the presence of 1,2-diamino ethane and 1,3 diamino propane. The aldehydes were investigated by elemental analysis ,IR spectroscopy ,^{1}H and ^{13}C NMR and related complexe were characterizated by elemental analysis , IR spectroscopy and X ray spectroscopy.



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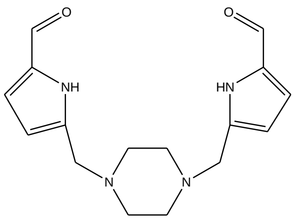

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Keywords: Mannich reaction; X-ray Crystal Structure; Schiff base complex

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$ZrCl_4$ Mediated Synthesis of Some 3,3'- Bisindolyl(aryl)methanes and Study of Their Photophysical Properties

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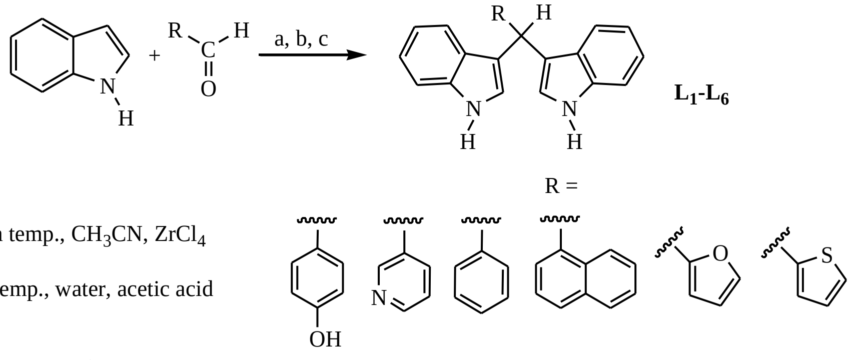
3,3'-bisindolylmethane (R = H, scheme shown below), the simplest form of a bisindol, is known to have diverse biological activities such as anti-cancer, anti-bacterial, and anti-inflammation [1]. Besides, this compound and its derivatives are used as intermediates in the synthesis of many organic compounds with pharmaceutical importance [2]. On the other hand, derivatives of 3,3'-bisindolylmethane with an aryl group on tetrahedral carbon atom bridging between two indole rings, commonly referred to as 3,3'-bisindolyl(aryl)methane, due to their affinity to a variety of metals and anions such as copper (II) and fluoride ions have found applications as colorimetric sensors.[7-10] Similar binding capability of these compounds to common protic and non-protic organic solvents and their dramatic color changes due to solvation of their ground or excited states have led to the development of simple and highly efficient solvatochromic combinations [3]. In this study, successful synthesis of a series of 3,3'-bisindolyl(aryl)methanes by modification of a previously reported synthetic method in the literature is reported. Main research goals included a detailed structural characterization of the products by means of NMR spectroscopy and X-Ray crystallography, and understanding the role of aryl substituent on the photophysical properties of these compounds.



a, b, c (except L_4) = room temp., CH_3CN, $ZrCl_4$

a, b, c (L4 only) = room temp., water, acetic acid

Keywords: Bisindolylmethane, anti-inflammation, solvatochromic, photophysical

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Cu (I) Complexes of Dihydrobis(2-mercapto-benzimidazolyl)borate and Dihydrobis(2-mercapto-benzothiazolyl)borate Ligands: Structural, Photophysical and Computational Studies

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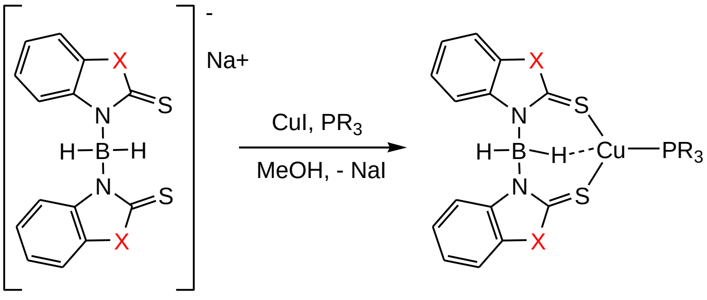
Since the discovery of Trofimenko's "scorpionate" ligands in 1966 [1], known as [hydrotris(pyrazolyl)borate], there has been great interest in their chemistry and application. These ligands could influence the properties of the transition metal center without getting directly involved in metal complex's reactivity. This view of the scorpionate ligands changed following the introduction of a new more flexible scorpionate ligand, [hydrotris(methylimidazolyl)-borate] or Tm, which is based upon a *N*-methyl-2-mercaptoimidazol-1-yl ring system. Newer scorpionate ligands have major differences compared to the Trofimenko's original ligand set [2]. They are more flexible and they are based on soft sulfur donor atoms. The flexibility of these ligands allow for B-H activation and in some instances formation of metalloboratranes. As our contribution to this field, we have developed some copper (I) complexes, supported with these ligands and phosphine donor ligands. Due to affinity of soft copper (I) ions to sulphur and phosphine ligands, the resulting complexes are highly stable and show interesting photophysical properties. We have synthesized eight copper (I) complexes with this ligand set and they are characterized fully with ^{1}H& ^{13}C NMR spectroscopies and single X-ray crystallography, whenever possible. Photophysical properties of these complexes, which is highly dependent on the nature of the phosphine ligands, will also be discussed.



NaBB; X = N-H

NaBB-2; X = S

PR$_3$ = Alkyl Phosphines

Keywords: Trofimenko, Scorpionate, pyrazolyl borate, metalloboratrane

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The role of weak intermolecular interactions in the assembly of a series of d^{10} Metal coordination polymers based on N, N'-Bis-pyridin-3-ylmethylene-naphtalene-1,5-diamine ligand; ultrasonic synthesis, spectroscopic and structural characterization

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The motivation of this work is to highlights factors that influence the supramolecular structures of d10 Metal coordination polymers. Two novel Hg(II) and Cd(II) 1D coordination polymers (CPs) have been constructed from metal iodide and a N, N'-Bis-pyridin-3-ylmethylene-naphtalene-1,5-diamine ligand using conventional method. These compounds were studied using X-ray crystallography, infrared spectroscopy and X-ray powder diffraction. These coordination polymers in nano-size were synthesized under ultrasonication and their morphology were characterized using scanning electron microscopy (SEM). Our analyses reveal the substantial role of weak hydrogen bonds and π-π stacking interactions in the assembly of these series of compounds. Coordination polymer consisting of $[Hg(L)I2]_n$ and $[Cd(L)I2]_n$ building blocks are both made up of 1D chains and their supramolecular crystal structures were studied by different geometrical and theoretical methods. The changes in the size of halides from Cl^- to I^-, which this change from Br- to I- is strikingly tangible, is accompanied by, not only changing the coordination geometry around the central metal atom which can be described as seesaw structure for 3 and 4 and distorted trigonal pyramidal for 1 and 2, but also causing changes in the type of weak intermolecular interaction in the final supramolecular assembly(from $\pi_{\text{Naphthyl}}\cdots\pi_{\text{py}}$ and C–H…π_{Naphth} in 1 and 2 to C–H…π_{Naphth}, Hg….π and N …π_{py} interactions in 3 and 4. In addition, Nanoplates of 1 and 2 were synthesized in methanol by ultrasonic irradiation and were further investigated by using scanning electron microscopy (SEM). Finally, these nanoplates were calcined at 500°C for 2 h and CdO nanoparticles brown precipitate was formed.

Keywords: *d^{10}* coordination polymer, Nano coordination polymer, π…π interactions, Cadmium oxide, Utrasonication

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Synthesis and characterization of some new Schiff base ligands and their binuclear nickel complexes

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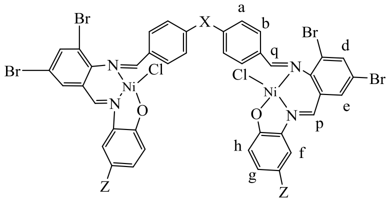
Schiff bases are condensation products of primary amines and carbonyl compounds. They are one of the most useful categories of organic compounds and have received considerable attention in theoretical and experimental investigations[1,2]. Schiff's bases are used in different areas such as catalysis, bioinorganic chemistry and drugs such as anti-corrosion, anti-cancerous, anti-HIV, anti-bacterial and anti-fungal material and DNA cleavage. Furthermore, their industrial potentials make them good choice for catalysis, transport, drug design, solar cells, chemical sensor, liquid crystal, and organic chemistry displays[3-8]. In the present research, some novel binuclear Ni(II) complexes were synthesized from some hexadentate imine ligands (NNO)$_2$ prepared *via* condensation of some diamines, 2-amino-3,5-dibromobenzaldehyde and 2-hydroxyaniline derivatives using reflux method. The compounds were elucidated using different physicochemical methods including analytical analysis, magnetic moment measurement, FT-IR, ^{1}H and ^{13}C NMR, UV/Vis spectroscopies mass and TGA.



Keywords: Schiff base, Nickel complex, 2-amino-3,5-dibromobenzaldehyde, 2-hydroxyaniline

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Synthesis and crystal structure determination of two new macrobicyclic salts containing hexahydropyrimidine moieties in the presence of Nickel(II) perchlorate and their theoretical studies

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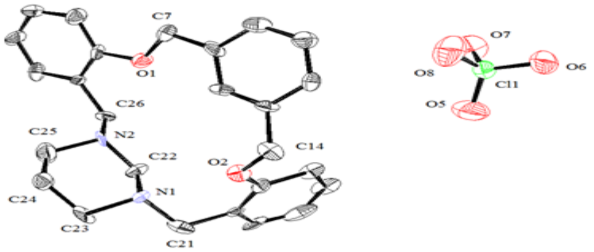
Macrocyclic structurally reinforced by the inclusion of bridging alkyl groups between nitrogen atoms in the macrocyclic ring. Reinforced macrocycles showed much greater rigidity than those nonreinforced analogueses[1]. The addition of an extra bridging group between nitrogen donors within macrocyclic ligands skeletons (to give a piperazine-like structure) leads to much more rigid ligands displaying selectivity for metal ions due to the match between the size of the metal ion and that of the macrocyclic cavity in comparison with conventional macrocyclic ligands[2].Two macrocyclic Schiff base ligands (L1, L2) and their related reduced forms (L3 and L4) have been prepared. In the presence of Ni(II) perchlorate in methanol, the reinforced macrobicyclic salts containing hexahydropyrimidine cation moiety have been developed. Here, it seems that Ni (II) perchlorate acts as oxidizing agent converting methanol to the formaldehyde which then, in turn, it bridges two nitrogen atoms of reduced forms of macrocycle producing final products. All Schiff-base ligands and their reduced forms together with related salts were characterized by elemental analysis, IR spectroscopy, ^{1}H and ^{13}C NMR, EI-Mass and in the case of [L3′](ClO4) salt by X-ray crystallography. The proposed mechanism for the formation macrobicycle ligand [L3′] from the reaction of macrocyclic ligand L3 and formaldehyde has also been studied via density functional theory (DFT).



Keywords: Macrobicycle Ligand; Hexahydropyrimidine Moieties; X-ray Crystal Structure; Density Functional Theory

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Synthesis, characterization, and in vitro cytotoxicity studies of antioxidant ferulic acid loaded on γ-Fe_2O_3@SiO_2 nanoparticles

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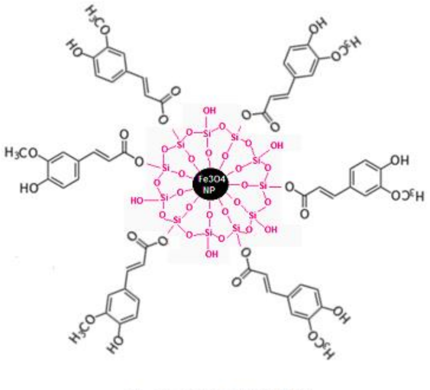
In this investigation, Fe_3O_4 magnetic nanoparticles (MNPs) were prepared via chemical coprecipitation reaction and the surface of Fe_3O_4MNPs was coated with silica by sol-gel process [1]. The surface of Fe_3O_4@SiO_2 MNPs was modified by an antioxidant agent, trans-ferulic acid, to achieve water-soluble MNPs for biological applications (Fig. 1). Fourier transform infrared spectroscopy (FT-IR) showed that the MNPs were successfully coated with SiO_2 and ferulic acid (FA) ligand. The morphology of γ-Fe_2O_3@SiO_2-FA MNPs were found to be spherical in images of transmission electron microscopy (TEM) and showed a uniform size distribution with an average diameter of 21 nm. The *in vitro* cytotoxic activity of γ-Fe_2O_3@SiO_2-FA MNPs and FA were investigated against the human cancer cells (MCF-7, PC-3, U-87 MG, A-2780 and A-549) by MTT colorimetric assay. The cytotoxic effect of MNPs on the all cancer cell lines was several times of magnitude higher compared to free FA except A-549 cell lines.



γ-Fe_2O_3@SiO_2-FA MNPs

Keywords: Magnetic nanoparticles, Ferulic acid, Cancer cell line.

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Component participation of iron-Tetra(2-pyridyl) porphyrin in activity of chloroperoxidase artificial enzyme

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For designing the pseudo-enzymes, one can look at the contribution of the components in enzymatic function as biomimetic approach. Previous studies demonstrated the role of iron metal at heme prosthetic group as catalytic foundation [1]. Also, the ligand attached to the axial position of heme activates it to perform enzymatic reactions [2]. Here, the chloroperoxidase activity of heme, iron ion (+3), synthesized iron (+3) – tetra(2-pyridyl) porphyrin complex and the synthesized non-metal tetra(2-pyridyl) porphyrin complex with cysteine and mixed surfactants “SDS-DTAB” (as hydrophobic pocket), were compared. The ascending order of activity of these compounds are “non-metal tetra(2-pyridyl) porphyrin”, hemin, “iron Fe (+3) – tetra(2-pyridyl) porphyrin”, iron ion (+3), respectively. Indeed, observation the little activity of non-metal Tetra(2-pyridyl) porphyrin is paramount of importance that can be attributed to Π-to-Π^* transitions and concluded that the central metal (iron) evolutes the chloroperoxidase function.

Keywords: Non-metal Tetra(2-pyridyl) porphyrin, Cysteine, SDS/DTAB, Biomimetic, Chloroperoxidase.

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Synthesis, characterization and catalytic properties of $MoO_2(acac)_2$ immobilized on Fe_3O_4/PANI nanocomposites

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The catalytic activity of nanoparticles (NPs) represents a rich resource for chemical processes, employed both in industry and in academia. NPs have applications in diverse fields, including energy conversion and storage, chemical manufacturing, biological applications, and environmental technology [1]. Polyaniline is one of the most versatile conducting polymers which have been extensively investigated due to its remarkable properties, such as tunable electrical conductivity, inexpensive monomer, facile synthesis and good environmental stability [2]. In this study, Fe_3O_4 magnetic nanoparticles were synthesized by hydrothermal method. Then the polyaniline was coated onto the magnetic nanoparticles. $MoO_2(acac)_2$ was then supported onto the resulting nanocomposite and heterogeneous catalyst Fe_3O_4/PANI/$MoO_2(acac)_2$ was prepared. The new catalyst was characterized by FT-IR, XRD and FE-SEM. Then the catalytic property of this compound was investigated in the epoxidation of cyclooctene as a model reaction. The various parameters such as type of solvent, type of oxidant, amount of oxidant and amount of catalyst were optimized for this reaction. The optimum conditions were found as 10 mg catalyst in dichloroethane with t-BuOOH as oxidant which gives 98% yield during 60 minutes. This catalyst was also successfully recycled for 4 times without significant reduction in epoxide yield.

Keywords: Fe_3O_4 magnetic nanoparticles, polyaniline, $MoO_2(acac)_2$, heterogeneous catalyst,epoxidation

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Synthesis and characterization of Fe_3O_4/PANI/AHS/Ag nanocomposites and its application in catalytic reductions of 2-nitroaniline and 4-nitroaniline

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Aromatic amines are important organic compounds used as astarting and an intermediates material for the manufacturing of a variety of chemicals such as biologically active natural products, pharmaceuticals, and dyes [1,2]. For this reason, catalytic reductions of nitro compounds in to aromatic amine with cost effective catalyst is important. In this study, polyaniline was coated onto the surface of magnetic nanoparticles and modified by AHS ligand (Sodium 4-amino 5-hydroxy 7-sulfonaphtalen 2-sulfonate). Then silver nitrate were loaded onto the surface of the modified polyaniline and reduced to silver nanoparticles by addition of $NaBH_4$. The structure and properties of Fe_3O_4/PANI/AHS/Ag nanocomposites were assessed by IR, XRD, ICP and FE-SEM. The catalytic reduction of 2-nitroaniline (2-NA) and 4-nitroaniline (4-NA) with $NaBH_4$ has often been used as a model reaction to evaluate the catalytic performance of nanoparticles. The reduction reactions of both 2-NA and 4-NA compounds were easily achieved due to the formation of a single product in each case and were determined by measuring the change in UV–vis absorbance at different interval of reaction time [3].The catalytic performance of the nanocomposite was tested for the reductions of 4-NA and 2-NA. The catalytic reduction results showed that the as-synthesized Fe_3O_4/PANI/AHS/Ag nanocomposites possessed superior catalytic activity for the reduction of 4-NA and 2-NA. Complete reductions of 4-NA and 2-NA took, 120s and 300s, respectively.

Keywords: nanocomposites, 2-nitroaniline, Reduction, 4-nitroaniline

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Iron porphyrinic framework as a highly efficient catalyst for oxidation of diverse alkanes

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Nowadays, one of the most important issues in organic synthesis is the selective oxidation of saturated hydrocarbons under mild conditions due to the inactivity of C-H bonds [1]. Among different catalyst used for oxidation reactions, metalloporphyrins are one of the active catalysts which oxidized different chemical reactions [2]. In this study, porphyrinic metal organic framework was prepared using iron chloride and the synthesized pyridyl porphyrin ligand. The prepared heterogeneous catalyst was characterized by XRD, FT-IR, UV-Vis, SEM, TGA-DSC and elemental analysis. The catalytic activity of the relevant prepared compound was evaluated by the oxidation of various substrates. It was found out that the prepared framework catalyzed oxidation of cyclooctane, cyclohexane, diphenyl methane and ethyl benzene with 65–100% conversions and 70–100% selectivities toward the desired product with a very small amount of catalyst. The effects of amount of catalyst on the oxidation of cyclooctane is represented in Fig 1. Based on the obtained results, the heterogeneity and reusability of the catalysts seems promising. High yields, clean reactions, high thermal stability and reusability of catalysts, make them good candidates for heterogeneous catalyst in various oxidation reactions.

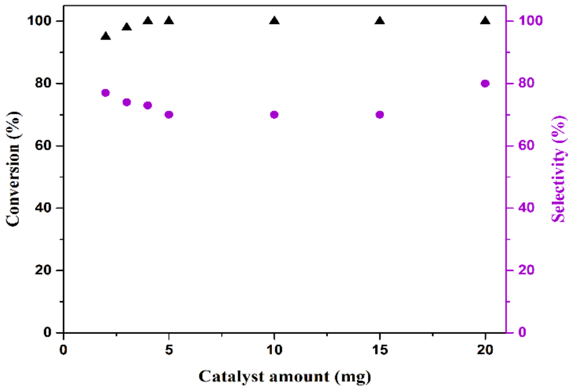

Fig 1. The effects of amount of catalyst on the oxidation of cyclooctane.

Keywords: Porphyrinic framework, oxidation, heterogeneous catalyst, alkanes.

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Epoxidation of various alkenes using cobalt porphyrinic framework as catalyst

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Alkenes oxidation is one of the important reaction in industry due to the importance and usefulness of epoxy precursor in the manufacturing of different commercial products and industrial production of chemicals such as epoxy resins, glue and polyether. Although epoxide selectivity is still a major challenge because of the byproducts formation in these reaction [1]. Metalloporphyrins are one of the best models which have been extensively explored as catalyst to oxidize various chemical reactions [2]. In this study, porphyrinic metal organic framework was prepared using cobalt chloride and the synthesized pyridyl porphyrin ligand. The prepared heterogeneous catalyst was characterized by means of XRD, TGA-DSC, UV-Vis, SEM, FT-IR and elemental analysis. The catalytic activity of the relevant prepared framework was evaluated by the epoxidation of cyclooctene, cyclohexene, norbornene and trans-stillbene with 55–100% conversions and 75–100% selectivities toward the desired product with a very small amount of catalyst. The effects of reaction time on the oxidation of cyclohexene is represented in Fig 1. Investigation of the stability and reusability of the catalysts revealed the heterogeneity character of the catalyst with no desorption during the course of oxidation reactions.

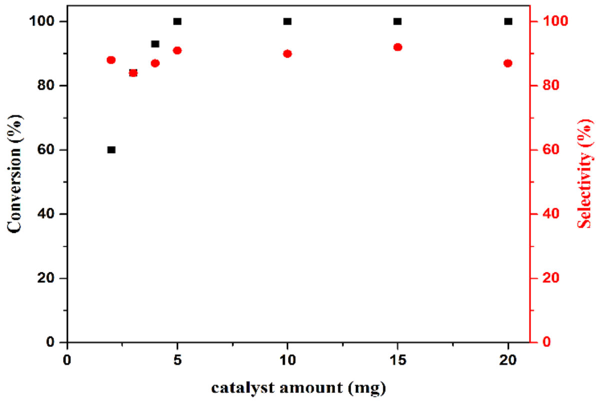

Fig 1. Kinetic oxidation profiles of cyclohexene with TBHP over the catalyst.

Keywords: Porphyrinic framework, heterogeneous catalyst, alkenes, epoxidation.

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Synthesis and characterization of sulfonated graphene as a highly active solid acid catalyst for esterification

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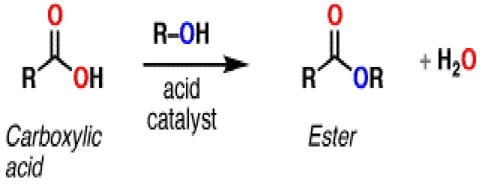
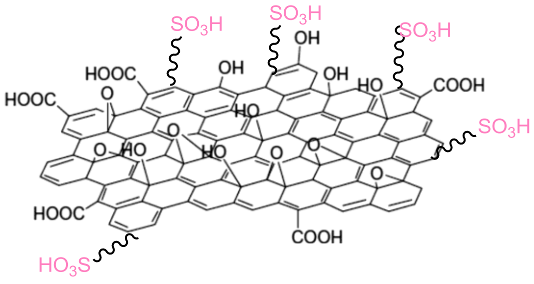
Graphene has enjoyed significant recent attention. Since it is a single atomic layer of sp^2 carbon atoms, graphene has a large surface area which makes it suitable for supporting different functional groups. Due to its large surface area and existence of oxygen functional groups on it, graphene oxide is a perfect support for immobilizing a large number of sulfonic acid groups which can exhibit high acidic properties. Therefore we prepared a solid acid catalyst based on graphene oxide with sulfonic acid agent on it. Characterization of this catalyst was performed by different physicochemical methods. The FT-IR spectroscopy and CHNS elemental analysis confirmed the grafting of sulfonic acid groups on these nano sheets. X-ray diffraction (XRD) analysis was used to identify crystal phase. Also shape and size determination of these nanoparticles were performed by transmission electron microscopy (TEM). The catalytic performance of this new graphene based solid acid catalyst as tested in the esterification of acetic acid with butanol and showed a high catalytic activity leading to 74% conversion of butanol and 100% selectivity to butyl acetate production.





Keywords: Graphene oxide, Sulfonic acid, Acid catalyst, Esterification

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Preparation and characterization of Ni-Mo-$Cs_{1.5}H_{1.5}PW_{12}O_{40}/SiO_2$ nanocatalysts

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The most popular heteropoly acids are those having the Keggin structure $H_3PW_{12}O_{40}$ (HPW). The main disadvantage of HPW is their very low surface area (<10 m^2 g^{-1}), which hinders accessibility to the acidic sites. Since the new hydrocracking catalysts are composed of HPW, it becomes necessary to overcome these drawbacks and a feasible way is to prepare supported HPW catalysts. One approach to obtain supported HPW catalysts is the impregnation of the support with a heteropolyacid solution followed by evaporation of the solvent. Silica has been widely favored as the supporting material for HPW, since it interacts weakly with the Keggin anions and thus preserves their structure. The Cs-exchanged Keggin-type heteropolyacid is well maintained at high temperatures, usually over 500°C. Conventionally, a suitable transition metal (M = Pt, Pd, Ni, Mo and Co) has been applied as the main active metal component, which is deposited on the acidic supports. In this research, Ni-Mo-Cs/HPW/SiO_2 nanocatalysts were prepared by sol-gel and impregnation methods with a solution containing the desired quantities of $Ni(NO_3)_2$, $(NH_4)_6Mo_7O_{24}.4H_2O$, Cs_2CO_3, tetraethyl orthosilicate (TEOS) and $H_3PW_{12}O_{40}$. The synthesized samples were characterized by X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDX). Morphology of the samples was studied by scanning electron microscope (SEM) and the surface area, pore volume and pore size of the catalysts were determined by BET method. The obtained results indicate that the HPW phase is loaded on the silica and the size of prepared samples is in nano-scale range. Surface area of the samples that synthesized by sol gel is more than synthesized by impregnation method.

Keywords: Nanocatalys, Hetropolyacid, Sol gel, SiO_2

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Nano tetraimine Pd(0) complex: synthesis, characterization, computational studies and catalytic applications in theHeck-Mizoroki reaction in water

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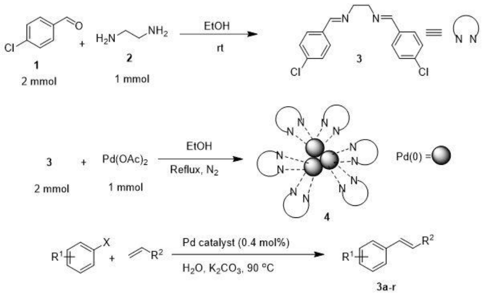
New nano tetraimine Pd(0) complex was successfully prepared by complexation of palladium acetate with a N,N-bisimine ligand. The structural features of the catalyst and ligand were characterized using some different microscopic and spectroscopic techniques such as FT-IR, XRD, XPS, UV–Vis, NMR, and the elemental analysis. The morphology of the catalyst was determined using FE-SEM, and TEM. The catalyst was effectively employed in the palladium-catalyzed Heck-Mizoroki reaction in water as a green solvent. The catalyst was reusable and recycled for six times without any decrease in its catalytic activity. Furthermore, we have theoretically explored the feasibility of two neutral and cationic pathways in the density functional theory framework.



Keywords: Nano tetraimine Pd(0) complex; catalyst, Heck-Mizoroki reaction, Grean chemistry

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Design and synthesis of three new 3D metal-organic frameworks for improved catalytic performance

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Metal-organic frameworks are newly emerged porous materials. These inorganic-organic hybrid materials have diverse crystalline structures, high surface areas, and large porosities. This dissertation is focusing on developing new design and synthetic strategies to construct novel MOFs for applications of gas storage, chemical sensing and heterogeneous catalysts [1]. Knoevenagel condensation of aldehydes with active methylene compounds is a useful transformation that has been widely employed for carbon–carbon bond formation in the synthesis of several fine chemicals [2]. Although the low thermal and chemical stability of MOFs as compared to their inorganic counterparts have restricted their use only under mild conditions, there have been several reports already that showed MOFs can be excellent heterogeneous catalysts for Knoevenagel condensation [3].

In this study three new functionalized MOFs, $[Zn_2(oba)_2(4\text{-bpdb})]_n$, $[Zn(oba)(4\text{-bpdh})_{0.5}]_n$, and $[Zn(oba)(4\text{-bpmb})_{0.5}]_n$ have been investigated for their performance as heterogeneous catalysts for the Knoevenagel condensation reaction. To characterize the possible base-type catalytic behavior of these MOFs, the Knoevenagel condensation reaction was performed in the presence of these MOFs by employing a 1 : 1.2 molar ratio of benzaldehyde and malononitrile in different solvents such as ethanol, methanol, n-hexane, … at room temperature. To the best of our knowledge, it is the first report that knoevenagel condensation is performed using functionalized MOFs. It can be deduced from these results that higher yields were achieved in polar protic solvents. Furthermore this study demonstrated that the basicity of azine functionalized pores is probably an important factor in the catalytic performance.

Keywords: Metal–organic frameworks, Knoevenagel condensation

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Synthesis, characterization and absorption ability of $MgFe_2O_4$/graphene magnetic nanocomposite for removal of methylene blue dye pollutants from aqueous solution

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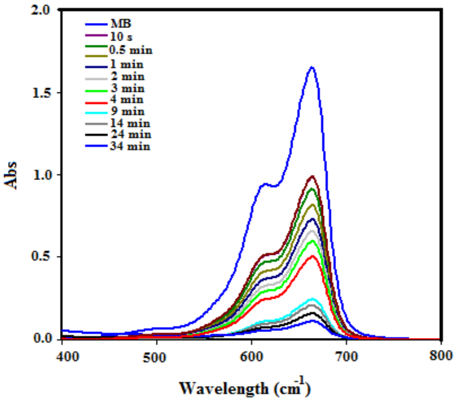
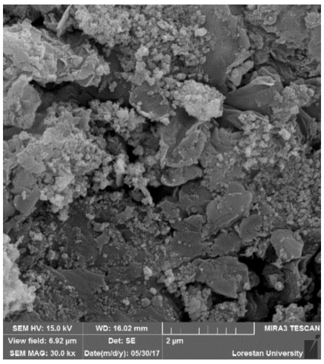
Organic dyes are widely used in various fields and seriously induce water pollution[1,2]. The treatment of industrial effluents is a challenging topic in environmental science, as control of water pollution has become of increasing importance in recent years [3].

In this work, the $MgFe_2O_4$/graphene magnetic nanocomposite was synthesized by hydrothermal method. The nanocomposite was characterized with different analysis such as FT-IR, XRD, SEM, EDAX and VSM. The SEM images show that the $MgFe_2O_4$ nanoparticles are uniformly dispersed on graphene sheets. The $MgFe_2O_4$/graphene nanocomposite used as an afficient adsorbent for removal of methylene blue organic dye . The result of adsorption experiments demonstrate that synthesize nanocomposite can effectively remove methylene blue organic dye pollutants from aqueous solution and removal efficiently of 94 % in 34 min.





Keywords: Graphene oxide**,** Magnesium acetate, Sodium acetate

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Preparation and photocatalytic properties of magnetically recoverable Ce–Ag–ZnO/ Fe_3O_4 nanoparticles

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Recently, many techniques have been developed for the removal of pollutants from wastewaters to limit their impact on the environment. Photocatalytic treatment of wastewater has proven to be an effective process for the degradation of dye pollutants.

Ce, Ag codoped ZnO/ Fe_3O_4 nanoparticles were synthesized following an eco-friendly synthesis method, at mild temperature and used as an effective photocatalyst for the photocatalytic degradation of harmful and toxic organic dye.

The prepared nanoparticles were characterized in detail using different techniques for morphological, structural and optical properties. The X-ray diffraction (XRD) patterns studies revealed hexagonal wurtzite ZnO and magnetite Fe_3O_4. Field emission scanning electron microscope (FE-SEM) micrographs show a spherical shape and nearly well distribution with an average particle size of 20–30 nm. Energy-dispersive X-ray spectroscopy (EDX) reveals the successful doping concentration of Ce and Ag. Ultra violet- visible spectroscopy (UV-VIS) shows a red shift in the absorbance spectrum with increasing the various co-doping concentration. Photoluminescence spectra (PL) studies were done under the excitation of 360 nm, which shows the existence of Ce–Ag–ZnO/ Fe_3O_4 reduces the emission intensity lines.

The photocatalytic activity of prepared nanoparticles was evaluated by the photocatalytic degradation of methylene blue (MB) dye. The photodegradation of MB proceeds much more rapidly in the presence of Ce–Ag–ZnO/ Fe_3O_4 compared to the bare ZnO nanoparticles. The presented work demonstrates that the prepared recyclable nanoparticles are promising material for the photocatalytic degradation of organic dyes and toxic chemicals.

Keywords: ZnO, Fe_3O_4, Recyclable nanoparticles, Photocatalyst

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Photo Degradation Of Azo Dye Congo Red by Hexagonal ZnO Nano Disc structure

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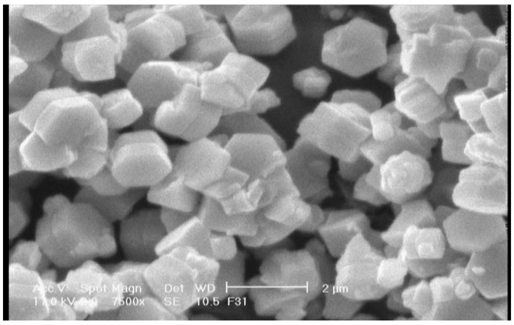
Dye pollutants are harmful species produced by industries and their removal is of importance from environmental point of view. Release of dye containing waste water in the ecosystem leads to huge aesthetic pollution and perturbations in aquatic life [1]. Most of the organic dyes are not easily degradable by standard biological methods. Recently photocatalytic degradation of various kind of organic and inorganic pollutant has been extensively studied using semiconductor metal oxides as photocatalysts [2]. ZnO is a wide bond gap oxide semiconductor with a direct energy bond gap of about 3.3eV, and consequently absorbs UV radiation through bond to bond transition [3]. In this study we report a simple method for the preparation of ZnO hexagonal nano disc structure. The samples characterized by SEM, XRD and BET. Congo red, a typical azo dye with two (-N=N-) azo bonds, is used to investigate the catalyst efficiency for photocatalytic elimination of pollutants and a 30 W high pressure Hg Vapor lamp is used as light source.



Keywords: Zinc oxide, Azo dye, Nano disc structure.

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Nanohybrid catalyst of porphyrin based on metal oxide semiconductors and their performance evaluation in the organic synthesis

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In the present study, we show the synthesis, structure and optical properties of a porphyrin and its cobalt complex[1,2] covalently assembled on $TiO_2/BiVO_4$ nanocomposite. The prepared catalysts were characterized by different techniques including FESEM, EDAX, XRD, DRS and FT-IR spectroscopy. The photocatalytic activity of catalysts were evaluated for the oxidation of various primary alcohols under visible light irradiation in the presence of oxygen source and environmentally friendly oxidant under different solvents conditions. Also, the effects of parameters such as solvent, amount of catalysts, reaction temperature, Effect of different oxidant, Effect of oxidant/substrate Ratios and utilization efficiency of hydrogen peroxide were investigated. The modification of TiO_2-$BiVO_4$ with porphyrin led to an increase in its photocatalytic activity under UV and visible-light. The photocatalytic activity of nanomaterials was then determined by GC-Mass. The stability of these photocatalysts was also investigated, and the results showed that they can be reused several times without appreciable loss of activity.

Keywords: Photocatalyst, Porphyrin, Nanocamposite

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Effect of additives on gelation time of silica network in SiO_2-NiO, and SiO_2-ZnO nanocomposites

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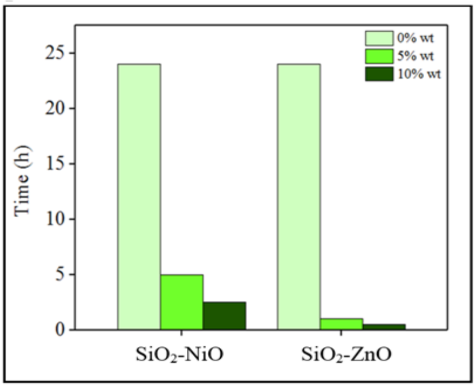
In this work, we report a study on gelation time and structural aspects of SiO_2-NiO and SiO_2-ZnO binary systems prepared by sol–gel method. These nanocomposites were prepared at 5 and 10 wt% and annealed at different temperatures from 200 to 800 °C. The solution required for the synthesis of SiO_2 sol consisted tetraethyl orthosilicate (TEOS), ethanol, water and HCl. The materials used as the NiO and ZnO precursors were hexahydrated nickel-nitrate $Ni(NO_3)_2 \cdot 6H_2O$ and zinc acetate dihydrate $Zn(OAc)_2.2H_2O$, respectively. These precursors were added to the SiO_2 sol solution and the gelation time was considered. Average gelation time from the 3 runs of the reactions varied from 30 min to 24 h. After aging the gel in air for 24 h, the impact of various annealing temperatures on crystal structure of the nanocomposites was also inspected. The crystal structures of the prepared samples were characterized by X-ray diffraction (XRD). These materials would be great candidates for sensor applications.



Keywords: gelation time, sol-gel, SiO_2-NiO, SiO_2-ZnO

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Synthesis, characterization and film deposition of the WO_3 nanowires

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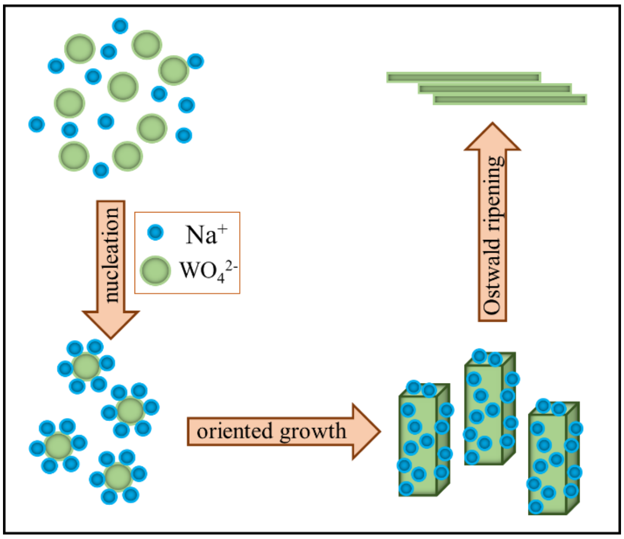
WO_3 nanowires were synthesized successfully via a one-step hydrothermal method. The details of morphology and crystalline nature of the prepared sample were characterized by scanning electron microscopy (SEM) and X-Ray diffraction (XRD). The WO_3 nanowires had uniform size with diameters around 30 nm and they had single morphology. Moreover, based on characterization and analyses, a possible growth mechanism of the WO_3 nanowires was also proposed. The investigation of the experimental parameters demonstrated that the sodium tungstate dihydrate ($Na_2WO_4.2H_2O$) played a crucial role in determining the structure and properties of the final products, which has acted as morphology director. The dip-coating technique was used to create a monotonic WO_3 nanowire thin film. Thin film was deposited on quartz substrate from powder sample dispersed in ethanol and dried in air. The simple preparation strategy, excellent morphology and improved features of the one-dimensional nanowire structures held substantial promise for rendering WO_3 as sensing element in future sensor applications.



Keywords: WO_3, Hydrothermal, Growth, Thin film

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Preparation and characterization of Ni/Ce-ZrO_2 nanocatalysts with different supports

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The acidic nature of ZrO_2 has been found to have an excellent effect on acid-catalyzed reaction. The acidic properties of ZrO_2 modify the surface properties of this compound such as crystallinity, surface area and pore distribution. In this research, Ni/Ce-ZrO_2 catalysts with different supports (SiO_2 and γ-Al_2O_3) were prepared by a two-step impregnation method. The synthesized samples were characterized by X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDX). Morphology of the samples were studied by field emission scanning electron microscope (FESEM) and surface areas of the catalysts were determined by BET (Brunauer-Emmett-Teller) method. The XRD patterns of the catalysts showed two groups of diffraction peaks. One group corresponded to the cubic crystal structure, and the other group corresponded to the tetragonal structure. Result showed that a mixed structure of the cubic Ce-rich solid solution and the tetragonal Zr-rich solid solution was formed instead of a homogeneous Ce-ZrO_2 solid solution. The obtained results indicated that the size of prepared samples was in nanometer range and the surface area of the catalyst with the silica base was more than that of the catalyst with the gamma alumina base.

Keywords: Nanocatalysts; Zirconium oxide; Silica; γ-Alumina

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Characterizing the synthesized graphite/magnetite nano-composites using ultrasonic waves

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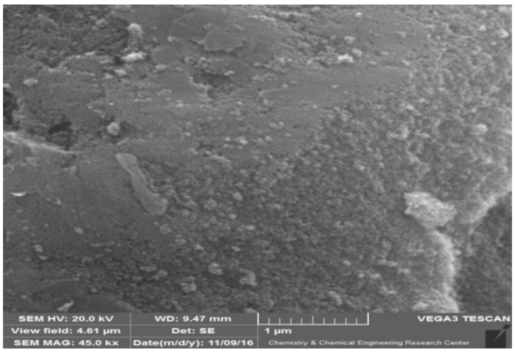
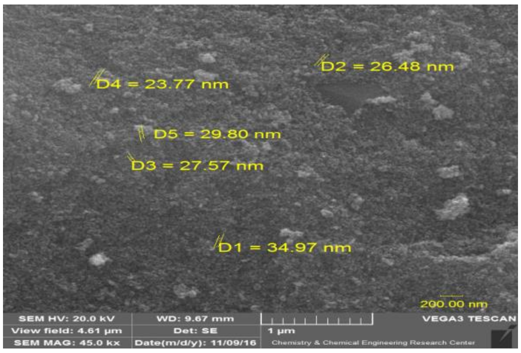
A composite material is made by combining two or more materials which they work together to give unique properties. However, each of the materials alone does not have the desired characteristics. In this study, the graphite/magnetite nano-composites were synthesized using ultrasonic waves in one step process with different weight percentage of graphite in relation to the Fe_3O_4. The prepared samples were characterized using SEM, BET, XRD techniques.

Finally, the synthesized samples were studied to use as precursor of supercapacitor to apply in energy storage devices. The fabricated supercapacitor electrodes were investigated using electrochemical methods such as cyclic voltmetery (CV), chronopotentiometry (CP) and electrochemical impedance spectroscopy (EIS) [1, 2].





Keywords: Nano-composite, Graphite, Magnetite, Ultrasonic waves

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Synthesis, characterization and crystal Structure of the new dihalooplatinum(II): A new precursor for the preparation of platinum nanoparticles

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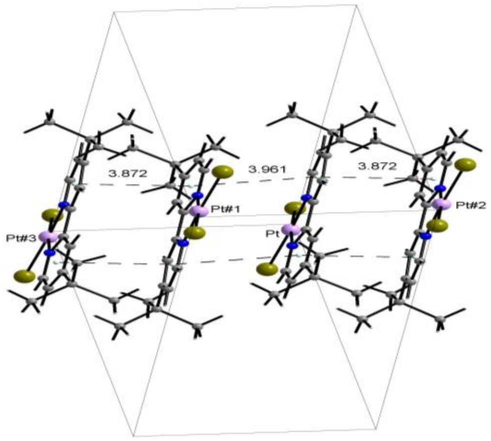
A good deal of scientific studies has been devoted to synthesize of noble metal nanoparticles due to their noteworthy properties and applications in a wide range of fields. Platinum nanoparticles are of particular interest in nanotechnology due to their high practical catalytic activities, such as the methanol oxidation, oxygen reduction and others [1]. It has been found that metal coordination complexes can be suitable precursors for the preparation of metal nanoparticles [2]. The application of platinum(II) complexes as a precursor for the preparation of platinum nanoparticles has not been investigated widely. In the present study, we have prepared some dihaloplatinum(II) complexes of $[PtX_2(NN)]$ (NN = diimine; X = Cl, Br, I). In addition, the platinum nanoparticles were obtained by the calcination of the dihaloplatinum(II) complexes. The resulting nanoparticles were investigated by X-ray powder diffraction (XRD), energy-dispersive X-ray (EDX) and field emission scanning electron microscopy (FESEM) analyses. The average particle size by use of Scherrer's equation is calculated to be about 27.5 nm. The crystal structure of the yellow polymorph of $[PtBr_2(bu_2bpy)]$ (bu_2bpy = 4,4'-di-*tert*-butyl-2,2'-bipyridine) will be discussed.



Keywords: Platinum, Nanoparticles, Diimine, Crystal structure, Polymorphism

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Synthesis and characterization of Ni-Cr-Al LDH and its sensing behavior

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In recent years, layered double hydroxides (LDH), also known as anionic or hydrotalcite-like clays, have growing interest for using in the wide fields owing to their attracted desirable properties, which include good biocompatibility, intense adsorbaility, high catalytic activity, low cost, and high chemical stability. Ni–Cr-Al layered double hydroxide was synthesized by the co-precipitation method in constant pH, at various temperatures and various Ni^{2+}/Cr^{3+} / Al^{3+} molar ratios in H_2O [1]. The samples (LDHs) characterized [2-3] by powder X-ray diffraction, FT-IR and TEM. Then its sensing properties were investigated at room temperature. In this research, the sensor response was recorded in the presence and absence and various concentrations of VOCs. Desirable properties for a sensor include high sensitivity, low detection limit, good reproducibility, long-term stability, fast current response, and low interference. Most of these properties exist in our sensor.

Keywords: LDH, Layered double hydroxide, Coprecipitation, Sensor

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Post-Synthesis Functionalization of Hollow Mesoporous Silica Nanospheres for an Anticancer Drug Delivery system

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Recently, hollow mesoporous silica nanospheres (HMSNs) have been studied as potential drug carrier materials as a result of their unique properties, such as large internal void space and well-ordered mesoporous shell pore channel. In this study, glycine functionalized hollow mesoporous silica nanospheres (gly-HMSNs) were successfully synthesized by a post-synthesis process. The prepared samples were characterized by FTIR, SAXS, N_2 adsorption-desorption, SEM, TEM and thermograviametric analysis techniques. The effect of the surface functionalization on the adsorption capacity and release profile of cisplatin (as an anticancer drug) was investigated. We found that the surface functionalization of HMSNs increases the loading capacity of drug. Moreover, release tests performed at two times in phosphate buffered saline (PBS, pH of 7.4) media showed a sustained and controlled release of cisplatin from the synthesized gly-HMSNs. The cytotoxicity effect of the as-synthesized gly-HMSNs was carried out in MCF-7 cell lines by MTT assay and the data proved that this material have a negligible toxicity. This results indicated that this support could be effective carrier for anticancer drug delivery systems.

Keywords: Hollow mesoporous silica nanospheres (HMSNs), Drug release, Cytotoxicity, Cisplatin

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Preparation of a novel, efficient, and recyclable catalyst, Polyoxometalate/zirconia nanocomposite, For Biginelli reaction

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This paper describes an improved procedure and simple method for the efficient and facile synthesis of 3,4-dihydropyrimidinones with using inexpensive heteropolyacid catalyst. Efficient catalysts are key materials in chemical technologies which supply useful substances to society and assist maintaining the environment as healthy as possible. HPAs have several advantages as catalysts which make them economically and environmentally attractive. They have very strong Brønsted acidity approaching the superacid region and this acid base property can be varied over a wide range by changing the chemical composition. Nevertheless, the main drawback of this kind of material for catalytic applications is sepration and reused, that is difficult. Therefore, for many catalytic applications, the dispersion of HPA onto a high surface area carrier is desirable. In this research, polyoxometalate supported on nano-zirconia was prepared and its catalytic performance was evaluated in three component condensation of benzaldehyde, ethyl acetoacetate and urea or thiourea to afford corresponding 3,4-dihydropyrimidin-2(1H)-ones(thiones).The structure of the synthesized nanocomposite catalyst was systematically characterized by various analytical and spectroscopic techniques such as (FT-IR) spectroscopy using the KBr pellet technique The phases present in the catalyst were analyzed using powder XRD The morphology of nanocomposite revealed by a scanning electron microscope (SEM). The biginelli reaction products were characterized by FT-IR, ^{1}H NMR and ^{13}C NMR and comparison of their physical properties with those reported in the literature. DHPM synthesised in excellent yields and high purity. The low cost catalyst has exhibited remarkable reactivity and reusability.

Keywords: Heteropolyacids, Nanocomposite catalyst , Nano-zirconia, Biginelli reaction, Reusability

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Evaluation of textural properties of γ-Al_2O_3 nanoparticles synthesized by Multi-step precipitation

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Mesoporous γ-Al_2O_3 is an important inorganic material used as an adsorbent and catalyst support in commercials catalytic applications, especially in hydrotreating catalysts. Hydrotreating is a precise process for the successful performance of oil refining. Hydrodemetallization (HDM), Hydrodesulfurization (HDS) and Hydrodenitrogenation (HDN) are examples of Hydrotreating processes [1]. It is know that asphaltene in the heavy oils have a determinant effect on the activity of a catalyst. So, the presence of large pores in support in the range 10-20 nm is important for Hydrotreating of large molecules such as asphaltene [2]. The present work aims to experimentally synthesize the high pore size of the alumina, which are suitable for Hydrotreating of heavy oils including Hydrodemetallization and Hydrodesulfurization. In this study, γ-Al_2O_3 nanoparticles were synthesized through a Multi-step precipitation method by varying the pH from 3 to 8, and repeating it alternatively. Textural properties of γ-Al_2O_3 nanoparticles were controlled through the number of pH swinging frequencies. Prepared samples were characterized by XRD and SEM techniques. In addition, specific surface area and pore size distribution of the obtained samples were determined by BET method. XRD patterns revealed that the sample prepared with high the number of pH swinging frequencies has a higher crystalline size. The most important γ-Al_2O_3 peaks in the XRD pattern correspond to 2θ of 37.6, 39.5, 45.8 and 66.8. All diffraction peaks of the samples show cubic structure. The results of BET analysis showed that synthesized γ-Al_2O_3 nanoparticles have a pore size between 14.7 nm and 12.3 nm.

Keywords: γ-Al_2O_3 nanoparticles, mesoporous, Multi-step precipitation method, Hydrotreating

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Synthesis, characterization and immobilization of a novel mononuclear vanadium (V) complex on modified magnetic nanoparticles as catalyst for epoxidation of allyl alcohols

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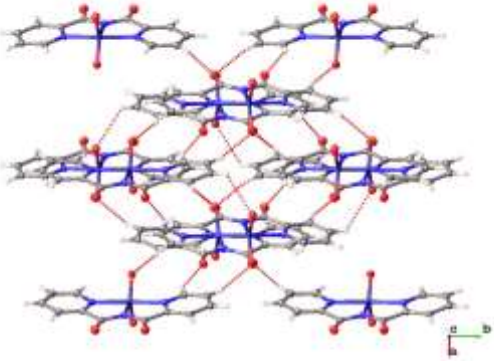
The coordination chemistry of vanadium is of current interest because of vanadium in metaloenzymes. Several vanadium complexes with polypyridyl ligands have been synthesized and used as anti-protozoa, anti-tumor, antiparasitic, DNA cleavage, and insulin mimetic activity[1]. Besides vanadium is also a relevant element in several industrial fields as homogeneous and heterogeneous catalysts [2]. In this study bis(2-pyridyl carbonyl)amid) VO complex designated as [VO_2(bpca)] was prepared from hydrolysis of 2,4,6-tris(2-pyridyl)-1,3,5-triazine (tptz) in the presence of VO(SO_4) in an alkaline solution. Single-crystal X-ray crystallography revealed that the coordination of V in complex is a distorted square-pyramid coordinated with three nitrogen of bis(2-pyridyl carbonyl)amid) ligand and two binding oxygen atoms. The prepared complex which successfully supported on modified Fe_3O_4 nanoparticles (nanocatalyst). The complex and nanocatalyst were characterized by means of FT-IR, XRD, VSM , SEM and TEM. The catalytic activity of [VO_2 (bpca)] complex and prepared nanocatalyst were evaluated by the epoxidation of geraniol, 3-methyl-2-buten-1-ol, trans-2-hexen-1-ol and 1-octen-3-ol with 70–98% conversions and 95–100% selectivities. Based on the obtained results, the heterogeneity and reusability of the catalysts seems promising. In addition, the in vitro antibacterial activity of [VO_2 (bpca)] complex have also been evaluated and compared.



Keywords: Vanadium (V) complex, Bis (2-pyridyl carbonyl)amid, Nanomagnet, Epoxidation, Allylalcohols.

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Synthesis and characterization of chitosan coated iron oxide magnetic nanoparticles for controlled delivery of nevirapine in biomedical applications

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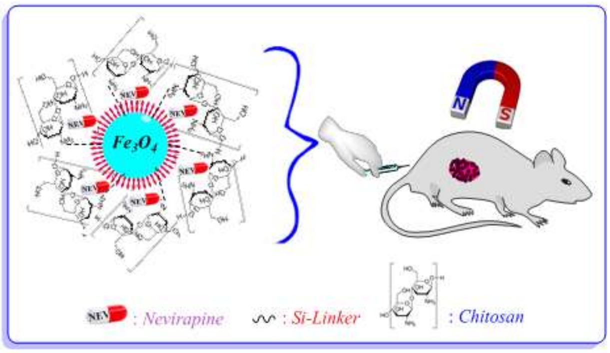
In the past decade, the synthesis of superparamagnetic nanoparticles has been intensively developed not only for its fundamental scientific interest but also for many technological applications: among others, magnetic storage media [1]. In this study magnetic iron oxide nanoparticles (MIONPs) were modified with Si-based linker, which resulted in formation of chlorine groups on the particles surface. The chlorine functionalized MIONPs can bind to chitosan [2-3]. The obtained nanomaterials were characterized by several techniques including fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), vibrational sampling magnetometer (VSM), field-emission scanning electron microscope (FE-SEM), energy-dispersive X-ray spectroscopy (EDX) and thermogravimetric analysis (TGA). The (Nevirapine = NEV) NEV-loading efficiency determined by UV–Vis spectrometer. The controlled delivery effect of Chitosan@MIONPs was tested for nevirapine in different conditions. The results show the high drug loading and the low release time for the prepared nanomaterials. The prepared NEV-grafted magnetic nanoparticles showed a superparamagnetic property with a saturation magnetization value of 35.7 emu g^{-1}, indicating an unlimited potential application in the treatment of cancer using magnetic targeting drug delivery technology.



Scheme 1. A schematic diagram for injection of new drug carrier to mice.

Keywords: UV-Vis, Nevriapine, Chitosan, Drug delivery.

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Synthesis, characterization and biomedical application of human serum albumin coated iron oxide nanoparticles for releasing drug at a controlled rate

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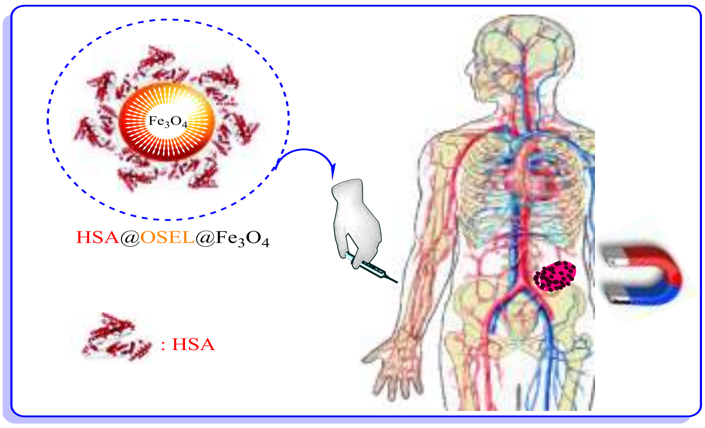
Human serum albumin (HSA) is the most abundant protein in plasma, and it can serve as a versatile carrier for drug delivery as well as for prolonging the active profile of fast-clearance drugs [1]. This work reports the synthesis and characterization of human serum albumin (HSA) coated iron oxide nanoparticles by chemical co-precipitation method to determine the optimum conditions in controlled drug delivery [2-3]. This nanosystem is well-suited for dual encapsulation of HSA@Fe_3O_4 and oseltamivir molecules, because the encapsulation is achieved in a way that is similar to common drug loading. Drug attachments were examined by Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), vibrational sampling magnetometer (VSM), field-emission scanning electron microscope (FESEM), energy-dispersive X-ray spectroscopy (EDX) and thermogravimetric analysis (TGA). The (Oseltamivir=OSEL) OSEL-loading efficiency determined by UV–Vis spectrometer. Moreover, HSA-based magnetic nanoparticles carrier systems represent an attractive drug loading and the low release time for the prepared nanomaterials in drug delivery.



Scheme 1. A schematic diagram for injection of new drug carrier to patient.

Keywords: HSA, UV–Vis, Oseltamivir, Drug delivery

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Nanostructured mesoporous Co-Ni Layered Double Hydroxide (LDH) and Brucite-Like Co-Ni Hydroxide: Preparation, Characterization, and Application as Heterogeneous Catalysts

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Layered materials have great importance in a variety of applications including catalysis, photocatalyst, and drug delivery [1]. Hydroxides of cobalt and nickel are well-known to crystallize in two polymorphs, α and β. The β-hydroxides are composed of neutral metal hydroxide layers similar to brucite in which M^{2+} is surrounded octahedrally by six hydroxyl ions, while the α-hydroxides are isostructural with hydrotalcite-like compounds (LDHs) and consist of positively charged layers of metal hydroxides that are separated by intercalated anions and water molecules in the gallery to restore charge neutrality [2]. In this study, nanostructured mesoporous α- and β-Co-Ni hydroxides were synthesized by a hydrothermal method. The samples were characterized by XRD, Fe-SEM/EDX, FT-IR, TGA, UV-vis and nitrogen adsorption-desorption isotherm. The samples were employed as heterogeneous catalysts in the oxidation of benzyl alcohol, *N*-formylation of aniline, and the Claisen–Schmidt condensation. In all of the three reactions, the conversion enhanced by increasing the amount of catalysts from 10 to 30 mg, and the catalytic activity of Co-Ni LDH was better than that of brucite-like Co-Ni hydroxide. In benzyl alcohol oxidation, the best conversion for Co-Ni LDH and brucite-like Co-Ni hydroxide was 90% and 80%, respectively, in solvent-free conditions. In *N*-formylation, the best conversion for both catalysts was obtained 95% in solvent-free conditions. However, the time required for Co-Ni LDH to reach this amount was a quarter of that for brucite-like Co-Ni hydroxide. For the Claisen–Schmidt condensation, the best result (70% for Co-Ni LDH and 50% for brucite-like Co-Ni hydroxide) was obtained at 90ºC.

Keywords: Co-Ni layered double hydroxide, Brucite-like Co-Ni hydroxide, Oxidation of benzyl alcohol, N-formylation of aniline, Claisen–Schmidt condensation

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Two new Copper(II) complexes with chelating N,O-type bidentate ligands: Synthesis, characterization, crystal structure and catalytic activity in azide-alkyne cycloaddition reaction

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1,2,3-Triazoles are an very important class of aromatic five-membered heterocyclic compounds which applied in agrochemicals, drug and industrial utilizations. Because of unique properties and impressive applications of these compounds, various synthetic methods have been developed for their synthesis recently. The Huisgen 1,3-dipolar cycloaddition reaction of terminal alkynes and azides that modified by Sharpless and Meldal in 2002, is a valuable, powerful and popular method for the synthesis of 1,2,3-triazoles [1-3].

In this study, two new copper(II) complexes, [CuL_2] and [$Cu(phox)_2$], were synthesized by reaction of 1-((4-bromophenylimino)methyl)naphthalen-2-ol, HL, and 2-(2′-hydroxyphenyl)-2-oxazoline, Hphox, ligands with copper acetate, respectively. The synthesized complexes were characterized using FT-IR spectroscopy, elemental analyses, and their solid state structures were confirmed by single crystal X-ray diffraction. The catalytic activity of the complexes was evaluated in azide–alkyne cycloaddition (AAC) click reaction in water without any additional reducing agents or bases. The [CuL_2] complex showed high catalytic activity in this reaction and 1,2,3-triazole derivatives were produced in moderate to good yields.

Keywords: Copper, azide–alkyne cycloaddition, 1, 2, 3-triazoles, N,O-bidentate ligands

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Synthesis, characterization and unveiling the biological activities of two novel orthopalladated complexes; interactions with DNA and BSA

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Two new orthopalladated complexes [Pd(L_1)(HQ)] (1) and [Pd(L_2)(HQ)](2), (L_1 =2-Biphenylylamine, L_2 = 3-phenylimidazi[1,5-a]-pyridine, and HQ = 8-hydroxyquinoline) are obtained in two steps by the reaction of palladacyclic dimer with 8-hydroxyquinoline. They have been synthesized and characterized by using IR, NMR and elemental analysis and thermal denaturation studies. The binding of the complexes with native calf thymus DNA (CT-DNA) were monitored by UV-V is absorption spectrophotometry, fluorescence spectroscopy. Our experiments indicate that these complexes could strongly bind to CT-DNA via partial intercalative mode. In addition, fluorescence spectrometry of the bovine serum albumin (BSA) with the complexes, showed that the fluorescence quenching mechanisms of BSA were static process. The results of site-competitive replacement experiments with specific site markers clearly helped us to conclude that complexes bind to site I of BSA.. Finally, the molecular docking experiment effectively proved the binding of Pd (II) complexes to DNA and BSA.

Keywords: Pd complexes; CT-DNA binding; BSA binding; Anticancer activity

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Palladium Schiff base metal complexes immobilized on GO- $MnFe_2O_4$ for reduction of para-nitro phenol

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Palladium Schiff base metal complexes have been covalently grafted on to GO- $MnFe_2O_4$ previously functionalized with 3-aminopropyltriethoxysilane. Potential catalytic behavior was tested in the reduction of para-nitro phenol to para amino phenol by an excess of $NaBH_4$ in an aqueous medium at room temperature. The reduction of para nitro phenol was monitored using UV-Vis absorption spectroscopy. The catalyst was characterized using infrared (IR), thermogravimetric analyses TGA, inductively coupled plasma atomic emission spectrometry (ICP-AES), X-ray diffraction and transmission electron microscopy (TEM). IR spectroscopy, thermogravimetric analyses and ICP-AES confirmed the successful incorporation of the metal Schiff base complexes onto GO- $MnFe_2O_4$. X-ray diffraction and TEM showed the intact structure of the GO- $MnFe_2O_4$ palladium Schiff base complex on the Go-$MnFe_2O_4$ showed high catalytic activity in reduction of para nitro phenol. The recycling results of these heterogeneous catalysts showed good recoverability without significant loss of activity and selectivity within four successive runs.

Keywords: Schiff base metal complexes; graphene oxide, reduction of para-nitro phenol

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Synthesis and Characterization of $Co_3(BTC)_2$-Polyaniline Composite

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Due to tunable compositions, porous structure, and high surface areas, metal-organic frameworks (MOF) have attracted significant attention as viable materials with potential for applications in, e.g., pollutant and gas separation, gas storage, and drug delivery [1]. However, the main obstacle for their application in energy and electronic systems is their low conductivity. Incorporating compounds that are good conductors such as conductive polymers (polyaniline, polypyrrole and polytiophene) can be considered as an efficient way to improve conductivity of MOFs [2,3]. In the present work at first, $Co_3(BTC)_2$ was prepared by hydrothermal synthesis method. After this, $Co_3(BTC)_2$-Polyaniline composite was synthesized by polymerization of aniline in the presence of MOF where ammonium persulfate was used as oxidant. The successful synthesis of the composite was confirmed by FTIR spectroscopy, SEM, EDX, and XRD techniques. The IR spectrum of the final product exhibited characteristic peaks at 1562 and 1494 cm^{-1} that are assigned to the quinine and benzene ring stress deformation, respectively. The peaks at 1524-1612 and 1370-1474 cm^{-1} region are attributed to asymmetric and symmetric vibrations of carboxylic groups of the MOF linkers. The presence of polyaniline and $Co_3(BTC)_2$ was also confirmed by energy disperse X-ray spectroscopy (EDX). A good agreement was obtained between X-ray diffraction patterns of the composite with polyaniline and cobalt MOF diffraction patterns. Due to high surface area and good electrical conductivity, this porous composite has excellent potential to be used as absorbent or supercapacitor.

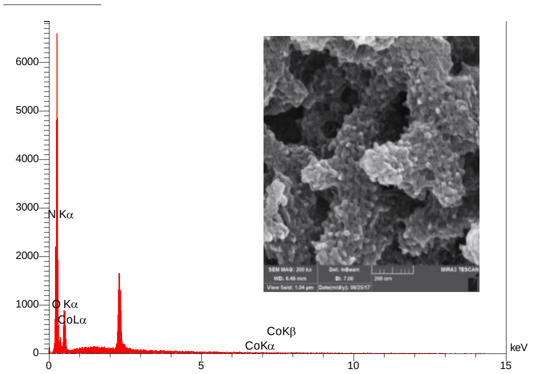

Fig. 1. SEM and EDX image of the $Co_3(BTC)_2$-Polyaniline composite.

Keywords: Metal-Organic Framework, Solvothermal synthesis, Polyaniline, Composite

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Synthesis and characterization Metal-Organic Framework (MOF) vanadate composite by modified sol-gel method for aromatic desulfurization of hydrocarbons as a model fuel

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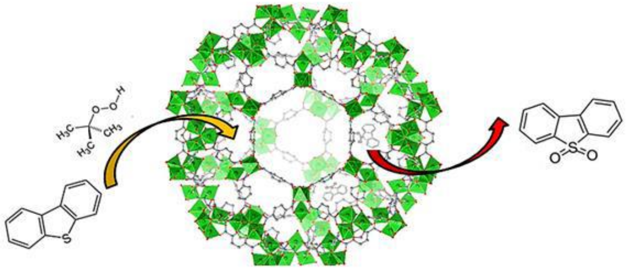
The ultra-deep desulfurization of gasoline and diesel fuel is continuous to attract attention in academia and industry owing to the environmental concern of these fuels. The majority of global petroleum reserves contain sour crudes, and there is a great demand to improve the efficiency of the desulfurization technology. According to new environmental regulations in several countries, the sulfur level in gasoline and diesel fuel must be reduced to below 10 ppm, which is called "S-free" fuel. The main objective of this work was to develop a new route for the preparation of advanced functional inorganic materials for aromatic desulfurization of hydrocarbons from simulated fuel. Metal-Organic Frameworks (MOFs) with unique properties, including crystallinity, large and tuneable pore size and strong interaction between polytopic ligands and metal ions became an important class of pore materials. These classes of compounds have found their way through science by their fascinating framework topologies and design flexibility in which lead to broad applications in gas storage, gas separation, catalysis, sensors, and drug delivery systems. In this work, MOF/vanadate composite was prepared by infiltration of vanadium alkoxide, and after characterization with XRD, BET, SEM, TGA-DTA, and IR was used a catalyst for oxidative desulfurization of dibenzothiophene from simulated fuel. Results showed that the prepared composite is an efficient catalyst for aromatic oxidative desulfurization of hydrocarbons.



Keywords: MOF; MIL-101(Cr); MOF-A520, Vanadate; Desulfurization; Dibenzothiophene

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Antibacterial activity of noble metal decorated nickel ferrite-mordenite nanocomposites

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Functionalized magnetic core-zeolitic shell nanostructures were prepared by hydrothermal and coprecipitation methods. The products were characterized by Vibrating Sample Magnetometer (VSM), X-ray powder diffraction (XRD), Fourier Transform Infrared spectra (FTIR), nitrogen adsorption-desorption isotherms, and Transmission Electron Microscopy (TEM). The growth of mordenite nanoparticles on the surface of silica coated nickel ferrite nanoparticles in the presence of organic templates, was also confirmed. Antibacterial activity of the prepared nanostructures was investigated by the inactivation of E.coli as a gram negative bacterium. A new mechanism was proposed for inactivation of E.coli over the prepared samples. In addition, the Minimum Inhibitory Concentration (MIC) and reuse ability were studied. TEM images of the destroyed cell wall after the treatment time were performed to illustrate the inactivation mechanism. According to the experimental results, the core-shell nanostructures which were modified by organic agents and then, functionalized with noble metal nanoparticles, were the most active which was predicted from the earlier studies [1, 2].

Keywords: Magnetic core-zeolitic shell nanostructure, Antibacterial activity, Nickel ferrite, Mordenite, E.coli

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Reduction and Dechlorination of Chlorinated ethylenes by nano Particles of Iron doped on Graphen Oxide Sheets

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In this paper, a new criterion for reducing chlorinated ethylenes is proposed. The proposed method is based on converting graphene oxide into magnetic sheets by nano zero valent iron particles. A laboratory study conducted to investigate to remove chlorinated ethylenes from aqueous solution. Dechlorination reaction of two important pollutants in the environment, 1,1,2-tri-chloroethene(TCE) and tetra-chloroetene(PCE) studied. The results showed that both pollutants converted almost completely in presence of magnetic graphene oxide surfaces.

Keywords: Magnetic graphene oxide surfaces, Graphene magnetic nanoparticles of iron, Removal of chlorinated contaminants

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$AlCl_3$ as a Highly Efficient Catalyst for Chemoselective Oxidation of Alkynes

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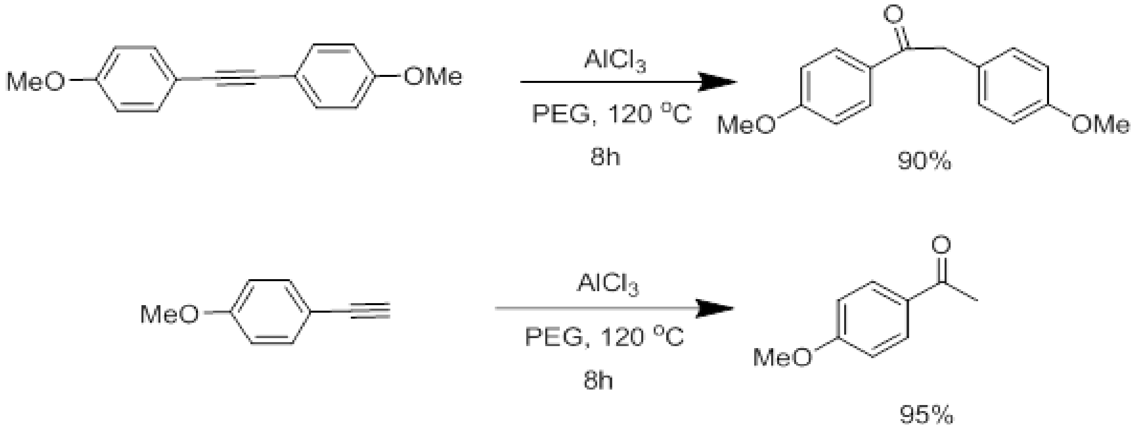
Catalytic hydration of C–C triple bond provides a perfect and environmentally benign approach for the preparation of carbonyl compounds with 100% atomic efficiency.[1] The classical methods for the hydration of alkynes have been carried out using mercury (II) salts as Lewis acidic catalysts in aqueous sulfuric acid.[2] However, the toxicity of mercury (II) and the requirement of strong acid have produced pollution problems that have limited its applications. As possible alternative catalysts, transition-metal complexes containing Rh, Ir, Pb, Pt, Au, Ag, Fe, Co have been reported to catalyze the hydration of alkyne in good yields.[3] In this paper, we demonstrate that $AlCl_3$ could act as an efficient catalyst in the oxidation of alkynes. Both of terminal and internal alkynes converted to corresponding ketones with high yield. To the best of our knowledge, this is the first report for the use of $AlCl_3$ for oxidation of alkynes to ketones with high efficiency.



Scheme1. Chemoselective oxidation of Alkynes

Keywords: $AlCl_3$, Oxidation , Alkyne,ketone

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Synthesis and characterization of Fe_3O_4@CuO and their catalytic activity towards oxidative amidation, enole carbamates and 2-amino benzothiazoles synthesis

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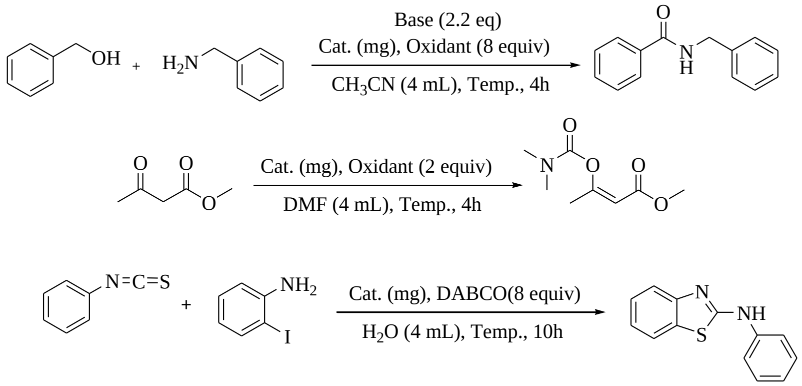
A robust, safe and magnetically recoverable CuO catalyst was synthesized by anchoring CuO onto Fe_3O_4 (Fe_3O_4@CuO) magnetic nanoparticles. The Fe_3O_4 magnetic nanoparticle-supported CuO catalyst thus obtainedwas characterized using scanning and transmission electronmicroscopies, thermogravimetric analysis, vibrating sample magnetometry, X-ray diffraction, and inductively coupled plasma atomic emission and Fourier transform infrared spectroscopies. Fe_3O_4@CuO was screened oxidative amidation, enole carbamates and 2-amino benzothiazoles synthesis. The Cu content of the catalyst was measured to be 0.28 mmolg^{-1} Cu. In addition, the Fe_3O_4@CuO catalyst can be easily separated and recovered with an external permanent magnet. The anchored solid catalyst can be recycled efficiently and reused five, eight and six times respectively with only a very slight loss of catalytic activity.



Keywords: Magnetic nanoparticles, Fe_3O_4@CuO, Oxidative amidation, Enole carbamates, 2-aminothiazoles

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Iron-Porphyrin/Cystein as pH switchable pseudo-enzyme

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Porphyrins can be widely used as active site biocomplexes, where biomimetic synthetic metal porphyrin is considered as being pseudo-enzyme. In this approach, many attempts have been made to improve and enhance the activity of these pseudo-enzymes by the environmental parameters change like temperature, ionic conditions, pH and the hydrophobic pocket for these compounds. The system consisted of the porphyrin metal-cysteine complex and polyethylene glycol (as hydrophobic pocket) has used to model the native chloroperoxidase enzyme (CLP). Porphyrin-iron-cysteine-polyethylene glycol in pH 3 for thionine as a substrate shows a similar activity and 28% native CLP enzyme efficency. This enzyme performs two catalytic reactions catalase by decomposing H_2O_2 as a substrate and as a peroxidase by oxidizing guaiacol with low levels of natural enzyme peroxidase (pH =7) and catalase (pH =7), respectively.

Keywords*:* Iron-Porphyrin/Cystein, Polyethylene glycol, Biomimetic, Chloroperoxidase, Peroxidase, Catalase.

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Structure and Biological Activity of Platinum(IV) Complex with Phenyl Pyridine

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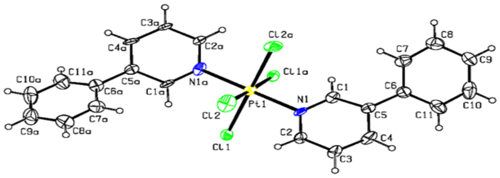
Pt-based drugs are considered as some of the most efficient chemotherapeutic agents, especially in the treatment of solid tumors [1-2]. Drug resistance and severe toxic side effects are two major limitations for pharmacological activity of this drug. Pt(IV) compounds, providing several advantages over Pt(II) drugs such as kinetic inertness, stability in the bloodstream, less reactivity towards biomolecules and therefore a reduction of unfavorable side effects, and efficiency in cisplatin- resistant tumors [3]. In this research, a novel platinum(IV) complex, $[Pt(phpy)_2Cl_4]$ were prepared from the reaction of H_2PtCl_6-$6H_2O$ with 3-phenyl-pyridine (phpy), in methanol. The complex was fully characterized and its structure was determined by the X-ray diffraction method. It crystallized in the Orthorhombic crystal system, with *C2cb* space group. This complex has two monodentate nitrogenous ligand with four chloride anions attached to a Pt(IV) metal in a distorted octahedral environment. This complex along with related ligand and salt was used for in vitro cytotoxicity evaluation against four cultures, NIH-3T3, Caco-2, HT-29 and T47D by MTT assay. Furthermore, their anticancer activity was investigated by flow cytometry.



Keyword: Cisplatin, Platinum(IV), Cytotoxicity, Flow cytometry, Crystal structure

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Influence of reaction time and calcination temperature on the characteristic property of gamma alumina

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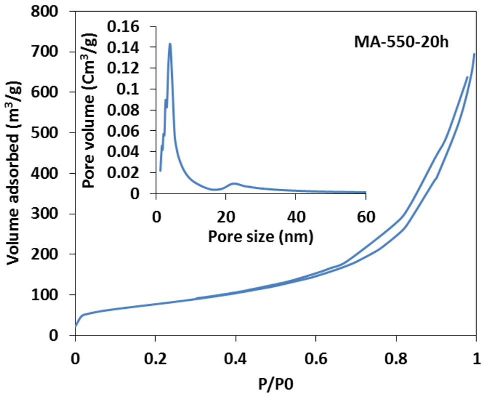
We studied the synthesis conditions for the mesoporous alumina formation from aluminum tri-sec butoxide in the presence of non-ionic (triblock poly(ethylene oxide)-poly(propylene oxide)- polyethyleneoxide, P123) template via Evaporation-Induced Self-Assembly (EISA) method at different reaction time (9 h and 20 h). Also, calcination at two different temperatures (550 and 600 °C) carried out in order to study the effect of calcination on their structural features. The nanostructures were studied by X-ray diffraction (XRD) and N_2 adsorption/desorption techniques. XRD patterns of the as-made nanostructures revealed the amorphous state (weakly crystalline ɣ-phase) of alumina after calcination. The results showed that surface area, pore size and pore volume appeared changes as the reaction time and temperature calcination changed. The obtained alumina mesophases have specific surface areas in the range of 216-283 m^2/g and narrow pore size distribution depending on the reaction condition. The maximum specific surface area (283 m^2/g) is achieved for mesoporous alumina when reaction time and temperature calcination were 20 h and 550 ^{o}C.



Keywords: P123, Reaction time, Calcination.

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Synthesis, Characterization and Thermal Behavior of $[Mn(H_2O)_6][Pb(dipic)_2].2H_2O$ as a Precursor for Preparation Paramagnetic Mixed Oxide Nanoparticles

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In the present study bi-metallic complex of $[Mn(H_2O)_6][Pb(dipic)_2].2H_2O$ where dipic is pyridine-2,6-dicarboxylic acid was synthesized and characterized by atomic absorption, conductivity measurement, elemental analysis, Fourier transform infrared spectroscopy (FT-IR), ultra violet-visible spectroscopy (UV-Vis). The thermal behavior of complex was studied by thermo-gravimetric analysis (TGA) and Differential scanning calorimetry (DSC). This complex was used as a precursor for preparation paramagnetic nanoparticles of Pb_2MnO_4 and PbO by thermal decomposition of $[Mn(H_2O)_6][Pb(dipic)_2].2H_2O$ at 600ºC. These nanoparticles characterized by FT-IR spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Magnetic behavior of nanoparticles was studied using vibration sample magnetometer (VSM) at room temperature.

Keywords: Bi-metallic complex, Thermal decomposition, Paramagnetic behavior, Mixed oxide nanoparticles, .$Pb_2MnO_4$and PbO Pb_2MnO_4 and Pb

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Synthesis and application of the natural zeolite modified with magnetic nanoparticles of $CoFe_2O_4$

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Zeolites are the group of minerals containing hydrated aluminosilicate of alkali and alkaline earth metals that have porous and uniform crystalline structures. Clinoptilolite is a natural zeolite that has attracted more attention due to widespread occurrence and good compatibility with the cement matrix to improve the mechanical characteristics. However, it is difficult to separate the clinoptilolite fine powder from water because it is suspended in it for a long time after wastewater treatment. It seems attractive to combine adsorption properties with magnetic properties to produce an adsorbent for the removal of pollutants from water [1-3]. In this work, at first $CoFe_2O_4$ magnetic nanoparticles were synthesized by hydrothermal method, using surfactant. Then, the natural zeolite of clinoptilolite was modified by $CoFe_2O_4$ magnetic nanoparticle. The prepared $CoFe_2O_4$ magnetic nanoparticles and the modified zeolite were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared (FT-IR). The applicability of the synthesized composites for removal of heavy metal ions from aqueous solutions was assessed. The effective parameters such as initial pH values, adsorbent dosage, contact time and initial concentration on the sorption process were studied and optimized. The results showed that the Langmuir isotherm equation is the best to describe the sorption process.

Keywords: natural zeolite, Clinoptilolite, magnetic nanoparticles, $CoFe_2O_4$, heavy metals

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Study on gas sensor with modified nano metal oxides for detection of specific gases and methods for preparing

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A resistive gas sensor under the influence of a target gas is considered as a system. The input to this system is a time-varying voltage applied to the sensor of heating element, which regulates, the operating temperature of the sensor. The output of the system is the transient response of the sensor to a gas present. The properties of the system change with respect to the nature and concentration [1]. In this paper, conductometric semiconducting metal oxide gas sensors have been widely used and investigated in the detection of gases, Investigations have indicated that the gas sensing process is strongly related to surface reactions [2]. Sensors showed fast response, stable, good selectivity, good recovery, repeatable and good sensitivity towards VOC exposure. In the following, the morphology of the nano powders was determined by scanning electron microscope (SEM) and the FTIR spectrum was studied. Eventually, successful discrimination among several target gas was studied.

Keywords: Gas Sensor, VOC, Metal Oxide

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Effect of alkoxide precursors on nano- boehmite properties prepared by sol-gel method and their adsorption properties for copper removal

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There are several methods for the synthesis of nanomaterials such as sol-gel, deposition, hydrothermal, solvothermal and etc. In this study, aluminum oxides with high surface area and large pore volumes were prepared by a facile method. This method provides the possibility to design nanoparticles with controlled morphology, high specific surface area and high purity. One of the advantages of this method is the utilization of green and safe materials. Boehmite (AlOOH), was prepared by aluminum alkoxide as precursors. These nanoparticles with high surface area and large pores was synthesized using sol-gel method via an easy and environmentally safe method in a short time. Also, for evaluation of the effect of chain length of alkoxide precursors on the product, aluminum propoxide ($Al(OC_3H_7)_3$), aluminum butoxide ($Al(OC_4H_9)_3$) and aluminum pentoxide ($Al(OC_5H_{11})_3$) was used. The application of these nanomaterials in the removal of heavy metals from water was studied and nanoboehmites were used to remove copper from aqueous solution. These nanoparticles were characterized by FT-IR, XRD, TGA, DTA, FE-SEM and TEM techniques. N_2 adsorption-desorption analyses were used for determination of the specific surface areas and pore volumes of the synthesized materials. The mesoporous boehmite which was prepared by aluminum propoxide, has large surface areas (671 m^2/g), pore volumes (0.312 cm^3/g), and narrow pore-size distribution.

Keywords: Sol- Gel, Boehmite, Alkoxide precursors, Alcohol, Nano powder, Adsorption

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Photocatalytic properties of nanohybrid Zn-TCPP@TiO2 in organic reactions

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Titanium dioxideś application is limited by its poor visible light harvesting capability, but it is an excellent photocatalyst. In this work, a visible light responsive photocatalytyst in organic reactions was developed using Zinc-porphyrin (ZnTCPP) supported on TiO_2. A Zinc-porphyrin dye with four carboxyphenyl moiety of ancillary (ZnTCPP) was studied as a sensitizer in combination with TiO_2. All intermediate nanomaterial and final nanohybrid compounds were characterized by FESEM, EDAX, XRD and FT-IR spectroscopy. The as-prepared nanohybrid photocatalysts have apparent adsorption in visible light region, making them active for visible-light-induced organic reactions. Nanohybrid ZnTCPP@TiO_2 shows extremely higher efficiency and shorter reaction time then TiO_2 nanoparticles. Remarkably, photocatalytic performance of the TiO_2 nanoparticles were enhanced from 70 to 90% by anchoring the TCPP on the TiO_2 in oxidation reaction. So, this nanohybrid compounds have potentials to be used as high performance heterogeneous photocatalyst under visible light irradiation with advantages of high activity, high selectivity, reusability and easily separation for organic reactions.

Keywords: TiO_2, Nanohybrid, Photocatalyst, Porphyrin, Organic reactions.

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Novel inorganic complex precursor for Fischer-Tropsch synthesis

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The Fischer–Tropsch synthesis (FTS) is highly noteworthy for production of clean fuel from syngas [1,2]. Conversion of the hydrogen and carbon monoxide to hydrocarbons at the presence of a catalyst is a fundamental step in the FTS process. Hence, selecting a suitable catalyst plays a key role in crop distribution [3,4]. The Mgo-supported Co–Zn catalyst prepared by thermal decomposition of inorganic precursor was tested in the Fisher-Tropsh synthesis (FTS); the structural properties and performance of the catalyst was compared to those of sample constructed via impregnation method. The Fisher-Tropsch was studied over prepared catalyst in the temperature range of 200–300 ◦C with H_2/CO molar ratio of 2 The Co–Zn/MgO catalyst presented higher activity than the reference catalysts prepared by impregnation method. The results revealed that the synthesized catalysts have higher catalytic activity comparison to those prepared via the convention al impregnation method. The effect of the preparation method on the structural properties shows that synthesizing the catalyst through inorganic precursor route is more appropriate. The characterization of both precursor and calcined catalyst was carried out using powder X-ray diffraction (XRD), FT-infrared, scanning electron microscopy (SEM), BET specific surface area.

Keywords: Fischer–Tropsch synthesis,Inorganic precursor, Impregnation.

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Investigating the Fenton reaction of Fe_3O_4@MCM-41 at degradation of aqueous pollutants

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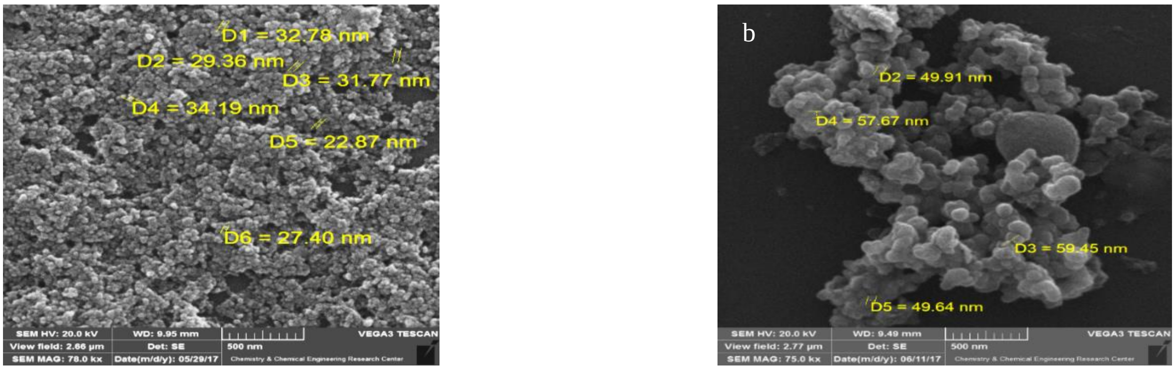
The Fenton reactions are kind of advance oxidation reaction including H_2O_2 with iron oxide structures that predominantly produces radicals of hydroxide ($^{\circ}$OH) as the oxidizing species. In this study the Fenton reactions of Fe_3O_4@MCM-41 structures were investigated. The Fe_3O_4@MCM-41 samples were prepared using co-precipitation method in alkaline ambient. The synthesized samples were characterized using SEM, EDX, XRD, UV–Visible techniques. Finally, the catalytic activities of the prepared samples were studied to remove methylene blue dyes from water as pollutant under irradiation of ultraviolet and visible light. The obtained results show that the prepared samples have more catalytic activity under light illumination [1,2].



SEM images of (a) Fe_3O_4 and (b) Fe_3O_4@MCM-41

Keywords: Fenton reaction, catalytic activity, iron oxide

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Preparation and characterization of KH_2PO_4/RHA as a new nanocomposite in the synthesis of symmetrical N,N′-alkylidene bisamides

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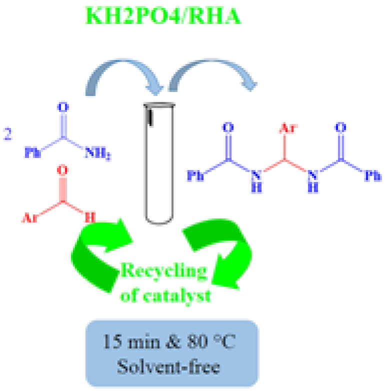
Development of new green routes in chemical synthesizes gained much attention with increasing concern about environmental pollution troubles. Heterogeneous catalysts and green solvents are keys to successful development of green chemistry in this regard [1]. Potassium dihydrogen phosphate (PDP) is a low cost, a non-toxic chemical compound with a high catalytic performance which has rarely been investigated. However, its practical application as a catalyst in aqueous media is limited due to the high solubility and difficulty of filtration and recovery of particles. The choice of an efficient support could significantly improve the activity, selectivity, and recycling of catalyst system [2]. Thus, the addition of support materials such as silica from rice husk ash (RHA) may enhance its catalytic activity. The extracted amorphous silica from RHA as an agricultural waste with low cost was employed as an excellent support for the PDP. The nanocomposite prepared through treatment of modified RHA with PDP. The synthesized nanocomposite was characterized by XRD, FESEM, FT-IR, and ICP. A simple, efficient and eco-friendly procedure was applied for the synthesis of N,N′-alkylidene bisamide derivatives in the presence of a catalytic amount of KH_2PO_4/RHA nanocomposite under solvent-free conditions.



Keywords: Nanocomposite, Potassium dihydrogen phosphate, Rice husk ash, N,N′-alkylidene bisamides

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Synthesis and characterization of cadmium sulfide nanospheres by hydrothermal method

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CdS with a direct band gap of 2.4 eV at room temperature has attracted tremendous interest due to it has attractive physicochemical properties and special orientation [1]. This material has immense potential applications in photoconductive optical switches, nanogenerators, solar cell, light emitting diodes [2]. A variety of methods can be used for the formation of CdS nanoparticle that includes chemical bath deposition, electrochemical deposition, sol-gel synthesis, hydrothermal route and solvothermal method [11- 15]. Among these methods hydrothermal method appears to be practical, convenient, cost effective approach to synthesis the CdS nanoparticles because it does not involve any special instrumentation and growth rate can easily control. In this present paper, CdS nanoparticles have been synthesized by hydrothermal method in 150°C for 96 h using $Cd(NO_3)_2·4H_2O$ and thiourea as raw materials and NH_4OH as a complexing agent. The obtained product was characterized by XRD,SEM, EDX and DRS techniques. XRD pattern confirms the formation of hexagonal structure of CdS with average grain size of 30 nm(Fig.1). EDX spectrum demonstrate that the products are well crystallized with high purity. SEM images depict the presence of nanospheres in the sample with a diameter range of 45 nm (Fig.2). From DRS spectrum of CdS nanoparticles of our present study (Fig.3), a well-defined absorption peak at 460 nm is observed. The exciton absorption observed at about 460 nm, which is blue shifted compared with the characteristic absorption of bulk CdS may be due to quantum confinement effects.

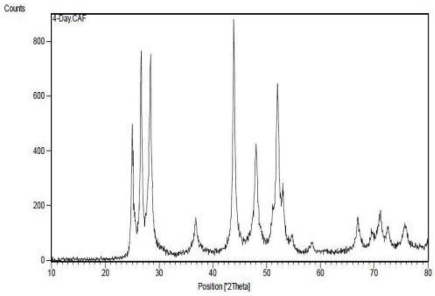

Fig.1 XRD pattern of nano CdS

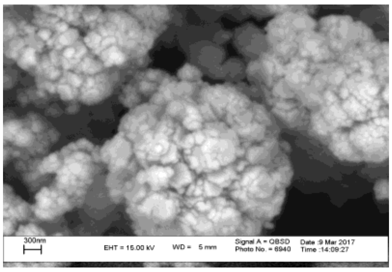

Fig.2 SEM image of CdS nanospheres

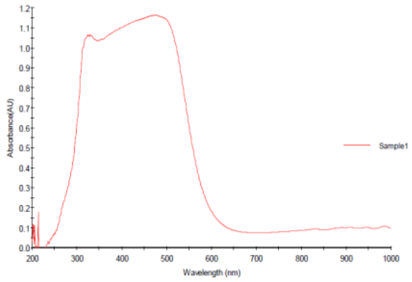

Fig.3 DRS spectrum of nano cdS

Keywords: Cadmium sulfide, hydrothermal method, nanosphere

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Synthesis of MOF(MIL101) as a Control and Drug Delivery

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Drugs in the form of chemical and bioactive compounds are widely used as therapeutic agents to improve health and to extend the lifespan of the human population. Many of these compounds are successful candidates for the treatment of severe illnesses such as cancer [1]. By making use of a drug delivery system (DDS), most of these issues can be overcome through the increment of drug solubility, protection from degradation, controlled drug release, provision of targeted delivery, and a decrease in toxic side effects. Finding an effective DDS for therapeutic agents has been an ongoing challenge in bioengineering. In this context, metal-organic frameworks (MOFs) have emerged as potential candidates owing to their distinctive characteristics, such as high pore volumes, large surface areas, multiple topologies and tuneable pore size and surface chemistry [2]. MOFs are synthesized in a self-assembly process from metal ions or clusters, acting as coordination centres that are interconnected by organic ligands [3]. In this study, MIL-101(Cr) was synthesized and characterized by IR spectroscopy and x-ray powder diffraction(XRD). Then different drugs was loaded in synthesized MOF and finally,the drugs release in PBS buffer was measured at 37^{0}C .

Keywords: Drug Delivery , Metal- Organic Framework , MIL101

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Investigation of Copper ion adsorption on TMOS xerogel

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Heavy metals such as Cu(II) produced in industrial activity cause environmental pollution. In this research, TMOS(tetra methoxy ortho silane) xerogel was produced by sol-gel method and used as adsorbent for removal of Cu(II) from waste water. Various parameters such as contact time, pH, amount of adsorbent, dose of adsorbate and temperature effect on metal adsorption was investigated. With attention to results, the optimum contact time for Cu(II) on TMOS was determined 60 minutes. Also, pH 5-6 was chosen as optimum pH for adsorption of this ion on adsorbent. different models of equilibrium adsorption isotherms were studied and their constants were determined. The results show that the Dubinin-Radoshkevich isotherm model was fitted well with adsorption data. From the kinetic studies, it became clear that Pesudo-second order model was fitted with adsorption data of Cu (II) on TMOS. Thermodynamic investigations were showed that the adsorption process of this heavy metal on adsorbent is spontaneous and exothermic. Also, desorption experiments show that TMOS xerogel is adsorbent with power of recovery. Although the results of heavy metal ions adsorption examined by TMOS xerogel is not impressive but by compared with other adsorbent; non-toxic, high mechanical strength and high surface area , the ability to recover and re-use and low cost can be as important factors for using this adsorbent for removal of heavy metal ions of the water resources.

Keywords: Xerogel, TMOS , Sol-gel, Adsorption, Cu(II) .

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Solid-state Conversion of a Thallium(I) Coordination Polymer to silver(I) Coordination Polymer Nanostructures

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The different method of coordination polymer synthesis is developed because of their wide range of structures and functions [1,2]. The need for environmentally friendly processes has brought forward alternative synthetic strategies, including mechanochemistry. [2] Mechanochemistry provides an alternative route, avoiding the use of large amounts of solvent, and is widely used in the synthesis of organic compounds, metal complexes, supramolecular co-crystals, polygons, nanomaterials, coordination polymers, metalorganic frameworks, and so on; therefore, it is worth investigating [1,3,4]. Mechanosynthesis has a significant potential in that sense as it offers short reaction times and avoids large quantities of solvent and high temperatures, also it is efficien [1,4]. The solid-state conversion of a Tl(I) coordination polymer synthesized by a sonochemical procedure, to Ag(I) coordination polymer nanostructures have been observed upon mechanochemical reaction of the compound [Tl_2L] (1) (L= Bis(4-hydroxyphenyl) sulfone), with $AgNO_3$. During this conversion, the reaction between Bis(4-hydroxyphenyl) sulfone and $TlNO_3$ in water and acetonitrile under ultrasonic irradiation results in the formation of a white powder which was dried at room temperature, in addition, compound (1) and $AgNO_3$ were mixed in a mortar and ground up for 30 minutes. Then the mixture was washed four times with distilled water until the unreacted $AgNO_3$ and produced $TlNO_3$ was removed, and the pure product was separated. The internal packing of these two compounds looked similar and low-energy structural changes allowed the conversion to occur smoothly. There are weak interaction planes in the crystal packing of 1, so the structure is not mechanically rigid, which allows Ag ions to penetrate the lattice and form stronger bonds.

Keywords: Coordination polymer, Mechanochemistry, Thallium(I), silver(I), Nanostructure

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Metal Organic Framework with formula $Zn_2(bdc)_2(dabco)$ as a drug delivery

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Metal organic frameworks (MOFs), also known as coordinationpolymers or coordination networks, are the unique of crystallinematerials formed by connecting metal centers and organic ligandsinto infinite arrays through dative bonds [1]. As one types ofporous materials, MOFs exhibited potential advantages over conventionalmaterials, such as tunable pore size and shape, adjustablecomposition and structure, biodegradability, excellent loadingcapacity and controllable drug release, and versatile functionalities,which enable MOFs to perform as promising platforms for variousmedical applications, including drug delivery[2],molecularsensing and bioimaging, and theranostics[3].In this respect, MOFs could be advantageous over other classical porous materials owing to their diverse architecturesand tunable porosity, along with modifiable framework functionality. Moreover, in a MOF-based DDS, the drug payload and release could be controlled by changing the ligand lengthor the connectivity and functionality. In this study, $Zn_2(bdc)_2(dabco)$ was synthesized and Then characterized by x-ray powder diffraction(XRD) and IR spectroscopy and effects of $Zn_2(bdc)_2(dabco)$ on the loading and release of drugs are investigated.

Keywords: Metal- Organic Framework , Drug Delivery, dabco, bdc

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Comparative catalytic activity of $\{Mo_{72}Fe_{30}\}$ nanoclusters in the oxidative dyes degradation

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Polyoxometalates (POMs) are attractive class of charged, nano-building blocks due to their wide range of structures, topologies and physicochemical properties[1]. Furthermore, because of their sizes, structures and properties, POMs are considered as intermediates between small molecules and metal oxide solids. Of particular interest in this respect are the nanoscaled Keplerate polyoxomolybdates of the {Mo11}n class with wide applications in science. The catalytic and photocatalytic activity of keplerate POM in different organic reactions have been well documented[2-4].

Nowadays, there are more than 10,000 kinds of dyes available commercially. However, many of them are toxic and even carcinogenic. Dyes are widely used in many industries, such as textile, paper and plastics. As a consequence, substantial volumes of waste water are contaminated by the dyes and needs to be decontaminated for recycles[5].

In this project, crystalline and noncrystalline forms of $\{Mo_{72}Fe_{30}\}$ nanoclusters were synthesized according to literature. After the characterization of these solids by different techniques such as FT-IR, Raman and diffuse reflectance spectra, as well as XRD, TGA and BET, a comparative study on the catalytic activity of these solids in the degradation of different dyes (RhB, Methlene-blue, Methyl Orange), at room temperature by H_2O_2 is presented.

Keywords: Keplerate polyoxomolybdate, $\{Mo_{72}Fe_{30}\}$, Dyes degradation

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Heterogeneous catalase-like activity of iron (III) based nanoball polyoxomolybdate

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Hydrogen peroxide is a strong oxidizer and a great bleaching agent that produced in different cellular biochemical pathways such as respiration [1]. Catalases are present in all aerobic organisms and protect them from oxidative stress by decomposition hydrogen peroxide to molecular oxygen and water [2]. So far many compounds have been used to catalyze H_2O_2 decomposition such as metal oxides [3] and metal complexes [4,5]. In this work a heterogeneous polyoxomolybdate (POM) catalyst containing Fe^{3+} is used to decompose H_2O_2 to O_2 and H_2O, both of which are essential to life. O_2 production was measured by a luminescence portable dissolved oxygen meter connected to an oxygen monitor with digital readout. The concentration of H_2O_2 at different time interval was determined by redox titration with $KMnO_4$. The catalase-like activity was examined at different acidic and neutral conditions, temperature from 25 to 50°C, different H_2O_2 concentrations and various amounts of Catalyst. It was found that this catalyst exhibited excellent catalytic ability and good reusability for H_2O_2 decomposition. According to IR spectroscopy and energy dispersive X-ray spectroscopy (EDS), no significant changes were observed after four times reuses of catalyst.

Keywords: Catalase-like activity, Polyoxometalate, Heterogeneous catalyst.

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Oxygen evolution reaction catalyzed by vanadium containing nanosphere polyoxomolybdate

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Molecular oxygen is the product of three very important enzymatic reactions: *i*) superoxide dismutation [1] *ii*) hydrogen peroxide disproportionation [2] and *iii*) water oxidation [3]. Polyoxometalate (POMs) contain anionic clusters of early transition metals (V, W, Mo, Nb and Ta) usually in their highest oxidation states bridged by oxide ions. Many researches provide evidence that POMs as robust, extensively tunable, molecular systems have considerable promise in the development of different oxidation catalysis [4]. In this work, oxygen evolution reaction was catalyzed by vanadium (IV) based polyoxomolybdate in the presence of Oxone® as an oxidant. The catalyst showed very high activity for O_2 production in aqueous solution of Oxone®, while, tetra-n-butylammonium Oxone® actually was inactive. No O_2 evolution was observed in the time course of the reaction in the presence of other oxygen sources including peroxides and periodate. The amount of evolved oxygen was affected by the catalyst and Oxone® concentration. A linear and direct correlation was observed between maximum evolved O_2 and catalyst concentration as well as low concentration of Oxone®. However, the slope of O_2 production decreased at higher oxidant concentration. Control experiments demonstrated that V could activate Oxone® to produce molecular oxygen.

Keywords: Oxygen evolution reaction, Polyoxometalate, Oxone®

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$\{Mo_{72}Fe_{30}\}$ nanoclusters catalyzed aerobic oxidative synthesis of benzimidazoles

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Molybdenum oxide based spherical hollow clusters of the type $\{(Mo)Mo5\}_{12}\{linker\}_{30}$ named also as Keplerates can be directly synthesized by the addition of linkers, such as $V^{IV}O^{2+}$ and Fe^{III}, to a dynamic library containing (virtual) pentagonal units in solution [1]. Benzimidazoles are very useful compounds in pharmaceutical industry, which exhibits significant biological activity against several viruses1, such as HIV, HSV-1, influenza, and human cytomegalovirus. Specifically, this nucleus is a constituent of vitamin-B_{12}[2]. In continuation of our research ongoing on catalytic applications of Keplerate POMs[3-5], in this work, catalytic activity of amorphous and crystalline $\{Mo_{72}Fe_{30}\}$ nanoclusters was compared in the synthesis of benzimidazoles under aerobic conditions. To explain different catalytic activity of two solids, different techniques such as FT-IR, Raman and diffuse reflectance spectra, as well as XRD, TGA and BET were used. The size of materials ranged between 4-25 nm according to TEM images.

Keywords: Keplerate polyoxomolybdate, $\{Mo_{72}Fe_{30}\}$, Benzimidazole

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Preparation of titanium dioxide photoelectrodes using different block copolymers and investigation of their performance on nanostructure solar cells

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At the end of last century, the possibility to use devices based on molecular components for the construction of a robust large-scale solar electricity production facility seemed utopic [1]. solar cells are highly promising power sources because the sun is a free source, pure, free of environmental impacts and accessible source of energy [2]. In this regard, the solar cells convert this energy into electricity. Nanostructured solar cells hold great promise towards new approaches for converting solar energy into either electricity (in photovoltaic devices) or chemical fuels. The use of nanostructures in photovoltaics offers the potential for high efficiency [3-4].

In this work we prepared titanium dioxide photoelectrode using different block copolymers and investigated its performance in nanostructured solar cells. Many wet chemical methods have been developed to fabricate micro/nanostructures of titanium dioxide such as sol–gel process. Firstly, we synthesized a stable TiO_2 sol and then deposited it on FTO substrate.TiO_2 photoelectrode identified by UV-Vis and SEM. In the following we investigated the performance of this photoelectrode in nanostructure solar cells.

Keywords: Photoelectrode, Nanostructure solar cell, Block copolymers, Titanium dioxide.

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Green, highly efficient and selective oxidation of oximes by a novel heterogeneous manganese nanocomplex supported on modified magnetic nanoparticle

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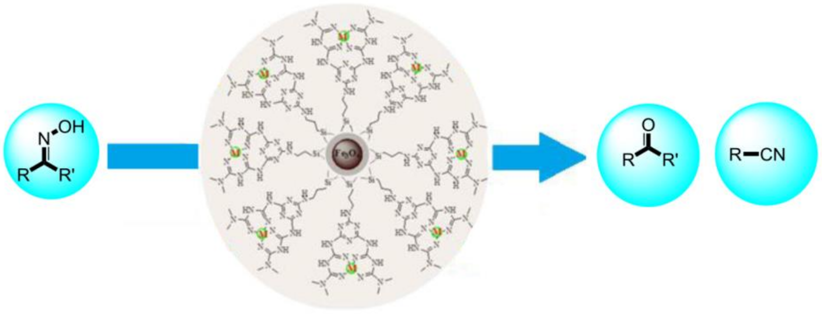
Owing to the growing environmental concerns and depletion of green chemistry, utilization of heterogeneous catalyst for green chemistry process in chemical synthesis and industry is receiving significant attention. The oxy-functionalization of C-H and C-N bonds of simple precursors, represent a powerful method to the synthesis of value-added products which find widespread [1-3]. The Fe_3O_4 magnetic nanoparticles modified with SiO_2/aminopropyl trimethoxy silane/cyanuric chloride utilized for anchoring metformin-manganese complex. The structure of novel complex well defined by elemental analysis, ICP, AAS, BET, FT-IR, EDX, SEM, TEM, DLS, XRD ,TG-DTG and XPS. The catalytic efficacy of the synthesized Mn-nanocatalyst was studied in the oxidation of oximes using molecular oxygen as ecofriendly oxidant. The nanocatalyst shows high catalytic activity and selectivity toward oxidation without any reducing agent. To achieve maximum efficacy of heterogeneous nanocatalyst, various parameters such as the ratio and amount of nanocatalyst, reaction time, temperature and solvents were evaluated.



Keywords: Supported Magnetic Nanoparticles, Heterogeneous catalyst, selective aerobic oxidation, green oxidant.

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5-7 September 2017

IMPLICATION-NOT logic-gate behaviours of g-C_3N_4 nanoparticles

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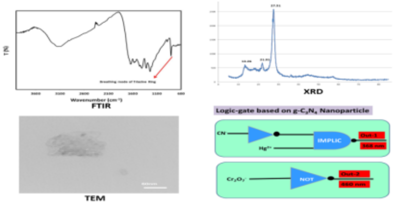
Recently, Graphitic-phase carbon nitride is emerged as a new type of semiconductors with high fluorescence quantum yield which exhibits unique photoluminescence (PL), photostability and excellent biocompatibility leading to attract worldwide attention in cell imaging, photocatalytic reactions and sensing processes [1]. Based on fluorescence properties of g-C_3N_4, these materials had been used in optical sensing processes for detecting metal ions and anions [2-3]. The ON-OFF fluorescence ability of g-C_3N_4 is suitable for designing logic-gate system. But, logic-gates behaviours of these materials were not investigated. In this work, the nanoparticles of g-C_3N_4 with good fluorescence properties were synthesized from nanosheet structures. The as-synthesized nanoparticles were characterized with FT-IR, TEM and XRD techniques. FTIR spectrum show the characteristic peaks of g-C_3N_4 structures in 810 cm^{-1} and 1200-1700 cm^{-1} wavenumber regions. In XRD pattern, two famous peaks centered at 13.1° and 27.4° were observed indicating the tri-s-triazine layered structure of g-C_3N_4. In addtion, TEM image elucidate the nanoparticle structure of g-C_3N_4 [4]. After characterization of the obtained nanoparticles, the fluorescence feasibility and ability of these materials for using in optical sensing processes was studied. According to the obtained results, g-C_3N_4 have two distinct emission peaks around 368 and 450 nm under excitation at 250 and 360 nm, respectively. The first emission peak at 368 nm was quenched by adding Fe^{3+}, Hg^{2+} and $Cr_2O_7^{2-}$. The quenched peaks in the presence of Hg^{2+} was returned to the initial level after adding CN^- ions. The second emission peak (λ_{emiss}=450 nm) significantly quenched by adding $Cr_2O_7^{2-}$. Based on these findings, two logic-gate behaviours for g-C_3N_4 nanoparticles were observed. Therefore, IMPLICATION-NOT logic-gate systems were designed for g-C_3N_4 nanoparticles in the presence of Fe^{3+}, Hg^{2+}, $Cr_2O_7^{2-}$ and CN^- ions.



Keywords: Graphitic carbon nitride, g-C_3N_4, Nanoparticle, Logic-gate, Fluorescence

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Sonochemical synthesis of Fe_3O_4/bentonite nanocomposites and investigation of their performance for removal of nitrate ions from water

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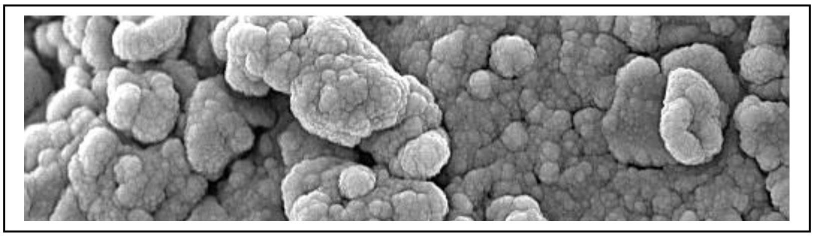
Bentonite is a clay with high adsorption efficiency for removal of water pollutions. In this research, activation of bentonite and synthesis of Fe_3O_4/bentonite nanocomposites with various amounts of Fe_3O_4 are reported. The prepared samples were characterized using variety of conventional techniques including, X-ray diffraction (XRD), scanning electron microscopy (SEM) and Energy-dispersive X-ray spectroscopy (EDX). Then the nanocomposites were used for removal of nitrate from water and several parameters such as pH, adsorbent amount, nitrate concentration and contact time were also studied. Recently magnetic sorbents are used to adsorb the pollutant of water and then easily separated with a magnet from the liquid phase. Based on the results, the best nitrate removal capacity is achieved at the lowest concentrations. The best nanocomposites was prepared with 50 % of nano Fe_3O_4. The optimum conditions for nitrate removal are: pH = 5, initial nanocomposite content = 2.0 g, contact times = 90 min and the nitrate concentrations = 100 mg/l. At this condition the maximum nitrate removal is 58%.



Keywords: bentonite, iron oxide, nanocomposites, sonochemical

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Synthesis and characterization of zinc oxide- bentonite nano composite and its performance in the decreasing of BOD, COD from industrial wastewater

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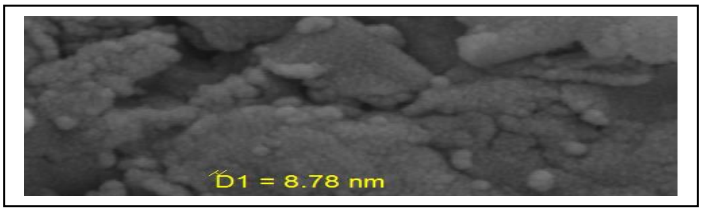
Bentonite is a type of aluminum phyllosilicaty clay minerals that naturally produced from various sources and mostly consists of montmorillonite or smectite group. Bentonite as a clay particle with unique properties such as high specific surface, exchange capacity cationic and adsorbent can be combined with nano-oxide and it can form an effective composite. In this research, activation of bentonite and synthesis of zinc oxide/bentonite nanocomposite with various amounts of ZnO are reported and their activities have been evaluated in the decrease of BOD, COD from industrial wastewater. For this research, zinc oxide nanoparticles were synthesized using gel containing citric acid and starch by sol-gel method. For synthesis of zinc oxide- bentonite nano composite, bentonite was added to the synthesis vase of zinc oxide nanoparticles. The prepared samples were characterized using variety of conventional techniques including, X-ray diffraction (XRD), scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR).The properties of nanocomposite have been investigated and the results proved that nanocomposite has the good efficiency at decreasing of BOD and COD.



Keywords: Bentonite, Zinc oxide, Nanocomposite, Industrial wastewater

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Preparation of bimetal nanocatalysts base on HZSM-5 zeolite for catalytic oxidation of volatile organic compounds

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One of the most promising ways to abate volatile organic compounds emissions to meet the requirements of air pollution control regulations is catalytic oxidation. Due to the low contaminant level and the large volume of gas to be treated, it is necessary to use highly active catalysts operating at low temperatures [1]. In this study, the catalytic oxidation of ethyl acetate has been investigated in a series of bimetal Ag–M (M: Fe, Co, Cr and Mn)-modified HZSM-5 zeolites. The objective was to find a catalyst with high superior activity, selectivity towards deep oxidation product and stability. The catalyst activity was measured under excess oxygen condition in a fixed bed reactor, between 150 and 450 ° C and ethyl acetate inlet concentration of 1000 ppm[2]. Both Fe–Ag–ZSM-5 and Cr–Ag–ZSM-5 catalysts exhibited high activity in the oxidation of ethyl acetate. The sequences of catalytic activity and catalytic stability were as follows: Fe–Ag–ZSM-5 > Cr–Ag–ZSM-5 > Co–Ag–ZSM-5 > Mn–Ag–ZSM-5 > Ag–ZSM-5 > HZSM-5. Total conversion of ethyl acetate was achieved at above 250 ° C. The catalysts were characterized by inductively coupled plasma atomic emission spectroscopy, X-ray diffraction, scanning electron microscopy, EDX and diffuse reflectance UV–vis spectra.

Keywords: Air pollution, Catalytic oxidation; VOC combustion; Bimetallic catalysts.

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Ultrasound-assisted fabrication of a nano porous porphyrin-based metal-organic framework

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Crystal engineering, the design and synthesis of supramolecular metal-organic frameworks is frontier field in research, not only for their variety of architectures and interesting molecular topologies but also because of their potential applications in zeolite-like catalysts, host-guest chemistry, gas storage, ion exchange, molecular recognition, photonic materials and magnetic. High quality crystals of metal-organic coordination compounds, such as those suitable for single-crystal X-ray diffraction measurements, can usually be obtained by a variety of approaches using wet solution chemistry and/or solvothermal methods[1]. High-energy ultrasound irradiation has been used for the synthesis of a zinc(II) MOF, $Zn_2(Zn\_TCPP)_3H_2O.2DMF$ (**1**), (TCPP = tetrakis(4-carboxyphenyl)porphyrin) in nano scale. The nano-structure was characterized by scanning electron microscopy (SEM), X-ray powder diffraction (XRPD) (Fig. 1), and elemental analyses. The utilization of high intensity ultrasound has found as a facile, environmentally friendly, and versatile synthetic tool for the coordination compounds[2,3].

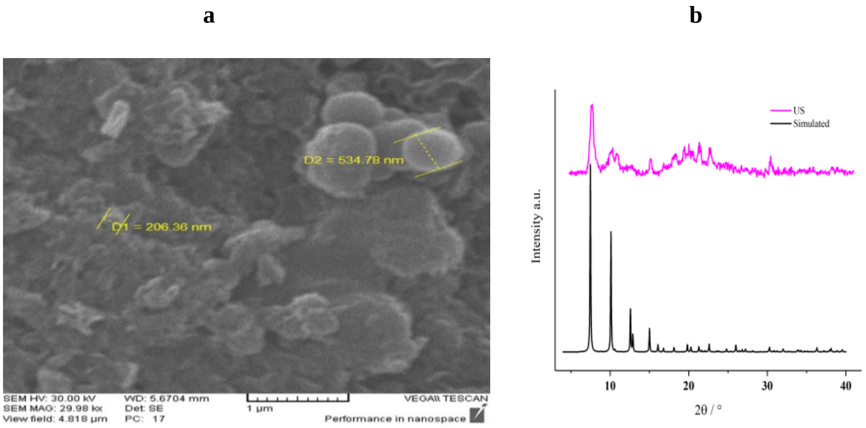

Fig. 1: (a) SEM photographs and (b) The XRD patterns of compound **1**.

Keywords : Metal_organic framework (MOF) , porphyrin , ultrasouninc

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Beta-zeolite as an effective adsorbent for poisonous of Congo Red dye

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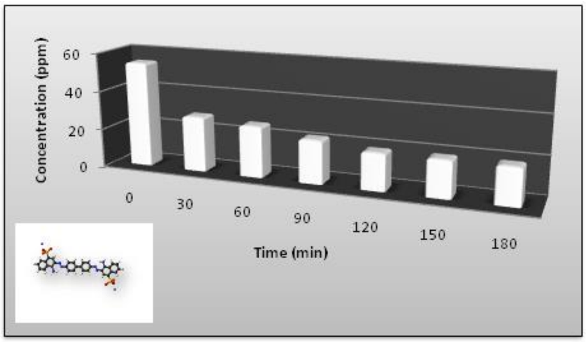
Zeolites have a wide area of applications as catalyst, adsorbent and ion exchange resin. Beta zeolite is one of the most useful zeolites that is not naturally available and should be obtained from a synthetic rout. Beta zeolite, with its intriguing framework architecture (*BEA) and 3-dimensional pore system, displays superior performance in refinery applications, environmental catalysis and a variety of organic reactions because of its vastly accessible pore volume, high adsorption capacity, strong acid sites and shape/size selectivity. In this report, through a two-step crystallization procedure, an ordered mesoporous aluminosilicate with cubic Ia3d structure has been synthesized from the assembly of as-synthesised zeolite beta precursors, utilizing cetyltrimethylammonium bromide (CTAB) as a template. The beta-zeolite was characterized by X-ray powder diffraction (XRD) and N2 adsorption–desorption. This mesoporous aluminosilicates was utilized as adsorbent of toxic dyes such as Congo Red. The Result showed that 30 mg of beta-zeolite decreased the concentration of Congo Red from 55 ppm to 19 ppm after 2h.



Keywords: Synthesis, Beta-zeolite, Adsorbent, Congo Red

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Novel synthesis of copper(II) oxide nanoparticles for non-enzymatic determination of glucouse

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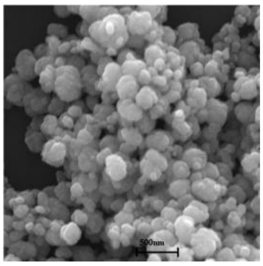
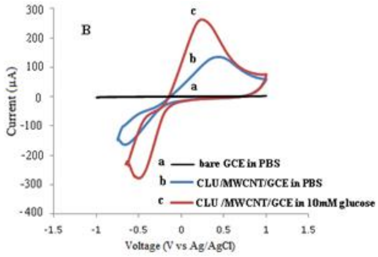
In past times, the chemical synthesis of inorganic materials with unusual and novel morphologies has attracted considerable attention because of their potential applications in various fields such as catalysts, medicine, electronics, sensors, ceramics, pigments, and cosmetics [1]. Metal oxides represent the most diverse class of materials with properties covering almost all aspects of materials science and physics. Copper oxide, as an important p-type semiconductor with the band gap in the range of 1.8 –2.5 eV [2] has obtained increasing interest because it has many potential applications. This material presents several applications and many efforts have been made to synthesize cupric oxide nanoparticles [3]. In this paper, for determining of a non-enzymatic glucose biosensor, CuO was applied for this purpose. These nanostructures were synthesized by a solvothermal method with the use of amino acids as additives. The synthesized nanoparticles were characterized by SEM and XRD. For fabricating the electrode, the nanoparticles were loaded on MWCNTs surface. Then these nanohybrides were loaded on glassy carbon electrode and used for sensing of different concentrations of the glucose. The best sensitivity obtained for the biosensor of CuO/ MWCNT with the amount of 139.67 μA/cm^2.mM.





Keywords: Copper oxide, Non-enzymatic glucose biosensor, Glassy carbon electrode.

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Fabrication of Nanodiamond-Coated SiO_2-based Substrate

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Nanodiamonds are emerging class of carbon nanomaterials which offer versatile properties such as high thermal conductivity, optical transparency, chemical inertness, high specific area, hardness and thermal stability. They have been synthesized by various methods such as: Detonation technique, laser ablation, plasma-assisted chemical vapor deposition (CVD), autoclave synthesis from supercritical fluids, chlorination of carbides, ion irradiation of graphite, electron irradiation of carbon 'onions' and ultrasound cavitation, with the first three of these methods being used commercially. As structural point of view, Nanodiamond (ND) particles consisting of a diamond core built up of sp^3 carbon, which may be partially coated by mixture of sp^2 and sp^3 carbon species. It was demonstrated that the surface of ND particles was covered with various Oxygen-containing functional groups. The functional groups present on the surface of ND particles can be used for covalent functionalization. In current study a novel approach for the fabrication of nanodiamond-coated SiO_2-based substrate is illustrated. In this regard, ND surface was firstly oxidized to establish a homogeneous layer of COOH groups, and then acyl chloride groups were created on the surface. The acyl chloride functionalized ND was subsequently reacted with amine-modified substrate to produce ND-coated SiO_2-based substrate. The resulting products were characterized by FT-IR, TGA, TEM, and SEM.

Keywords: Nanodiamond; Surface modification; SiO_2-based substrate

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Electrochemical synthesis of polypyrrole /CeO_2nanocomposite

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The preparation of organic–inorganic nanocomposites has been regarded as an important strategy to improve the mechanical, thermal, and chemical resistance of the polymers. Polypyrrole is one of the important conductive polymers that widely used in energy storage systems, biosensors and electronic [1]. Cerium is the rare-earth element with excellent redox properties. The cerium (IV) oxide finds extensive applications in catalyst supports, oxygen ion conductors in solid oxide fuel cells, and UV absorbents. Therefore, the synthesis of CeO_2 and its composites have been of special interest to researchers [2-4].
In this research, polypyrrole/ CeO_2nanocomposite was synthesized electrochemically. First nano-crystalline particles of CeO_2 have been synthesized by chemical precipitation method from cerium nitrate solution in the presence of sodium hydroxide and polyethylene glycol. The prepared CeO_2 nanoparticles were characterized by X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The size distribution of the particles was about 19 nm. Polypyrrole/ CeO_2nanocomposite have been obtained through cyclic voltammetry from pyrrole and synthesized CeO_2. The presence of CeO_2 in nanocomposite was studied by Energy Dispersive X-Ray Analysis (EDX) and SEM.

Keywords: Cerium (IV) oxide, Nanocomposite, Polypyrrole, Chemical precipitation, Electrochemical synthesis

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Sonochemical synthesis of CuS-NPs using aminoacid as biological agent

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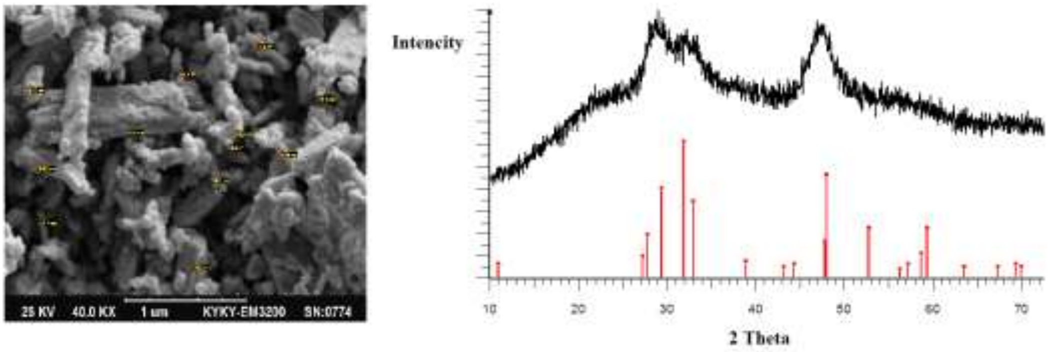
During the past decade the synthesis of semiconductor nanoparticles has become a major field of research due to their unique chemical, optical and electronic properties. Nanoparticle size can be controlled by using controlled release of nuclei of nanoparticles. Controlled release of nuclei can be obtained by controlling the reaction conditions such as ultrasonic irradiation time and use of chelating agent in sonochemical process. To prepare the nanoparticles, the solution of histidine (0.2 M) and sodium sulphide (0.1 M) was mixed with the solution of $Cu(NO_3)_2.3H_2O$ (0.1 M) under vigorous stirring. Then the mixture was kept under the ultrasonic irradiation at room temperature for 30 min. The resulting precipitate was then centrifuged and washed with alcohol. To obtain the powder of CuS nanoparticles, the precipitate was then dried at 60 °C. The nanoparticles were characterized by IR, XRD and SEM image. The XRD spectra confirmed the formation of CuS-NPs which have *Covelite* structure. The broadening of the peaks in XRD pattern indicates that the crystallite sizes are below 100 nm that confirms by SEM image. We successfully synthesized nano cooper sulphide by facile, useful and inexpensive method with biological organic chelating agent. One of the advantages of utilizing histidine is the growth controlling of particles. Synthesis of CuS-NPs using histidine as a bio-system is a novel and versatile route that has not yet been reported.



Keywords: Sonochemical method, Histidine, biological chelating agent

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Synthesis and Characterization of $Ag_3PO_4/Fe_3O_4/C_{60}$ Nanocomposite and Study of Their Antibacterial and Catalytic Activities

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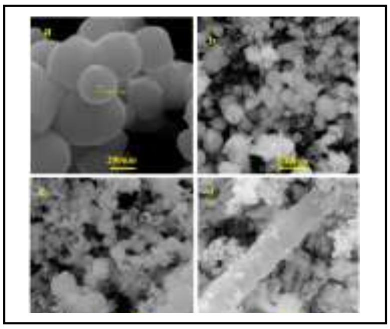
The $Ag_3PO_4/Fe_3O_4/C_{60}$ nanocomposite has been synthesized by a facile and effective hydrothermal method. This new nanocomposite was characterized by FT-IR, Raman spectroscopy, X-ray diffraction (XRD), UV–vis spectroscopy, Brunauer–Emmett–Teller (BET) specific surface area, and vibrating sample magnetometer (VSM). Morphology of nanocomposites was investigated by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The $Ag_3PO_4/Fe_3O_4/C_{60}$ nanocomposite showed good antibacterial activity against a few human pathogenic bacteria. The catalytic activity of the $Ag_3PO_4/Fe_3O_4/C_{60}$ nanocomposite for rapid and efficient reduction of toxic nitro compounds into less toxic corresponding amines by using NaBH4 as the hydrogen donor was also investigated. Our results show that $Ag_3PO_4/Fe_3O_4/C_{60}$ magnetic nanocomposite has exhibited higher catalytic activity better than Ag_3PO_4/Fe_3O_4 and Ag_3PO_4 respectively.



Keywords: C_{60}; Silver phosphate; Magnetic; Antibacterial Activity; Catalyst; Reduction of phenols

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Synthesis and Characterization of $BiVO_4/Fe_3O_4/C_{60}$ Nanocomposite and Study of Catalytic Activity

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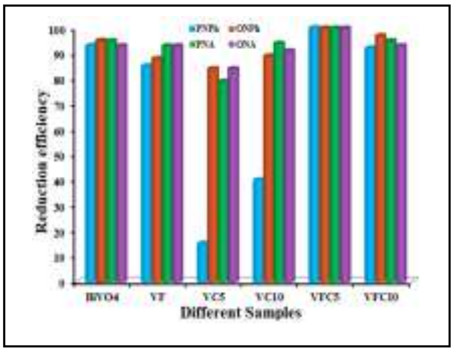
The $BiVO_4/Fe_3O_4/C_{60}$ nanocomposite has been synthesized by a facile and effective hydrothermal method. This new nanocomposite was characterized by X-ray diffraction (XRD), FT-IR spectra, Raman spectroscopy, vibrating sample magnetometer (VSM), Brunauer–Emmett–Teller (BET) specific surface area and UV–vis spectroscopy. Morphology of nanocomposites was investigated by scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). In this study, reduction of phenols and anilines on $BiVO_4/Fe_3O_4/C_{60}$ catalyst has been investigated. The catalytic activity of the $BiVO_4/Fe_3O_4/C_{60}$ nanocomposite for speedy and efficient reduction of toxic nitro compounds into less toxic resultant amines by NaBH4 as the hydrogen donor was also investigated. Our consequences show that $BiVO_4/Fe_3O_4/C_{60}$ magnetic nanocomposite has exhibited higher catalytic activity better than pure $BiVO_4$ and $BiVO_4/Fe_3O_4$.



Keywords: C_{60}; BiVO4; Magnetic; Catalytic activity; reduction of phenols; anilines

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Synthesis and characterization of Ni(II) complex immobilized on Fe_3O_4 nanoparticle: a reusable nanocatalyst and its application in the oxidative coupling of thiols and oxidation of sulfids

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Magnetic NPs have many unique magnetic properties such as superparamagnetic, high coercivity, low Curie temperature and high magnetic susceptibility [1]. Fe_3O_4 nanoparticles are a good candidate as a support material for heterogeneous catalysts because of their tremendous properties: abundance of unique activities, simple synthesis and functionalization, high stability, high surface area, low toxicity, price and simple separation by magnetic forces [2-3]. Oxidation of sulfides and oxidative coupling of thiols are very important in organic chemistry; their products are useful in medical and biological applications [4-5]. Ni(II) complex stabilized on magnetic iron oxide nanoparticles was prepared and characterized using FT-IR, TGA, XRD, VSM and SEM methods. This compound acts as a highly active and selective catalyst for the oxidation of sulfides and thiols. All of the processes were produced in short time with excellent revolutions in the presence of this nanocatalyst. Separation can be easily done using a simple magnetic separation process. The use of non-toxic, green and inexpensive materials, the compatibility of this method with the environment and the simplicity of separating the processes are one of the most important advantages of this catalyst.

Keywords: Magnetic nanoparticles, Nickel(II)complex, Oxidation, Sulfides, Thiols

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Effect of structure-directing agents on the synthesis of mesoporous alumina with adjusting pore size as a drug carrier

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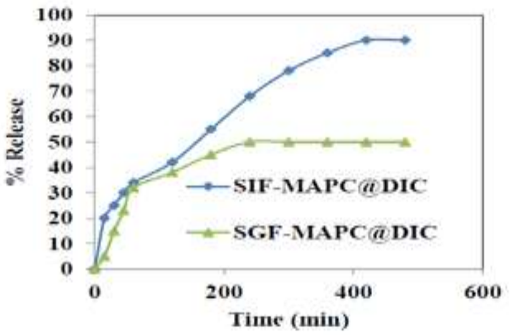
Mesoporous alumina structure has been successfully prepared by using mixed surfactants of nonionic block copolymer P123 ($EO_{20}PO_{70}EO_{20}$) and (cethyltrimethylammonium bromide, CTAB) as dual structure-directing agents through an acid-catalyzed sol-gel process. Effects of preparation parameters on the formation of the mesostructures have been extensively investigated. SEM and N_2 sorption measurements showed that the mixed surfactants system led to the product with high surface area (354 m^2/g) and large pore volume (0.80 cm^3/g). It is found that the morphologies of the resultant materials of P123/CTAB are favorable for the formation of alumina mesostructured (MAPC). Furthermore, the inner channel surface of MAPC due to its high surface area as a drug carrier is suitable for adsorption of acidic drugs such as diclofenac (DIC). The DIC was efficiently (90%) released into SIF as in vitro medium after 450 min. This carrier exhibited control release of a model drug under basic pH conditions.



Keywords: Alumina, DIC, P123/CTAB

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Delay in progression of Parkinson using new nifedipine/sol-gel alumina nano drug

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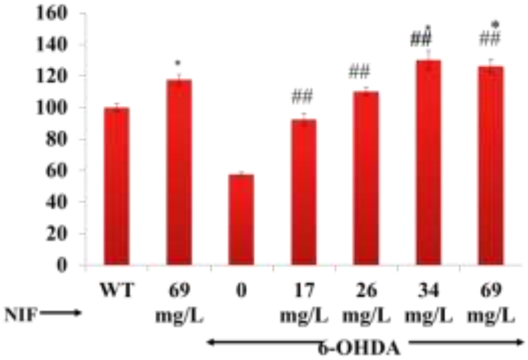
Alumina as a thermal and chemical substance has attracted the attentions. In this study, γ-alumina obtained from a simple rout by using aluminum nitrate and NaOH as starting materials. The sample was calcinated at 500 °C. Nifedipine as a poorly soluble drug was loaded on the prepared sample to reach a new formulation. The sample was characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), N_2 adsorption-desorption isotherms (Brunauer-Emmett-Teller (BET)-Barrete-Joynere-Halenda (BJH)) and field emission scanning electron microscope (FE-SEM). XRD proved that the drug is well-dispersed into the pores which its initial surface area was 203 m^2/g. Particle had average size of 20 nm. The potential of the new formulation in viability of SH-SY5Y cells were tested from oxidative stress caused by parkinsonian toxin 6-OHDA and found that the formulation neutralizes 6-OHDA toxicity and significantly enhances cell survival. Cell survival increased up to 130% by increasing the drug dose to 34 mg/L.



Keywords: Mesoporous alumina; Template-free; 6-OHDA; Nifedipine; Parkinsonian

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A facile synthesis of cubic-like porous magnesia for release of nifedipine drug

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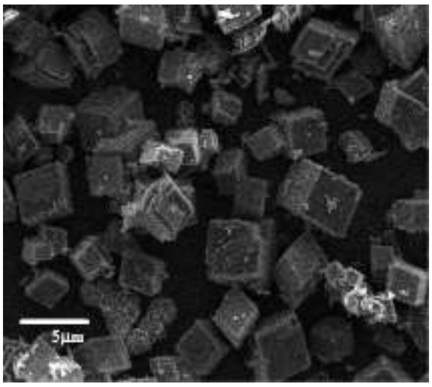
Porous magnesia (MgO) with cubic-like macro-nanostructure was synthesized by hydrothermal process at 130 °C during 4h in the presence of urea and an amino acid directing agents. Calcination temperature took place at 600 °C and the sample was used as carrier for drug delivery of nifedipine as a low soluble drug with undesirable release properties. The obtained MgO was characterized by analytical techniques such as X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscope (SEM) and N_2 adsorptione-desorption isotherms (Brunauer-Emmett-Teller (BET)-Barrete-Joynere-Halenda (BJH). Surface area of the sample was 35 m^2/g and the XRD was in accordance with the JCPDS of 89-7746. Nifedipine drug was incorporated into the magnesia pores by a post impregnation method to reduce its toxic effects by controlling the drug release property. The release profile was obtained in simulated gastric fluid (SGF) and intestinal fluid (SIF). The new drug showed 100% of release in both mentioned environments after 15 h of soaking time. It is clear that the new formulation enhanced substantially the solubility of this drug.

Keywords: Magnesium oxide, Nifedipine, Drug Release, cubic



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Influence of Surface functionalization of mesoporous TiO_2 for enhance release of poorly water soluble drug simvastatin

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The main aim of this study was to prepare pure TiO_2 as a drug carrier to improve the release rate of simvastatin with poor bioavailability property. In the present study, mesoporous titania was synthesized through evaporation-induced self-assembly method by using non-ionic pluroinc P123 as structure directing agent. The surface of mesoporous TiO_2 was modified through grafting with 3- aminopropyl triethoxy silan (APTES). Simvastatin was selected as the model drug and its release from both unmodified and modified TiO_2 was evaluated in in simulated gastric fluid (SGF, pH = 1.2) and simulated intestinal fluid (SIF, pH = 6.8) at 37 ^{o}C. The resulting materials were characterized by Fourier transform infrared spectroscopy (FT-IR), N_2 adsorption-desorption, X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM) and UV-Vis spectrometry. FT-IR spectroscopy revealed ionic interaction between carboxyl groups of simvastatin and the aminopropyl groups of the grafted APTES. In vitro release studies showed slower release rate of simvastatin from the functionalized carrier in applied media. Also, the release profiles modeled with Korsmeyer-Peppas to evaluate the kinetic of drug release.

Keywords: Mesoporous TiO_2, Surface functionalization, Simvastatin, Drug release

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Isocyanides Behavior toward Organolithium Compounds

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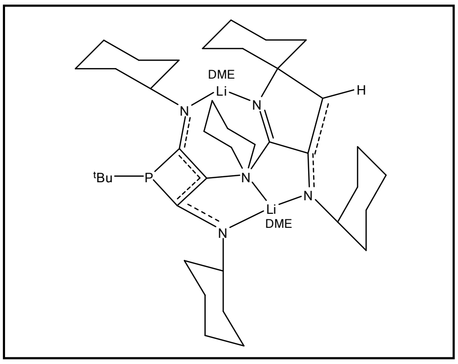
Alkyllithium compounds are widely used as very strong bases, nucleophiles and reagents for metallation in organic synthesis. Alkanes are very weak acids, hence their corresponding lithium-derivatives are extremely strong bases. The metalation uses the fact that the strong bases are capable to deprotonate organic molecules if they have "acidic" protons. Such "acidic" protons in organic molecules are mostly found at positions where a negatively charged anion is stabilized by a suitable functional group. Treatment of organolithium compounds with isocyanides leads to the formation of metalated species. Quenching of such reactive aldimines with electrophiles leads to ketenimines [1]. The reaction of Grignard reagent with isocyanides leads to dimerization by carbon-carbon coupling [2]. All base initiated dimerization show head-to-head coupling of molecules as a common feature. In this study, we present the reaction of cyclohexyl isocyanide (chosen due to its stability toward deprotonation) with $^{t}BuPLi_2$ in THF at room temperature. The reaction started obviously with dimerization first. The monomer unit may be described as a vicinal dilithiated amine. However the dimerized intermediate was able to react with three additional isocyanide molecules obtained with crystallization from DME. The involved cyclohexyl ring was observed in a spirocyclic system. The reason is not a simple deprotonation but a carbene formation followed by carbene insertion into carbon-hydrogen position due to the base stability of cyclohexyl group.



Keywords: Isocyanide, Organolithium compounds, Dimerization

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19th Iranian Inorganic Chemistry Conference
Chemistry & Chemical Engineering Research Center of Iran
5-7 September 2017
www.IICC19.ccerci.ac.ir

Synthesis and characterization of metal complexes by pentadentate N4S Schiff base ligand

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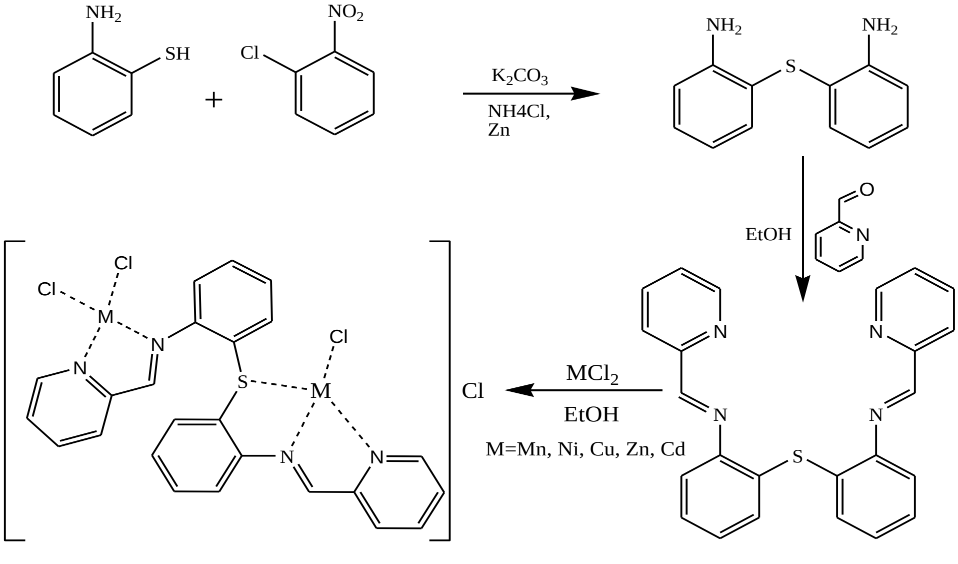
Transition metal complexes with thioether Schiff base ligands have been prepared since the beginning of the development of coordination chemistry and there is continuing interest in these complexes [1,2]. Symmetrical linear pentadentate Schiff base ligands that have N4S donors or have thioether and pyridine groups in their structure are very rare. It is known that N and S atoms play a key role in the coordination of metals at the active sites of numerous metallo-biomolecules [3]. In this work we synthesized 2-((2-nitrophenyl)thio)aniline from 1-chloro-2-nitrobenzen and 2-aminothiophenol and then prepared 2,2’-thiodianiline. N4S Schiff base ligand prepared by reaction of 2,2’-thiodianiline with pyridine-2-carbaldehyde. Mn(II), Cu(II), Zn(II) and Cd(II) Schiff base complexes of this ligand were synthesized. The Schiff base ligand and related complexes were characterized by IR, UV-Vis, NMR, Mass spectrometry, conductivity and elemental analyses.



Keywords: Schiff base, Schiff base complexes, N4S Ligand, pyridine-2-carbaldehyde

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Synthesis and characterization of Schiff base ligand containing two thiophene pendant arms and related complexes

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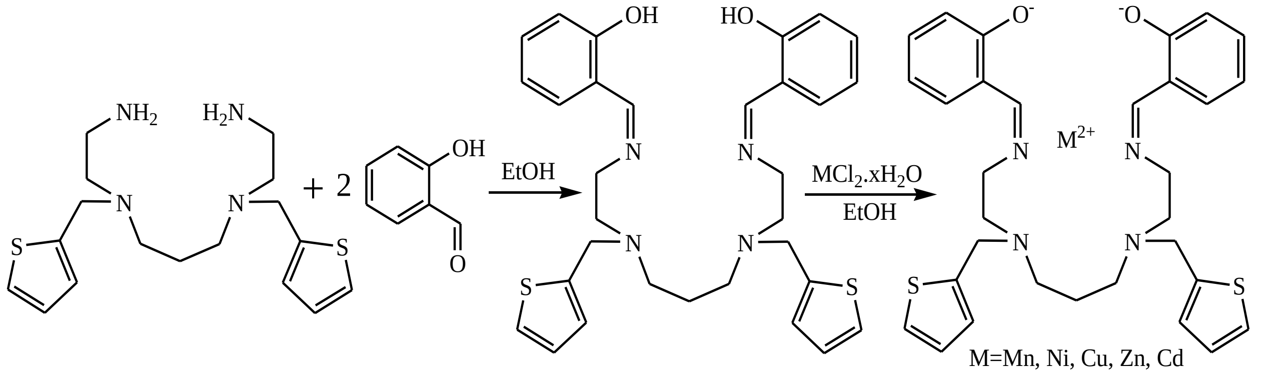
N, S and O donor Schiff base ligands are polydentate ligands that have hard and soft donors in its structure. These ligands are promising from the viewpoint of coordination chemistry because of their ability toward complexation and involvement in a wide range of biological and non-biological processes. The presence of both hard and soft donors in these Schiff base ligands allow coordination with a wide range of transition metal ions and several metal complexes with these Schiff base ligands have been reported [1–3]. In this work we synthesized a diamine containing two thiophene pendant arms and then prepared related Schiff base ligand by reaction of this diamine with salisylaldehyde. Mn(II), Cu(II), Zn(II) and Cd(II) Schiff base complexes of this ligand were synthesized. Diamine, the Schiff base ligand and related complexes were characterized by IR, UV-Vis, ^{1}H NMR, conductivity and Mass spectrometry.



Keywords: Schiff base, Schiff base complexes, N4O2S2 Ligand, Pendant arm.

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Molecular structure of novel hetero-ligand cobalt complexes

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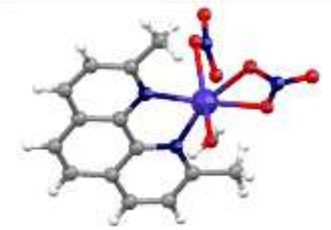
Transition metals ions are known to play very important roles in biological processes in the human body. For example, Cobalt is metal center part of vitamine B_{12}, a co-enzyme that plays significant roles in some biochemical processes. Cobalt complexes with nitrogen donor ligands, such as phenanthroline and /or bipyridine do exhibit antimicrobial properties and these metal complexes can control cancer cell division by significantly reducing DNA synthesis [1-3]. In our research, two novel cobalt complexes $[Co(dmphen)(NO_3)_2(H_2O)]$ (**1**) and $[Co(dmbipy)(NO_3)_2(H_2O)]$ (**2**) were synthesized by treatment of $Co(NO_3)_2.6H_2O$ with 2,9-dimethyl-1,10-phenanthroline (dmphen) and 6,6́-dimethyle-2,2′-bipyridine (dmbipy) respectively. In complex **1**, Co^{II} metal ion is six coordinated in a monoclinic geometry by two N atoms from 2,9-dimethyl-1,10-phenanthroline and four O atoms from two nitrate anions and one aqua ligand (Fig.). In complex **2**, Co^{II} metal center is also six coordinated in a tricilinic geometry by similar coordination environment as complex **1**. The stability of these complexes was evaluated by DFT method and compared with other related cobalt complexes.



Keywords: Cobalt complex, Crystal structure, Phenanthroline, Bipyridine

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Synthesis, characterization and crystal structure of a halo bridged copper(II) complex

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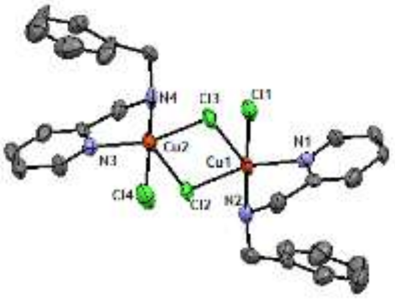
Binuclear complexes of copper(II) have been the subject of extensive investigation because of their wide use in various fields. These compounds have vast biological applications and good catalytic roles in many reactions [1]. Some of these complexes were designed and their structural properties were investigated in our research group. The synthesized binuclear copper (II) complexes containing halide ions as bridging ligands, reveals solvatochromic, halochromic and thermochromic behaviors [2]. In this report, in continuing our study on holo bridged complexes, the reduced Schiff base, *N*-(pyridin-2-ylmethyl)benzylamine (L), has been prepared and used as a bidentate ligand for the synthesis of chloro bridged dinuclear copper(II) complex, [LCu(μ-Cl)]$_2$. The complex has been characterized by FT-IR spectroscopy, conductivity measurements and elemental analysis. Crystal structure of the complex is also determined by X-ray crystallography that shows each copper(II) center has a square pyramidal coordination environment consisting of two bridging chloride anions, one terminal chloride anion, and two neutral nitrogen donors from the chelating ligand (L).



Keywords: Binuclear, Copper(II), Crystal structure

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Phthalocyanine complexes immobilized on polysilsesquioxane particles: a new and efficient catalyst for the oxidation of benzyl alcohol

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Recently, there has been intense interest in the preparation and application of functional polysilsesquioxane particles[1,2]. These polysioxane -immobilized ligand systems have great potential in the extraction and separation of metal ions and dyes from aqueous solution and as supported ligands for catalysts [3,4]. In this regard we have prepared two types of polysilsesquioxane particles. After studying the structures of these two polymers by different spectroscopic and microscopic analysis, nitro and amino metallophthalocyanines of copper and cobalt have been successfully anchored onto the surface of them and they used as catalysts in oxidation of benzyl alcohol with t-butylhydroperoxide. The optimization results showed that the activity of the prepared catalysts depend on the solvent, oxidant and the central cations of the catalysts.

Keywords: Polysilsesquioxane, Metallophthalocyanines, Benzyl alcohol, Catalyst, Oxidation

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Optimization of epoxidation of cyclooctene using polysilsesquioxane supported $MoO_2(acac)_2$ by box-behnken design

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Epoxidation of cyclooctene using molybdenum complexes is an important reaction that is interest for researchers[1,2]. According to importance of subject in this research, experimental design was used to optimize catalytic epoxidation of cyclooctene using a new catalyst. For this purpose, a polysilsesquioxanes were prepared using a base catalyzed sol-gel process. After studying the polymer structure, its functinal groups were changed to diethylenetriamine (dien) and then used to support $MoO_2(acac)_2$ complex. This supported catalyst was applied to the epoxidation of cis-cyclooctene with tert-butyl hydroperoxide (TBHP). The optimal design of experiments using box-behnken method was employed to evaluate the effects of individual process variables such as reaction time, amount of catalyst and volume of TBHP and their optimum values with this method were found to be 18min, 10mg and 0.4ml (in 1.5 ml of 1,2-dichloroethane and 0.5 mmol cyclooctene) respectively, to achieve a conversion of 89%. The product yields were studied by Gas Liquid Chromatography.

Keywords: Polysilsesquioxanes, Epoxidation, Cyclooctene, Box-behnken design

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Synthesis and Characterization of the New Chemically Responsive Gold(I) Complexes

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Many gold(I) complexes are found to be luminescent at room temperature in the solution phase, and some of them are emissive in the solid state. Recent interest in these complexes has been driven by possible applications in OLED display technology as dopant emitters [1] and in sensor development for luminescence detection [2]. Recent years have witnessed interesting developments starting from solvoluminescence to on-off switching of luminescence arising from the switching of intra- to intermolecular Au···Au interactions [3]. The luminescent properties of these complexes heavily rely on the nature and distance of Au···Au centers. Herein we synthesized and characterized the new gold(I) complexes with 2-vinylpyridine (2-Vpy) (**1**) and 2-ethynylpyridine (2-Epy) (**2**) with interesting solvochromic behavior. These complexes were characterized by ^{1}H NMR and ^{13}C NMR and their absorption and emission spectra were studied. Their ^{1}H NMR data show vinyl Hydrogens for **1** and ethynyl Hydrogens for **2**, which tells us our ligands are coordinated to the gold center through the nitrogen atom.

Keywords: Gold(I), Solvochromic, 2-vinylpyridine,2-ethynylpyridine.

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Synthesis and Characterization of a new group of complexes based on Naphthalimide ligands

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Chromophore ligands-appended, transition metal complexes have enjoyed significant attention over the years due to the wide variety of both fundamental and applied studies that are possible with such systems. The interactions of photoactive units, be they covalently linked in simple dyad systems, can allow studies into electron and energy transfer mechanisms [1,2]. Among these kind of organic chromophores, we can sign 1,8-Naphthalimide derivatives which have significant absorption, emission and photophysical properties [3]. In this study, in order to improve the properties of these chromophores, the design and synthesis of a new group of chromophores based upon 1,8-Naphthalimide derivatives and the study of their interaction with metallic centers such as Au(I), Ag(I) and Pt(II), were investigated. As we expected, by entering the metallic center, a new group of electronic transitions were engendered in the system and the complexes demonstrated interesting photophysical properties, so that they can be used as better tools in bioimaging applications in comparison with those observed for parent organic chromophores. All the ligands and complexes were characterized using NMR spectroscopy and ESI-Mass spectrometry and their solid state structures were determined by X-ray crystallography method.

Keywords*:* 1,8-Naphthalimide derivatives**,** Transition metal complexes, Photophysical properties.

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Synthesis, Characterization and Spectral Investigation of New Platinum Complexes Containing Phosphine Ligand

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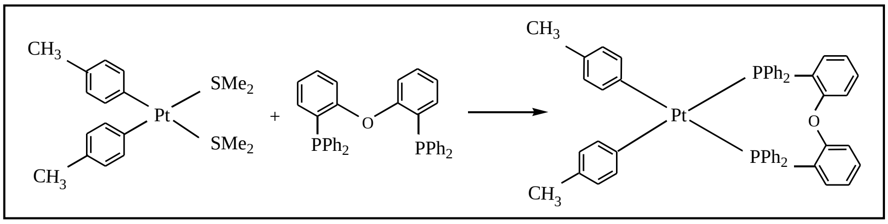
The square-planar of platinum(II) complexes have been increasing importance after the discovery of the anti-tumor property of *cis*-dichlorodiammine platinum(II) [1]. Also, platinum complexes are relatively easily oxidized or reduced in two-electron processes between the three main oxidation states. Since the predominant geometry for the (II) oxidation state is square planar and for the (IV) oxidation state is octahedral. Furthermore, oxidative addition reaction was accompanied by the addition of two species to the platinum(II) and reductive elimination reaction was accompanied by the loss of two fragments from platinum(IV) [2,3]. In this work, new platinum complexes containing phosphorous donor atoms were synthesized by the reaction of [PtCl$_2$(DMSO)$_2$] and [(p-MeC$_6$H$_4$)$_2$Pt(SMe$_2$)$_2$] with phosphine ligand in a 1:1 molar ratio. In these complexes the ligand was coordinated to metal via the phosphorous donor atoms and formed new complexes of platinum with square planar geometry. It was shown that these platinum(II) complexes contain 1:1 metal to ligand stoichiometry. These platinum complexes have been characterized by FT-IR, ^{1}H NMR, UV-Vis and elemental analysis. The molar conductivity measurements showed that these complexes were non-electrolyte. The photoluminescence of these platinum(II) complexes were investigated in dichloromethane.



Keywords: Platinum, Ligand, Phosphorous Donor

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New Platinum Complexes Containing Nitrogen Donor Atoms: Synthesis, Characterization and Luminescence Studies

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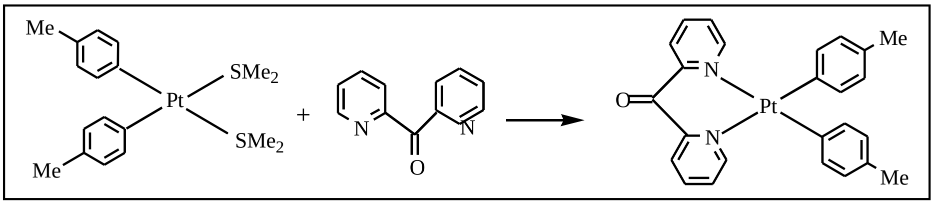
Organometallic chemistry is essentially related to organic chemistry and coordination chemistry. The existence of metal-carbon bonds in the structure of coordination compounds is a basic parameter for introducing of organometallic complexes [1]. Moreover, ligands have a key role for designing of orgnometallic compounds in coordination chemistry and one of the most important metals for synthesis of organometallic complexes is platinum [2,3]. In this work, new platinum complexes containing dinitrogen ligand were synthesized by the reaction of $[(p\text{-}MeC_6H_4)_2Pt(SMe_2)_2]$ with dinitrogen ligand in a 1:1 molar ratio. In synthesized organoplatinum complexes, the ligand was coordinated to the metal center via nitrogen donor atoms. Moreover, the MeI was used as a reagent for investigation of oxidative addition reaction on the platinum(II) complex and formation of the platinum(IV) complex with octahedral geometry was suggested. It was shown that these platinum(II) and platinum(IV) complexes contain 1:1 metal to ligand stoichiometry. The molar conductivity measurements showed that these complexes were non-electrolyte. The photoluminescence of the platinum(II) and platinum(IV) complexes were investigated in dichloromethane. These organoplatinum complexes have been characterized by FT-IR, ^1H NMR, UV-Vis and elemental analysis.



Keywords: Platinum, Luminescence, Nitrogen Donor

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Amino acid-Functionalized MCM-41 mesoporous silica for drug delivery

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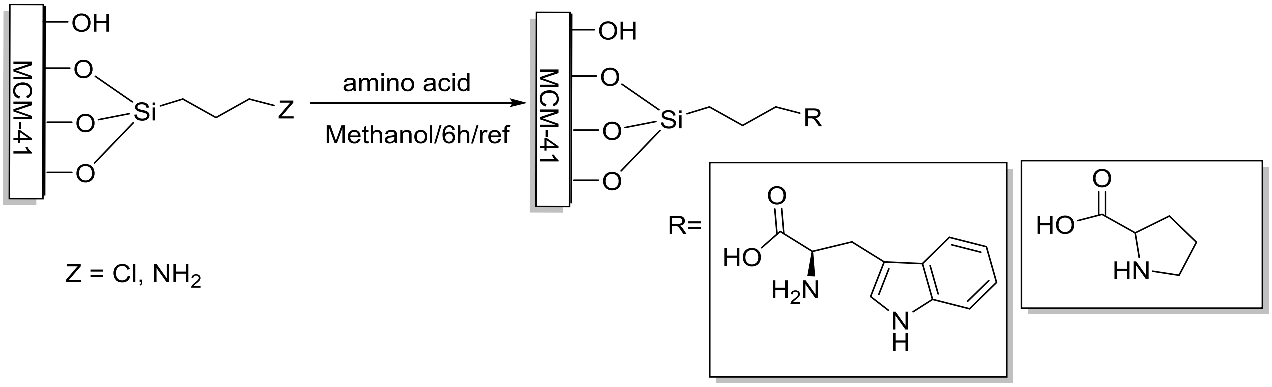
Design and synthesis of surface functionalized ordered mesoporous silica materials have attracted much attention in recent years, due to their applications in the fields of catalysis, adsorption, ion-exchange and medical devices.[1] Controlled drug release aims at optimizing drug efficiency while simultaneously reducing adverse collateral effects.[2] Recently we used modified MCM-41 as catalyst for the regioselective aminolysis of styrene oxide.[3] In this work, mesoporous MCM-41 silica is functionalized by L-proline and L-tryptophan. These grafted materials were studied as potential carriers for controlled drug release, using clarithromycin as a test drug (Scheme 1).



Scheme 1. Amino acid- functionalized MCM-41

Keywords: MCM-41, Amino acid, Drug delivery

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Influence of isocyanide ligands on the luminescence properties of cycloplatinated(II) complexes

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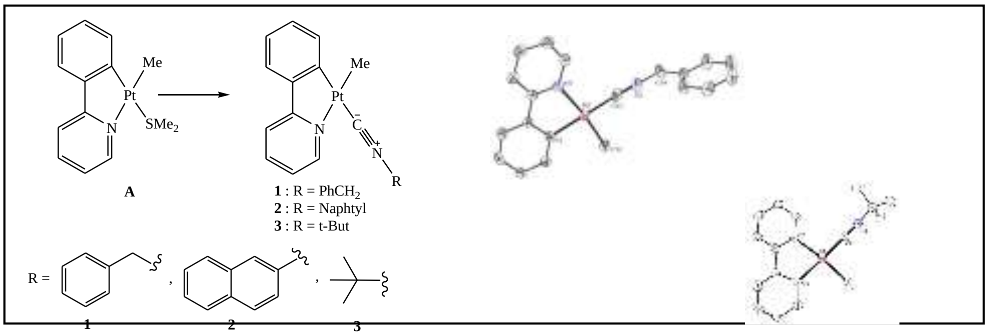
Isocyanides with general formula of –CNR (alkyl or aryl), exhibit an important class of strong field ligands, being powerful carbon σ-donors and weak π-acceptors [1]. The complexes of isocyanides with various late transition metals were reported and photophysically investigated [2]. Particularly, cycloplatinated(II) complexes containing isocyanide ligands have shown to be strong luminescent materials at room temperature [3]. There are enough evidences which indicates that R substituent in isocyanides considerably affects the steric, electronic and consequently photophysical properties of such complexes [4]. Herein, we have designed a new non-chelating L-X (L and X are neutral and anionic, respectively) system including two strong carbon σ-donors *i.e.* methyl (X) and -CNR (L, R= benzyl, naphtyl and t-butyl). The new complexes were characterized by NMR spectroscopy and X-ray crystallography. The complexes were photophysically studied and the obtained data were theoretically supported by DFT methods.



Keywords: Isocyanide ligands, Cycloplatinated complexes, Photophysical properties, DFT calculations.

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Assembly of platinum(II) rollover complexes with diphosphine ligands

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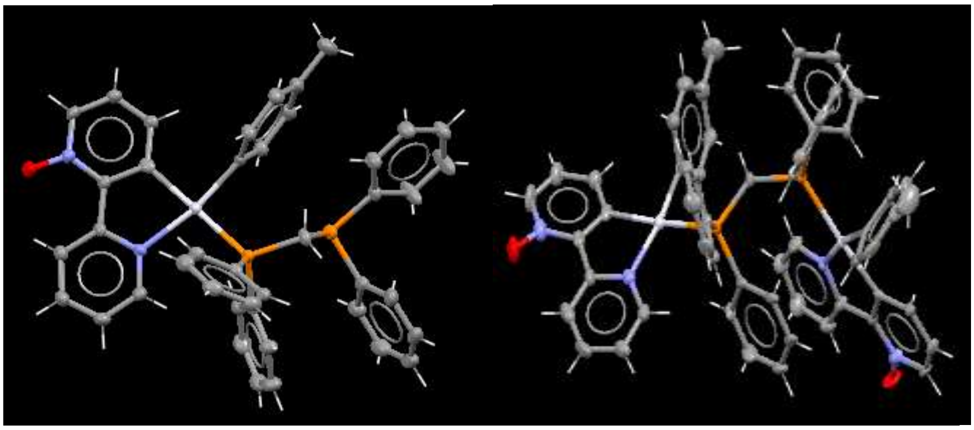
Diphosphines are an important class of tertiary phosphine ligands in organometallic chemistry and have found wide applications [1]. In general, diphosphines are versatile and robust ligands that are known to have various coordination modes [2]. Cyclometalated complexes have been studied in depth, and almost every *d*-block transition metal has its own representative, partially, this is because cyclometalation reactions are envisaged as intramolecular analogues of intermolecular C–H activation [3]. In the case of rollover cyclometalation the process is slightly different and is possible only with ligands that are at least bidentate; the reaction must involve partial decomplexation of the ligand, rotation and the activation of the C−H bond, and formation of the metallacycle [4]. Herein we report some aspects of the reactivity of platinum(II) rollover complexes with different bidentate phosphine ligands, in order to check the influence of different lengths of the backbone on the properties of the complexes, and also look for peculiarities due to the rollover scaffold.



Keywords: Diphosphine ligands, Rollover cyclometalation, Organoplatinum, X-ray structure determination.

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Structure-Reactivity Studies, Characterization, Crystal Structure and luminescence Properties of Some Organotin Complexes Based on the N-Donor Ligands

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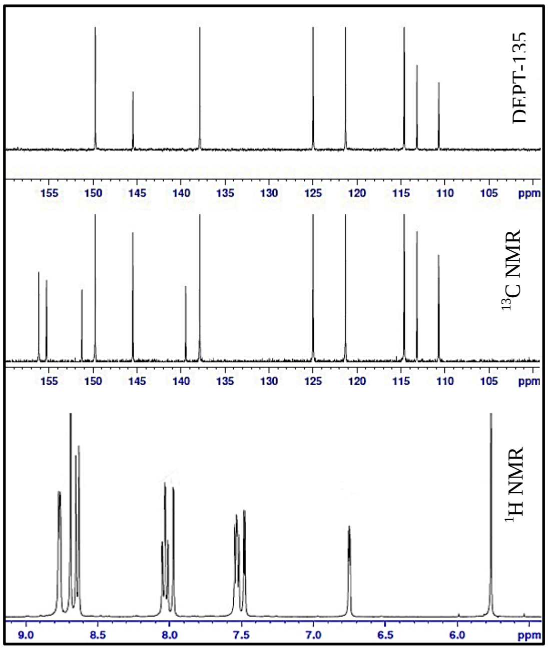
The preparation and coordination behavior of organotin(IV) compounds with polypyridyl ligands which coordinate through nitrogen atoms have been extensively investigated. Most of these complexes show biological activities, such as antifungal, antibacterial and antitumor activity. They usually form 1:1 and 1:2 adducts; the resulting adducts usually exist in the trigonal bipyramidal or octahedral geometries. In spite of the well-known chemistry of organotin complexes; the variety of structures containing the phenanthroline and 2,2'- bipyridine ligand is more diverse than those of substituted diimine ligands [1]. Herein, we report the reaction of some organotin(IV) dihalides R_2SnX_2 with diimine and terpyridyl ligands in different molar ratios to provide more information about their structural properties. The resulting products have been fully characterized by elemental analysis, multinuclear NMR (^{1}H, ^{13}C, ^{119}Sn) and DEPT-135 NMR spectroscopy and X-ray crystal structure determination. The solution luminescence properties of complexes have also been investigated. The results will be presented.



Keywords: Organotin, Crystal Structure, N-donor, NMR

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Pyridine-2-thiolate as a versatile ligand in platinum chemistry

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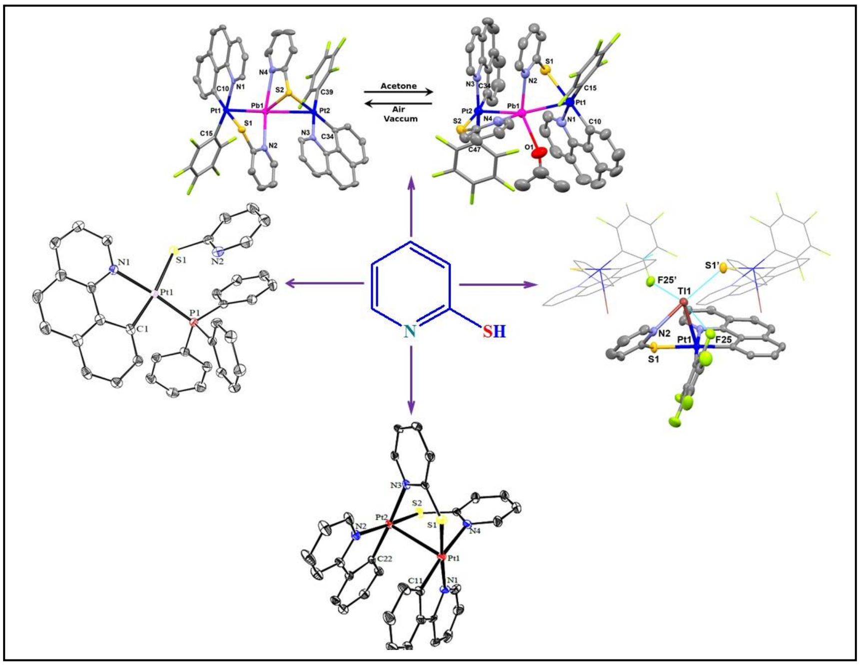
Pyridine-2-thiol (HS-2-py) is a versatile ligand, since both sulfur and nitrogen atoms can act as coordinating sites [1]. Meanwhile, pyridine-2-thiol can be deprotonated to give a pyridine-2-thiolate (S-2-py) ligand to coordinate with metals through the sulfur atom to leave the pyridine moiety free [2]. This ligand can behave as auxiliary ligand in transition metal complexes (especially in platinum compounds) while it has been believed that it plays important roles in the facility of tuning both steric and electronic properties of these complexes [3]. The present contribution revealed that the organoplatinum complexes comprising pyridine-2-thiol ligand can be a good target in photophysical studies, fundamental reactions such as C–S bond coupling, C–H reductive elimination and protonation reaction or considered as promising anticancer agents for drug development.



Keywords: Pyridine-2-thiol ligand, Organoplatinum, Photophysical properties, Organometallic reactions.

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Structural investigation of coordination aspects for complexes containing 2-(pyridin-2-yl)oxazolidine unit by CSD and introducing a new silver one: Supported by spectral and theoretical studies

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Oxazolidine derivatives are biological active compounds such as antidiabetic [1], anticonvulsant [2], antitubercular and aldose reductase inhibitors [3]. Fungicidal activities of this compounds were also established [4]. For extending this field, in this work, all coordination modes of 2-(pyridin-2-yl)oxazolidine-based ligands were extracted by CSD[1] and also a new silver complex of 2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol (L), $[Ag_2L(NO_3)_2]$ was prepared and identified by elemental analysis, FT-IR and ^1H NMR spectroscopies. Structure of complex was evaluated by density functional theory (DFT) at B3LYP/LANL2DZ level. The experimental and theoretical studies give raise a structure of figure 1. In this complex the ligand acts as tridentate. Two silver atoms have different environment and geometries including tetrahedral and trigonal. Molecular orbital energy diagrams of complex and related HOMO and LUMO orbitals were performed.

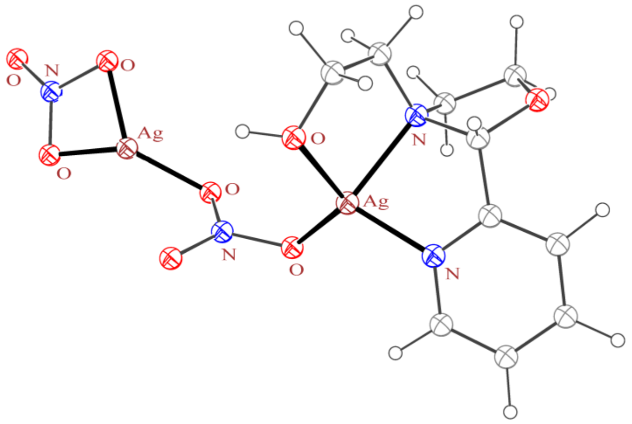

Figure1. Optimized structure of complexe.

Keywords: Silver, Coordination chemistry, Theoretical studies, Oxazolidine, CSD

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Solid-state conversion of a silver coordination polymer nanostructures to another one upon 2-aminopyridine addition

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Coordination polymers provide a unique opportunity for developing advanced functional materials. Solid-state structural transformations involving coordination polymers induced by light, heat, guest removal, uptake or exchange, expansion of coordination numbers, oxidation of metal centers, condensation, or reactions between the ligands are very fascinating and one of the hot topics in solid- state chemistry [1,2].

Solid-state structural transformation of Ag_2tp (1) coordination polymer [3] nanoparticles, prepared by sonochemical procedure, to $[Ag_2(\mu_4\text{-tp})(apy)_2]$ (**2**) (where tp = terephthalate dianion, and apy = 2-aminopyridine) [3] coordination polymer nanoparticle has been observed upon solid-state mechanochemical reaction of compound 1 with 2-aminopyridine. This change in coordination-mode was confirmed by single-crystal X-ray diffraction analyses of compounds 1 and 2. Powder X-ray diffraction experiments showed that the structural transformation occurs in the batch powder samples. These nanostructures were characterized by scanning electron microscopy (SEM), powder X-ray diffraction (PXRD), IR spectroscopy. These structural transformations normally involve significant rearrangement of molecular components in the crystals, including rotation, bending, swinging, sliding, shrinking, or swelling. In summary, by solid-state structural transformation, we successfully prepared $[Ag_2(\mu_4\text{-tp})(apy)_2]$ (2) by mechanochemical process.

Keywords: Solid-state, Coordination polymer, Structural transformation, Nano structure

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Synthesis and characterization of metal complexes with Schiff base ligand (SNS) derived from Thiophene-2-carbaldehyde

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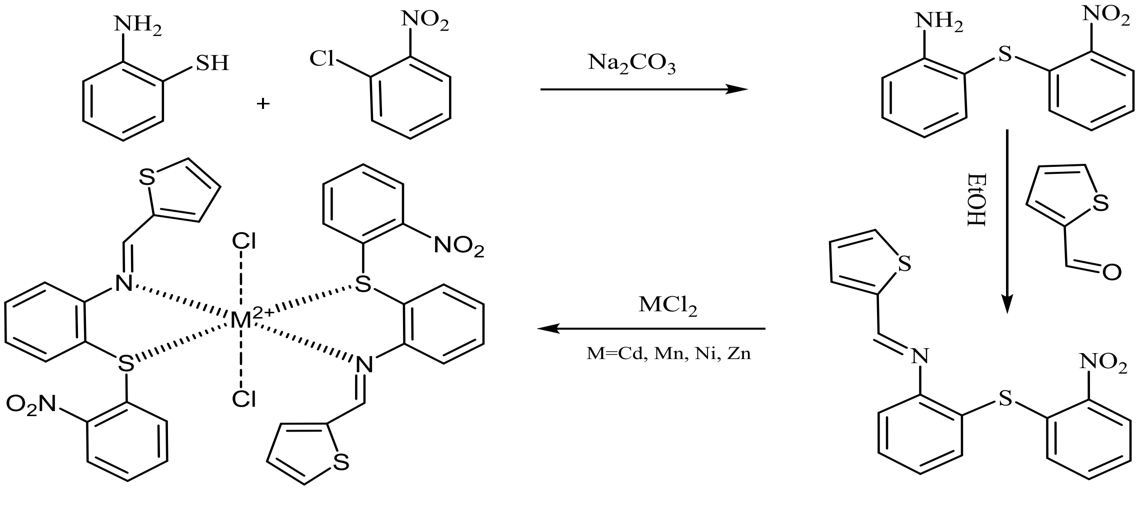
Schiff bases (imines) constitute one of the most widely used families of organic compounds, not only as synthetic intermediates but also in coordination chemistry[1]. It is known that N and S atoms play a key role in the coordination of metals at the active sites of numerous metallo-biomolecules[2]. Thiophene derivatives have intensively antibacterial and antitumor activities[3]. In this work we synthesized 2-((2-nitrophenyl)thio)aniline from 1-chloro-2-nitrobenzen and 2-aminothiophenol. Then SNS Schiff base ligand prepared by reaction of 2-((2-nitropheyl)thio)aniline with thiophene-2-carbaldehyde. Ni(II), Mn(II), Zn(II) and Cd(II). Schiff base complexes of this ligand were synthesized. 2-((2-nitrophenyl)thio)aniline and the Schiff base ligand were characterized by IR, NMR and Mass spectrometry and the synthesized complexes characterized by IR, UV-Vis, NMR, Mass spectrometry and conductivity. The results show that the ligand is coordinated to metal ions through imine N and thioether S atoms (Scheme).



Keywords: Schiff base, Schiff base complexes, SNS Ligand, Thiophene-2-carbaldehyde

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Synthesis, crystal structure and DFT study of novel hetero-ligand copper(II) complex

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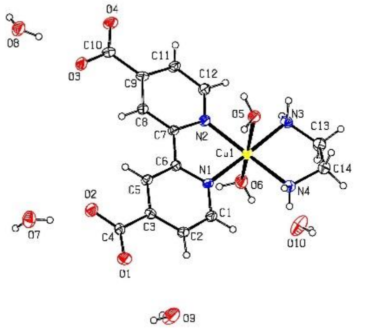
Spherical geometry around copper center in Cu(II) complexes is an interesting subject as building-blocks to construct novel coordination architectures [1-2]. However there are only a few reports on theoretical study on coordination chemistry of Cu(II) compounds with various ligands in the literature.

In this study, a new copper(II) complex with the ligands 2,2'-bipyridine-4,4'-dicarboxylic acid (bpydc) and ethylene-diamine (en) with formula of $[Cu(bpydc)(en)(H_2O)_2].4H_2O$ (**1**) has been synthesized. The complex was characterized by IR, UV–Vis spectroscopy, and single-crystal structure, where the structure refinement demanded six coordination environment around Cu(II) in a distorted octahedral geometry. DFT calculation was applied for determination of relative stability of four, five and six coordination copper complexes that it was confirmed the stability advantage of coordination number of 6 over 5 or 4.



Complex **1**

Keywords: Copper(II) complex, Nitrogen-donor ligands, Single-crystal XRD, DFT calculation.

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Tetracoordinated Hg (II) complex: Synthesis, structure analysis and spectroscopic studies

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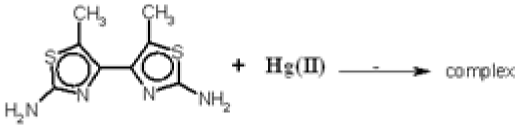
For the past decade, the reports have been made on the use of transition metal complexes. Mercury (II) compounds have current interest due to their possible applications as materials with non-linear optical properties. Due to these features, understanding the coordination chemistry of the mercury(II) ion is crucial for the rational development of materials with specific biological and physical properties. The tolerance for many different coordination numbers and geometries is typical of the coordination chemistry of Hg(II) ions. The mercury(II) ion is a distinctly ‘soft’ cation, showing a strong preference for Cl, Br, I, P, S and N-type ligands. Also, there are some examples reported in the literature describing the influence of weak intermolecular interactions on the coordination geometry of the metal center and the formation of unusual coordination geometries around the Hg(II) ion. We report here the synthesis and characterization of Hg(II) complex containing the 4,4′-btz ligand.



Keywords: Tetracoordinated, Hg (II), complex, structure analysis

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Aluminium Synthesis, Characterization and Antibacterial Activities of (III) Schiff-base Complex

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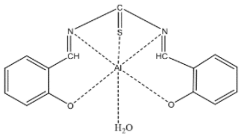
Metal complexes of Schiff base derived from the reaction of substituted salicylaldehydes with aliphatic aromatic amines represent a series of compounds containing nitrogen, sulphur and oxygen donor atoms that has been widely studied. Over the past few years, there have been many reports on their applications in biology including antibacterial, antifungal, anticancer, antioxidant, anti-inflammatory, antimalarial and antiviral activity[1,2]. In this paper, attempt to prepare free ligand was unsuccessful. The typical preparation of aluminium (III) complex, 1 mol of Al $(NO_3)_3.9H_2O$ and 2 mol of salicylaldehyde ($C_7H_6O_2$) were dissolved in 10 mL of ethanol to form homogeneous solutions. Few drops of ammonia solution were added until pH 6-8. Then thiourea solution was added dropwise to the above solution with stirring. The mixture was allowed to reflux under stirring for 8 h (Scheme 1). After that, the resulting mixture was cooled in room temperature and filtrated under reduced pressure. The complex was characterized by elemental analysis (CHNS), FT-IR, UV-vis spectroscopy, Magnetic moment, antibacterial activity and conductivity measurements. Conductance measurements showed the electrolytic nature of this complex. The complex shows better activity against all tested bacteria in which Bacillus substilis shows relatively better activity.



Scheme 1. synthesis of aluminium (III) complex

Keywords: Schiff-base complex, Antibacterial activity, Complexation.

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Synthesis and crystal structure of a novel cuprous thiocyanate anionic coordination network template by a cationic cupric complex

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Copper(I) pesudohalide coordination networks exhibit promising electronic and optical properties [1]. Three polymorphs of Copper(I) thiocyanate are known, which could be described as 3D networks containing four coordinated Cu and S atoms [2]. CuSCN has attracted attention as a transparent solution processable p-type semiconductor for solar electric power applications [3]. Recently, Copper(I) thiocyanate coordination polymers gained much research attention aiming at new electronic and optophysical properties [2,4]. The present research work introduces the first 3D anionic copper(I) thiocyanate coordination polymer templated by a cationic copper(II) complex. The $[Cu(en)_2]@[Cu_4(SCN)_6]_n$ (en = ethylene diamine) is crystallized in the monoclinic Pn space group. The cell parameters are a=9.987(2) Å, b=10.194(2) Å, c=11.714(2) Å and β=102.63(3)º.

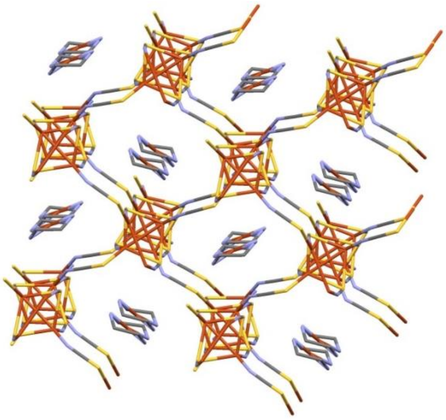

Fig. 1. The crystal packing of $[Cu(en)_2]@[Cu_4(SCN)_6]_n$.

Keywords: Coordination polymer, Copper(I), Thiocyanate, Template, Synthesis, Crystal structure

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Anion-controlled structural motif of cadmium coordination polymers

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Self-assembled coordination polymers (CPs) which contains metal cations and multitopic organic ligands have aroused a high degree of attention. This class of compounds provides numerous opportunities to modify properties such as gas storage, separation, luminescence, catalysis, sensors and so on [1]. The structural assemblies can be influenced by many factors, such as the organic ligand, coordination geometry of metal center, counterion, solvent, and temperature [2]. Anions have a major influence on the solid-state structure of coordination polymers in many ways [3]. In the case of an anion, it can act as either a coordination ligand or counterion balancing the framework charge depending on its coordination ability [2].

In this regard, we consider self-assembly of bridging bis-pyridyl schiff base ligand (**L$_{py}$**) as an organic tecton and cadmium metal ion as a metallic tecton. In this work, coordination polymers (**1**) and (**2**) have been synthesized from the reaction of bridging ligand and cadmium(II) sulfate and perchlorate, respectively. These coordination polymers have been characterized by several spectroscopic methods as well as X-ray structural analysis. Our results show that the structural motif and topology of two resulted coordination polymers depend on the anions used. As shown in Figure, in the case of coordination polymer (**1**), three-dimensional motif with sulfate anion as ligand was obtained while the topology of coordination polymer (**2**) is an one-dimentional interdigitate motif with perchlorate anion as guest molecules.

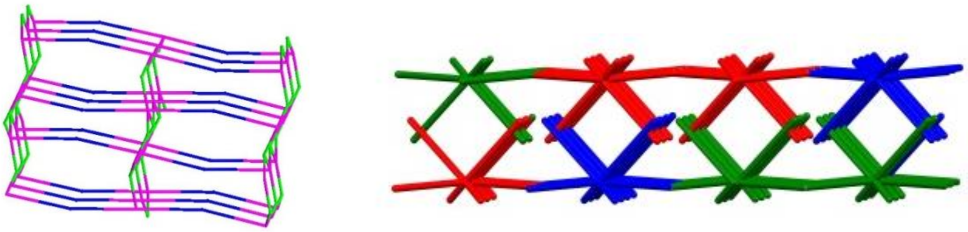

Fig. Schematic representation of the structural motif of coordination polymer**1** (left) and **2** (right).

Keywords: Coordination Polymer, Anion Effect, Cadmium, Structural Motif

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Topological different ladder structure of cadmium coordination polymers

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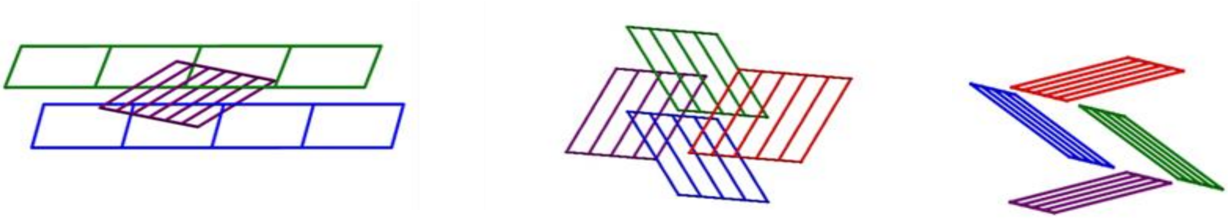
Nowadays, novel functional coordination polymers (CPs) have gained attention due to their potential applications in the realms of gas absorption, catalysis, luminescence, sensing and also in industrial and material science [1]. The complicated structures of coordination polymers constructed by the assembly of metal ion and organic ligands are quite difficult to predict and control during their synthesis. Some physical or chemical factors, such as temperature, counterion, pH value, metal-to-ligand ratio, solvent, etc., have unpredictable impacts on the structures and properties of the resulting solid-state structures [2]. In this context structural changes in response to the solvents have been observed in some coordination polymers [3].

In this work, the main scope is preparation of new coordination polymers based on a bridging bis-pyridyl schiff base ligand (**L_{py}**) as an organic tecton and cadmium as a metallic tecton. Herein, two coordination polymers of cadmium nitrate by different synthetic methods have been synthesized and characterized by spectroscopic methods and x-ray structural analysis. Our results show that compound (**1**) was a three-dimensional interpenetrated ladder network (1D+1D → 3D), while compound (**2**) was a one-dimensional non-interpenetrated ladder coordination polymer.



(a) (b) (c)

Fig. Topological representation of coordination polymers **1**(a) and **2** (b, c) in different orientations.

Keywords: Coordination polymer, Cadmium, Topology, Interpenetration

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Synthesis and characterization of a new Cu(II) proton transfer complex with 2,6–pyridine dicarboxylic acid and 3-(aminocarbonyl)pyridine

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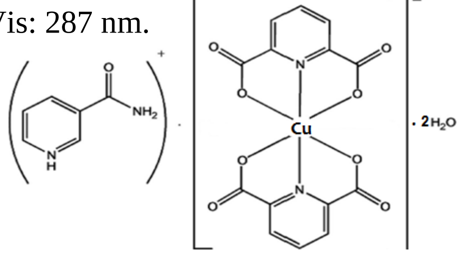
Anionic carboxylic acids and cationic amine fragments interacted together by intermolecular non–covalent interactions like (N−H···O) hydrogen bonds (HBs) results in the formation of a proton transfer ligands (PTLs). In following, the reaction of PTLs and metal salt in water or other solvents leads to the formation of respective coordination compounds [1, 2]. There are a few reports of Cu(II) complexes with pyridine–2,6–dicarboxylic acid (*H_2pydc*) [1(b), 3]. In this work, first of all, the new PTL as (dipicH)(acpyH)$^+$ was prepared from the reaction of (*acpy* = 3–(aminocarbonyl)–Pyridinium) with (*dipicH$_2$* = 2,6–pyridinedicarboxylic acid) in water (ratio 1:1). Then, the complex of Cu(II) with the proposed formula [Cu (*acpy*)(*pydc*)$_2$].2H$_2$O,[$C_{13}N_3H_{11}O_5$] was prepared from the reaction of Cu(NO$_3$)$_2$.3H$_2$O with mixture of (*acpy*) and (dipicH$_2$) in water (0.5:1:1). A solution of (*acpy*) (122 mg, 1 mmol) and (*dipicH$_2$*) (167 mg, 1 mmol) in water (15 ml) was heated at 353 K for 1h. It was then filtered off and the obtained solution kept at RT for 1 week that the needle like colorless crystals of (dipicH)(acpyH)$^+$ were obtained. Also (121 mg, 0.5 mmol) of Cu(NO$_3$)$_2$.3H$_2$O was dissolved in water (5 ml) and added to that solution of PTL (289 mg,1mmol). The resulting mixture was heated for a further 2 h. It was then filtered off and the filtrate kept at RT until the cubic Blue crystals [Cu (*acpy*)(*pydc*)$_2$].2H$_2$O were obtained after 4 days (MP: 271 ℃). The product characterized by FTIR, UV–Vis spectroscopies, and CHN-SO elemental analysis. CHN-SO: C% (Calc.: 43.65, Exp.: 44.63), N% (Calc.: 9.7, Exp.: 8.55), and H% (Calc.: 3.69, Exp.: 4.21). FTIR (KBr) Wave No. (cm^{-1}): 1660, 1710 (C=O Stret.), 1380 (C–O Stret.), 3040, 3140 (OH Stret.), 3000–3600 (N–H stret); UV–Vis: 287 nm.



Keywords: Proton transfer complex; 3–(aminocarbonyl)–Pyridinium , 2,6–pyridine dicarboxylic acid; Hydrogen bonding.

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Inhibition of Mild Steel Corrosion in Acidic Media Using Some Thiourea Derivatives

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Acid solutions are widely used for the removal of rust and scale in several industrial processes such as acid pickling, chemical and electrochemical etching, industrial acid cleaning, cleaning of oil refinery equipment, oil well acidizing and acid descaling, resulting in huge economic losses and many potential safety questions due to metallic corrosion [1]. The use of inhibitors is one of the most practical methods for corrosion protection of metallic objects in acidic media, as well as for reduction of acid consumption occurring during the course of corrosion [2]. The inhibitive effects of 1,1′-(pyridine-2,6-diyl)bis(3-(benzoyl)thiourea) (L1), 1,1′-(pyridine-2,6-diyl)bis(3-(2chlorobenzoyl)thiourea) (L2) and 1,1′-(pyridine-2,6-diyl)bis(3-(4-chlorophenyl)thiourea) (L3) on the corrosion of mild steel in 1 M HCl solution were investigated by chemical and electrochemical measurements such as weight loss, Tafel polarization technique and quantum chemistry analysis. The inhibition efficiencies obtained from different methods were in good agreement with each other. The Tafel polarization method revealed the mixed-mode inhibition of inhibitors. The adsorption of studied compounds on mild steel surface was found to follow the Langmuir isotherm. The values of the Gibbs free energy of adsorption strongly supported spontaneous chemical and/or physical adsorption of inhibitor molecules. The kinetic (E_a, ΔH^*, ΔS^*) parameters were calculated and discussed to describe the mechanism of adsorption. ΔH^* plus sign indicates that the dissolution process of steel is endothermic process. Molecular modeling was used to correlate corrosion inhibition properties and calculated quantum chemical parameters.

Keywords: Mild Steel; Thiourea; Corrosion; Inhibitor; Polarization; DFT

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Synthesis, characterization and spectroscopic Studies of new complexes of palladium with BSA and DNA

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Four new complexes of palladium with general formula $[Pd(C,N)(N_3)(Nu)]$ (C,N= biphenyl-2-ylamine or N-tertiarybuthylbenzylamine, Nu= isonicotinamide or 4-dimethylpyridine) have been synthesized by the cleavage of orthopalladated dimers of general formula $[Pd(C,N)(m\text{-}N_3)]_2$ and characterized with several methods including FT-IR, ^{1}HNMR, elemental analysis, UV-Vis spectroscopy, then the fluorescence quenching reactions of complexes with bovine serum albumin (BSA) in pH 7.20 Tris–HCl buffer solution were studied and the interaction of them with calf thymus deoxyribonucleic acid (DNA) have been studied by electronic absorption titration, fluorescence and viscosity measurement. Also in order to determination of protein binding site of mentioned complexes, site-competitive replacement experiments with specific site markers including Warfarin, Ibuprofen and Digoxin have been done. By the analysis of fluorescence spectrum and fluorescence intensity, it was showed that these complexes have an ability to quench the intrinsic fluorescence of BSA. Further our complexes showed the ability of interaction with binding site I of BSA. In addition, fluorescence resonance energy transfer (FRET) between complexes and BSA have been calculated. Absorption spectra of complexes titration with CT-DNA and viscosity measurement data showed the partial intercalation and groove binding of them to DNA.

Keywords: *BSA interaction,* Palladacycle, Fluorescence spectroscopy.

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Comparative studies on the interactions of antidiabetic drug, metformin and its platinum(II) complex with BSA using multi-spectroscopic methods

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In this study, an attempt has been made to study the interaction of an antidiabetic drug metformin (Met) and its platinum(II) complex with bovine serum albumin (BSA) employing UV–Visible absorption, fluorescence, CD spectroscopy. In fact, in this work we evaluated the effect of metal ion on the metformin drug for new drug design study, because the development of new drugs based on complexes has the advantage that such species (metabolized or not) can interact with biomolecules at two levels, i.e. metallic ion and ligand. Metformin caused the quenching of fluorescence of BSA based on static quenching mechanism while the Pt(II) complex with BSA leaded to the fluorescence quenching of BSA via both static and dynamic quenching mechanisms. The thermodynamic parameters showed that hydrophobic forces and hydrogen bond play main roles in Met–BSA binding reaction and the binding of Pt(II) complex with BSA is by hydrogen bonding and van der Waals force. The conformational changes in the structure of BSA because of interaction with the Pt(II) complex and Met were investigated by circular dichroism (CD) and UV spectroscopy. Competitive studies using site markers of warfarin and ibuprofen results predicted that the binding sites of the drug and its platinum complex with BSA were located in site I (subdomain IIA).

Keywords: Platinum(II) complex, Bovine serum albumin, Metformin, Spectroscopic study

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Spinel copper ferrite nanoparticles as an efficient and magnetically recoverable catalyst for synthesis of 1,2,3-triazoles

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One of the most active research areas in nanoscience, nanotechnology and advanced materials is the synthesis of functional magnetic nanoparticles (MNPs) which can easily be separated and recycled from the reaction solutions by an external magnet [1, 2]. we have synthesized $CuFe_2O_4$ magnetic nanoparticles and demonstrated that these magnetic nanoparticles are excellent catalyst for the azide–alkyne cycloaddition reactions. Because of the magnetic properties of the prepared $CuFe_2O_4$ nanoparticles, it could be easily recovered by means of an external magnetic field and reused upto three cycles in reaction with no significant loss in catalytic activity. According to catalyst leaching investigation, the reaction process is heterogeneously done in the presence of $CuFe_2O_4$ nanoparticles.

Keywords: Nanparticle; Copper ferrite; Magnetically recoverable; Azide- alkyne cycloaddition

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The green synthesis of 5-substituted 1*H*-tetrazoles in PEG catalyzed by Ni(II) immobilized on Fe_3O_4 as a recyclable and non-corrosive catalyst

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The integration of nanotechnology with green chemistry offers innovative prospects to meet current demands for ecological and economic sustainability [1]. Fe_3O_4 have been extensively studied in organic synthetic chemistry and material sciences, because of their high potential in catalysis and numerous applications in biomedicine [2]. Tetrazoles are an important class of polyazaheterocyclic compounds. They have been attracting much attention, due to their wide applications such as pharmaceuticals, catalysis technology and use as ligands in coordination chemistry[3-4]. We report application of Ni(II) complex immobilized on Fe_3O_4 for the synthesis of 5-substituted 1H-tetrazoles via [3+2] cycloaddition reactions of various organic nitriles with sodium azide in PEG as solvent (green solvent)[5]. Nanocatalyst can be easily recovered by an external magnetic field and reused for subsequent run for at least 5 times with less deterioration in catalytic activity.

Keywords: Tetrazoles, Magnetic nanoparticles (MNPs), Ni(II) complex

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Synthesis and spectroscopic studies of novel water soluble complex $[RuL(\eta^6\text{-p-cymene})Cl]^+Cl^-$ and investigation of that in catalytic activity for transfer hydrogenation of carbonyl compounds in green chemistry field

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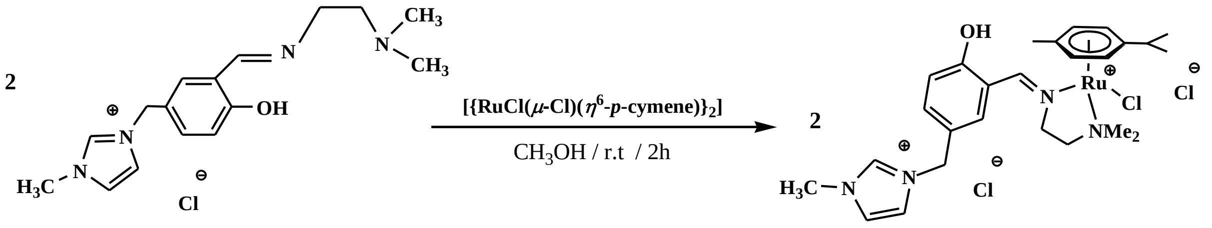
Water soluble complexes have variety applications in green chemistry, because of their high solubility in most solvents and specially in water. For example the η^6-arene-ruthenium(II) complexes with high solubility in water represent an important class of compounds, well-known for promoting a great variety of catalytic reactions, such as C-H activation [1], nitrile hydration [2] or transfer hydrogenation processes [3]. Therefore in this project, new water-soluble arene-ruthenium (II) complex, namely $[RuL(\eta^6\text{-p-cymene})Cl]^+Cl^-$ has been synthesized. By the reaction of Schiff base ligand wrought salicylaldehyde with *N*,*N*-dimethylethylenediamine in methanol at reflux condition for 4 h. Then treatment of the dimeric derivative $[\{RuCl(\mu\text{-}Cl)(\eta^6\text{-}p\text{-cymene})\}_2]$ with two equivalents of ligand in methanol at room temperature allowed the preparation of novel mononuclear water-soluble Ru (II) complex. This complex was characterized by IR, ^{1}HNMR, ^{13}CNMR spectroscopy and elemental analysis. Then the catalytic activity of the complex has been evaluated in the transfer hydrogenation of ketones and aldehydes under aqueous conditions with good yield.



Keywords: η^6-arene-ruthenium(II) complex, Transfer hydrogenation, Aqueous catalysis

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Novel water soluble complex, $[C_{23}H_{25}VO_4N_4^+]Cl^-$ with tridentate task-specific ionic liquid Schiff base ligand: Synthesis, characterization and survey of catalytic activity

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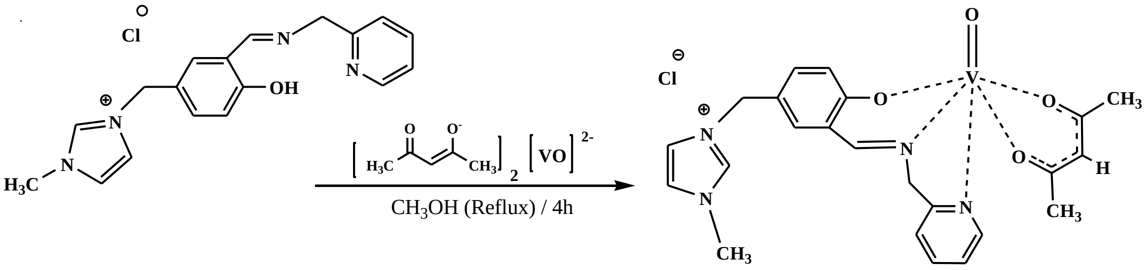
Schiff base complexes can be widely employed as catalysts, i.e. in the epoxidation of alkenes or the enantioselective oxidation of organic sulfides [1]. By reaction of chlorosalicylaldehyde with N-methylimidazole, the water soluble salicylaldehyde methylimidazolinium chloride was prepared. Then the reaction of 2-aminomethyl pyridine with this aldehyde resulted to synthesis of task-specific ionic liquid Schiff base ligand, (N-methylimidazolinium chloride salicylidin-2-methyl pyridine imine). Finally the vanadium (IV) Schiff base complex $[C_{23}H_{25}VO_4N_4^+]Cl^-$ was synthesized by reaction of this tridentate Schiff base ligand and $VO(acac)_2$ in 1:1 stoichiometry. The aldehyde, ligand and complex had been characterized by IR, ^{1}HNMR, and UV-Vis spectroscopy and mass spectrometry, as well as elemental analysis. Paramagnetic property of complex was also studied by magnetic susceptibility measurements. This complex was used as a catalyst in epoxidation of cyclooctene and oxidation of methyl phenyl sulfide [2]. The reaction parameters such as solvent, oxidant, alkene/oxidant ratio and the amount of the catalyst were optimized [3] and the results showed that it was highly active in these oxidation reactions. The effect of ionic nature of task specific ionic liquid Schiff base complex was also investigated in two mentioned reactions.



Keywords: Vanadium (IV) complex, Ionic liquid, Oxidation reaction, Methyl phenyl Sulfide

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Synthesis of Zn(II) and Cd(II) complexes with the new macroacyclic Schiff-base ligand containing two piperazine moieties: spectroscopic, antibacterial properties

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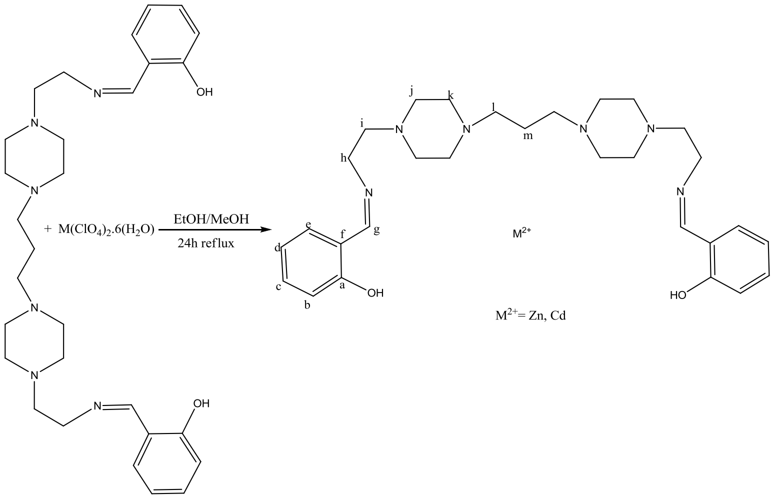
The new diamine 2,2'-(4,4'-(propane-1,3-diyl)bis(piperazine-4,1-diyl))diethanamine (A^1) was synthesized by reaction of 2-aminoethylpiperazine and 1,3-dibromopropane. The Schiff base ligand L^1 was synthesized by the condensation of 2-hydroxybenzaldehyde and (A^1). Its corresponding Zinc (II) and Cadmium (II) macroacyclic Schiff-base complexes were prepared by the reaction of metal ions and L^1 in methanolic/ethanolic solution. All products were characterized by elemental analysis, mass spectrometry and spectroscopic methods such as FT-IR, ^{1}H and ^{13}C NMR. The complexes were tested for *in vitro* antibacterial properties against some Gram-positive and Gram-negative bacteria. The complexes exhibit antibacterial properties and in some cases even more than those of Tobramycin and Tetracycline as standards [1-2].



Keywords: Schiff-base complexes, piperazine, antibacterial activity

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Supramolecular Study of Salophene with Fullerene

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Fullerene–porphyrin supramolecular systems have become an active area of research for the generation of acceptor-donor system with unique photophysical and photochemical properties [1]. Besides, porphyrin is a most famous 22-π electrons because of highly conjugated aromatic characteristics, planarity and formation of very stable metal complexes with various metals so the chemical and physical properties of porphyrin can be turned using various metals for the central atom and peripheral substitution[2]. On the other hand, Schiff base ligands and their complexes are versatile compounds which are widely used in a wide variety of fields for many years [3]. Having a highly conjugation system with 22-π electrons, Salophene can be a good candidate instead of porphyrin for studying the acceptor-donor supramolecular chemistry with fullerenes. In this research, experimental study and calculation of HOMO-LUMO gaps for a series of symmetrical Salicylaldehyde-based Schiff bases were undertaken (Fig. 1).

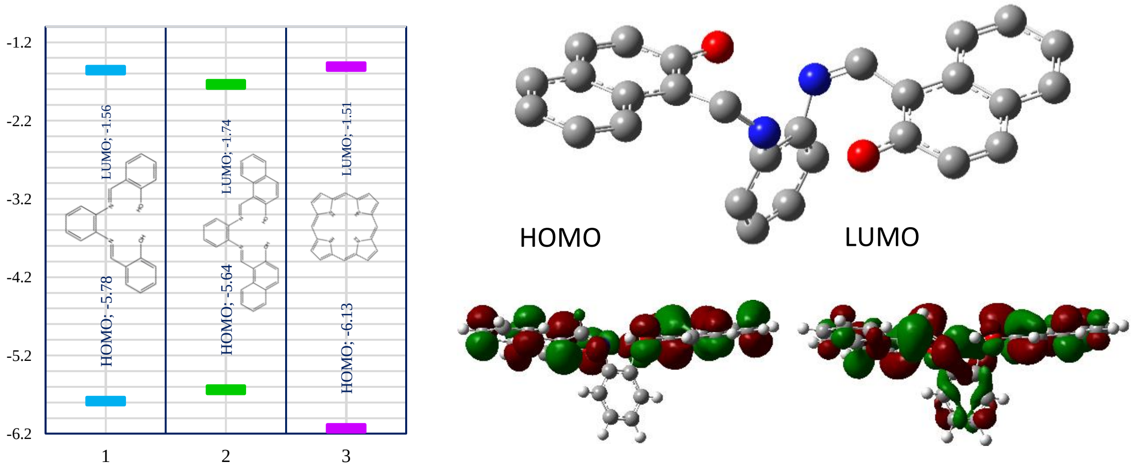

Fig 1- Calculated E_{HOMO}, E_{LUMO} levels, energy gap (E_g) values of the studied compounds obtained by B3LYP/6-31G* level.

Keywords: Supramolecular Chemistry, Schiff-Base Ligands, Fullerene, Porphyrin, Salophene

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Mixed Ferric, Silicon, and Manganese oxide nanostructures as novel adsorbent for removal of Methylene blue from waste water

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Organic dyes are the most common pollutants in wastewater emanating from textile, paper, plastic, leather, and food industries [1]. These dyes, dissolved in water, and also consume dissolved oxygen and hinder light penetration, affecting aquatic life severely [2]. Therefore, it is essential to eliminate these dyes before the discharge of wastewater. Mixed oxide nanoparticles of Fe, Si, and Mn were synthesized using a combined sol-gel - hydrothermal method. Estimated revealed the adsorption process by the electrostatic force between the cationic dye molecules and negative charge at nanoparticle surface. The highest dye adsorption capacity of the mixed oxide nanostructures associated to their high specific surface area, and the presence of surface Si-O groups. The optimize conditions of pH value, temperature, dye condition, adsorbent dose, contact time, and quantity of adsorbent [3].

Keywords: Mixed Metal oxide, Dye-adsorption , Mesoporous materials

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Mesoporous Ceria Supported Gold Nanoparticles

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Cerium oxide is widely used as a catalyst and/or catalyst support for many important catalytic supports for many important processes such as the water gas shift reaction, steam reforming and chemical fuel production. Gold displays the most dramatic size-dependent properties of the late transition metals. Because of this strong size dependence, stabilizing gold nanoparticles at their optimum size is critical. Doping of CeO_2 with elements of different ionic radii or oxidation states improve the exchange of oxygen in the oxide network by decreasing the energy barriers for oxygen migration. Its stability is mainly due to the ability to shift easily between reduced and oxidized state $Ce^{3+}\leftrightarrow Ce^{4+}$ which results in rapid formation and elimination of oxygen vacancy defects. The synergy between the ceria and the modifier can be achieved throughout different mechanisms such as creation of oxide vacancy, formation of solid solution, integration between segregation oxide and the deposition of metallic particles over the surface. Ceria supported gold nanoparticles (Au-CeO_2 NPs) were prepared by a simple deposition precipitation method. X-ray diffraction (XRD) and Fourier-transform infrared spectroscopy (FT-IR) indicated the formation of gold nanoparticles over phase pure cerianite ceria support. The presence of gold nanoparticles was well identified by UV-DRS study. In addition, the field emission scanning electron microscope (FE-SEM) images revealed that the maximum numbers of particles having spherical shape were approximately 10 nm size.

Keywords: Gold nanoparticles, Ceria support, Nano-structured materials, Catalysts.

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Green synthesis of Pd-ZnO nanoparticles using Cystoseira brown algae

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Metal and metal oxide nanoparticles have been intensively studied due to their favorable physical and chemical properties. The improvement in the optical, electronical, magnetic and chemical properties of these particles have been originated from their nano-scale sizes. Metal oxide supported metal particles have many potential applications in electronic and catalysis and also for gas sensing and hydrogen storage [1-3]. Pd/ZnO was used as photo-catalyst in degradation of organic dyes and as a catalyst in the C-C coupling reactions and oxidation of alcohols [4]. Controlling the factors influencing the size, shape, composition and morphology of the particles and the use of environment-friendly precursors are two challenging parts in the preparation of M/M'O compounds. Green synthesis is one of the newest methods for the synthesis of nanoparticles [5]. Herein we have reported a facile and green method for the preparation of ZnO and Pd/ZnO nanoparticles with the help of Cystoseira brown algae. This algae is abundant on the Persian Gulf off-shores. The prepared nanoparticles were characterized by SEM, XRD, EDX methods. XRD pattern showed that ZnO nanoparticles are pure with hexagonal structure and a mean particle size of 21 nm. It also showed a cubic structure for Pd and a mean particle size of 4.9 nm for it. SEM images showed that the morphology of ZnO particles were flower-like and Pd particles were sat as spherical particles on them.

Keywords: Algae, Palladium nanoparticle, Zinc oxide nanoparticle

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Sol-gel derived nano-porous gamma alumina as a carrier for *in vitro* drug delivery of valsartan

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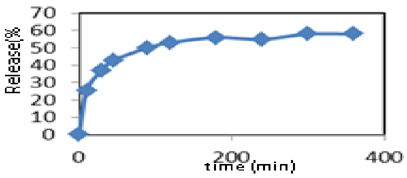
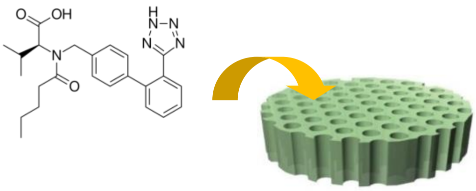
Valsartan is an angiotensin II receptor antagonist used for treatment of high blood pressure, congestive heart failure and to increase the chances of living longer after a heart attack [1]. Nano-porous alumina is a great platform for delivery of broad types of drugs like nifedipine, celecoxib and ibuprofen [2-4]. In current research nano-porous alumina (with surface area of 383 m^2/g) was synthesized via sol-gel method [3]. Sample characterizations carried out by FT-IR, BET and SEM. Valsartan was loaded on nano-porous alumina with the ratio of 1:3 and the nano-drug-carriers were abbreviated as Val@MA. FT-IR spectra confirmed the loading of the drugs into the carrier framework. The release of Val from MA was investigated in simulated body fluid (SBF) during 24 hours via UV analysis and it was observed that 58% of the drug was released with an initial burst release of 26% in the first ten minutes. The results demonstrated the substantially enhanced release of valsartan which was well known as a very slightly soluble drug.





Keywords: Valsartan, Alumina, SBF.

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Hemoglobin selective enzyme for conversion of aldehydes to carbocyclic acids

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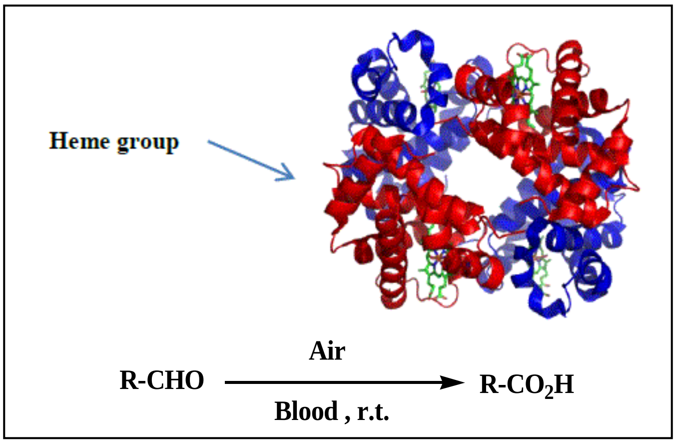
In this study, hemoglobin was applied as an enzyme which is useless animals product to oxidation different aldehydes as hydrocarbons instead of using some methods which have suffer from one or some disadvantages such as the requirement of strong acidic or basic conditions, stoichiometric or super stoichiometric amounts of costly or hazardous oxidizing agents, heavy-metal toxicity and high-temperature. in order to achieve this purpose, for the first time a new aerobic route was introduced for the selective oxidation of a variety of aromatic aldehydes as hydrocarbon to the corresponding carboxylic acids by molecular oxygen in the presence of hemoglobin in the water solvent. The mentioned method was proceeded under mild reaction conditions. A variety of analyses were used for this method such as ^{1}HNMR, mass and UV-Vis spectroscopies. A new type of (HbFe^{+3}) was introduced with UV-Vis spectra and mass spectroscopy. Also the obtained acidic product was characterized by ^{1}HNMR analysis. The results showed the selective oxidation of different aldehydes by Hb. Our suggestion for Hbs selectivity is based on its ring size which is related directly the size of aldehyde to get close to Hbs complicated structure.



Keywords: Hemoglobin, Enzyme, Aldehyde, Oxidation

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Hybride inorganic-organic functionalized SBA-15 as controlled releaser for Lovastatin

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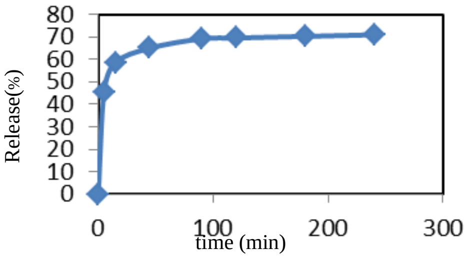
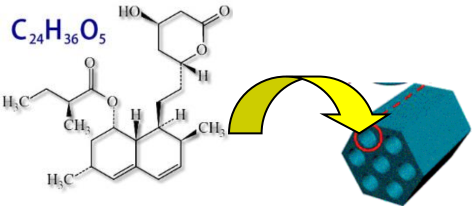
Lovastatin is a group of statins used along with a proper diet to help lower "bad" cholesterol and fats (such as LDL, triglycerides) and raise "good" cholesterol (HDL) in the blood [1]. It is usually well tolerated, with the most common side effects being, in approximately descending order of frequency. In the present study, Lovastatin (LOV) as a very low water soluble drug was loaded on hybride inorganic-organic NH_2-functionalized SBA-15 with the ratio of 1:3. Analyses of the samples were carried out by FT-IR, X-ray diffraction (XRD) and N_2-sorption. N_2 adsorption-desorption result showed that before grafting, SBA-15 demonstrated surface area of 787 m^2/g and pore diameter in range of 4 and 10 nm. After grafting, the surface area decreased to 215 m^2/g [2]. In vitro study was accomplished in simulated body fluid (SBF) for releasing of LOV. It was observed that the solubility of the drug increased to 79% after 4h of soaking time.





Keywords: Lovastatin, SBA-15, SBF.

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TiO_2 magnetic composite: Synthesis and dye removal in aqueous solution

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Ferrites as a stable spinel-type material, has potential applications in the field of gas sensors, biomedicine, pigments and photocatalyst. In recent years, ferrites as a magnetically photocatalyst for pollutant removal has received increasing attention [1-3]. In this work the TiO_2 composite with cobalt and manganese ferrite was synthesized. The prepared sample was characterized by X-ray diffraction (XRD), fourier transform infrared (FT-IR) spectroscopy, field emission scanning electron microscopy (FE-SEM) and energy dispersive X-ray analysis (EDX). The adsorption and photocatalytic efficiency of the sample for removal of methylene blue, congo red, methyl orange dyes was examined. The results indicated that the sample is a promising candidate for effective photodecolorization of dyes in aqueous solution. For the prepared sample a good removal of the congo red *via* adsorption experiment (62%) was observed. The results indicated that 93, 73 and 97% of the congo red, methyl orange and methylene blue in aqueous solutions were removed *via* photocatalytic decolorization after 180 min/respectively. The prepared sample demonstrated the high removal ability after five repeated utilizations.

Keywords: TiO_2, Magnetic composite, Photocatalyst, Adsorption, Dye removal.

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Study on the interaction of a new water-soluble asymmetric cationic metalloporphyrin with ctDNA

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Interaction of porphyrins and metalloporphyrins with DNA has a considerable interest due to their medical applications. Cationic porphyrins can extremely bind to DNA and photo dynamically modify the target site of a DNA molecule by a mechanism similar to that of anti-cancer antibiotics based on the DNA cleavage [1].

In this work, the interaction of 5-(1-dodecyl pyridynium-4-yl)-10,15,20-tris(1-methyl pyridynium-4-yl)-21H,23H-porphyrin Nickel (II) complex (NiMDTMPyP) with calf-thymus DNA (ctDNA) was investigated in trs buffer at 35 °C by UV-vis absorption, resonance light scattering (RLS) spectroscopy and viscosity measurement.

Then multivariate curve resolution-alternating least squares (MCR-ALS) method was applied to extract information from overlapping responses of the reaction participants from spectroscopic data, which was obtained by the UV–vis method. Its output provides the pure spectra of NiMDTMPyP and NiMDTMPyP–ctDNA complex, and concentration profiles.

The obtained results at low [porphyrin]/[DNA] mole ratio, decrease in the relative viscosity of ctDNA, much small red shifts ($\Delta\lambda$= 3.4 nm) and hypochromic effect (H = 38.6%) in spectra titration and gradually increase in the intensity of RLS signal suggest that mention porphyrin could be bind to ctDNA in an outside binding mode [2,3]. The apparent DNA binding constant of this porphyrin was evaluated by monitoring the changes in absorbance with increasing concentration of DNA, which were fitted to the McGhee-von Hippel model for the cooperative non-specific binding model. The apparent binding constant was determined as 6.7×10^{5} M^{-1}.

Keywords: porphyrin, outside binding mode, MCR-ALS method

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DFT calculations of the binuclear Schiff base nickel complexes

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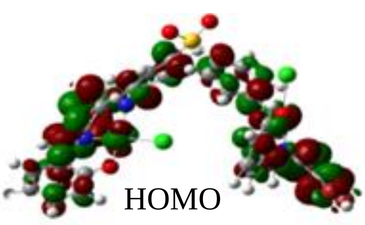
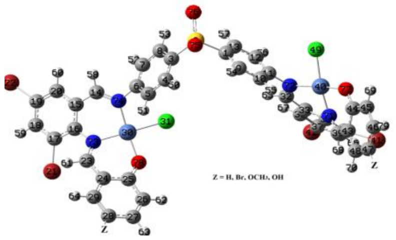
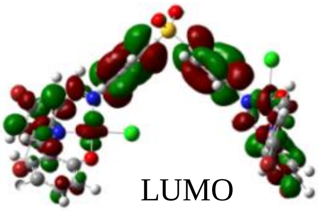
Schiff bases are one of the most useful categories of organic compounds and have received considerable attention in theoretical and experimental investigations and used in different areas such as catalysis, bioinorganic chemistry and drugs.[1-7]

In the present research, DFT calculations were carried out at the B3LYP levels of theory with a double basis set LANL2DZ for nickel, and 6-31+G(d,p) and 6-311+G(d,p) basis set for the other atoms. The geometries of the nickel complexes were obtained based on the optimized structures which confirm the magnetic moment measurements and demonstrate tetrahedral and square planer geometries. The calculation of the FT-IR vibrational frequencies, ^{1}H NMR and ^{13}C NMR chemical shifts of the compounds were carried out and compared with those obtained experimentally. The results of this comparison demonstrated good agreement between the theoretical and experimental data, which can be strong evidence of the accuracy of the experimental analytical data and validity of the applied mathematical model. Finally, the frontier molecular orbitals (HOMO and LUMO), ionization potential energy (I), electron affinity (A), electrophilicity (ω), electronegativity (χ), hardness (η) and softness (S) of the compounds were investigated.







Keywords: Schiff base, Nickel complex, DFT calculation, 2-hydroxyaniline, HOMO, LUMO

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Anticancer activity of platinum(II) and (IV) complexes with dipyridylamin

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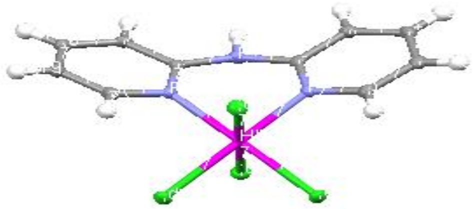
After the discovery of Cisplatin by Rosenberg in 1969, significant research efforts have been focused on development of Platinum complexes due to their potential antitumor activities. Platinum coordination complexes are biologically important for their anticancer activity, being effective on tumor types including testicular, ovarian, and colon cancers. The three Platinum anticancer drugs currently available on the marke , Cisplatin, Carboplatin and Oxaliplatin. Because of severe side effects and other deficiencies, however, alternative Platinum anticancer drugs are under development. Awidevariety Pt (IV) complexes have potential as powerful anticancer drugs, and they can be administered orally. Most Platinum complexes, which have been used as therapeutie agents often contain amine ligands. Variations in the nature of the amine group can have significant effects on the activity of these kinds of complexes. In this research, a novel platinum (IV) complex, [Pt Cl_4(2, 2'-dipyridyl amine)].DMSO were prepared from the reaction of H_2PtCl_6-$6H_2O$ with 2,2'-dipyridyl amine , in DMSO. The complex was fully characterized and its structure was determined by the X-ray diffraction method. It crystallizes in the Orthorombic crystal system, with *Cmcm* space group. This complex has two monodentate nitrogenous ligand with four chloride anions attached to Pt(IV) metal in a distorted octahedral environment and this complex along with three previously reported analogous complexes were used for in vitro cytotoxicity evaluation against four cultures , NIH-3T3, caco-2, HT-29 and T47D by MTT assay.



Keywords: Platinum (II), Platinum(IV), Anticancer, Cytotoxicity

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Theoretical study of substituent effect in *trans*-(NHC)PtI_2(*para*-NC_5H_4X) complex: a Platinum-Based Anticancer Drug

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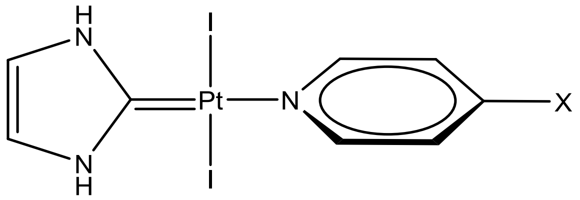
In this work, the substituent effect on the energy decomposition analysis (EDA) in *trans*-(NHC)PtI_2(*para*-NC_5H_4X) complex, a platinum-based anticancer drug, was investigated with MPW1PW91 method. The calculations of systems contain main group elements described by the standard 6-311G(d,p) basis set. For Pt element standard Def2-TZVPPD basis set was used and Pt described by effective core potential (ECP) of Wadt and Hay pseudo-potential with using the Def2-TZVPPD basis set. Energy decomposition analysis (EDA) was used to clarify the nature of the NHC… *trans*-PtI_2(*para*-NC_5H_4X) chemical bond in title complexes were investigated. The bonding interactions between the NHC ligand *trans*-PtI_2(*para*-NC_5H_4X) complex were evaluated using energy decomposition analysis (EDA) in the Multiwfn 3.3.5 software package. The instantaneous interaction energy (E_{int}) between the two fragments was calculated as**:** $\Delta E_{int} = \Delta E_{polar} + \Delta E_{els} + \Delta E_{Ex}$ where E_{polar} is the electron density polarization term (the induction term) calculated by subtracting E (SCF last) from E (SCF 1^{st}). E_{els} and E_{Ex} are the electrostatic interaction and the exchange repulsion terms, respectively. The substituent effect on interaction energies, the electron density polarization term, electrostatic interaction and the exchange repulsion terms were studied.



Keywords: substituent effect platinum-based anticancer drug, EDA.

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Hybrid of fullerene and ferrocene/ruthenocene/osmocene; a theoretical study

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Recently, interest in ferrocene−containing compounds has been extended to the magnetic, electrical, and nonlinear optical properties (NLO). Based on the fact that ferrocene is a good donor in NLO activity, an idea of the hybrid of the ferrocene and fullerene is highly intriguing [1]. Because fullerene is an electron deficient compound and has exceptionally strong *p*−aromaticity. In this work we investigate the complexes with formula $[M(Cp)(\eta^5\text{-}C_{60}Me_5)]$; ($M=Fe^{2+}$, Ru^{2+} and Os^{2+}), theoretically. The geometries of complexes in the gas-phase were fully optimized with def2-SVP basis set at M06-L and BP86 levels of theory using the Gaussian 09 set of programs. The different types of interaction energies [2] were calculated and corrected for the basis set superposition error (BSSE). The calculated interaction energies show that the (Cp)M···fullerene interactions are smaller than those of Cp···M(fullerene). EDA-NOCV and NBO calculations were also performed on complexes. The results of energy decomposition analysis for all complexes show that the M•••(Cp)fullerene interaction is more covalent than electrostatic.

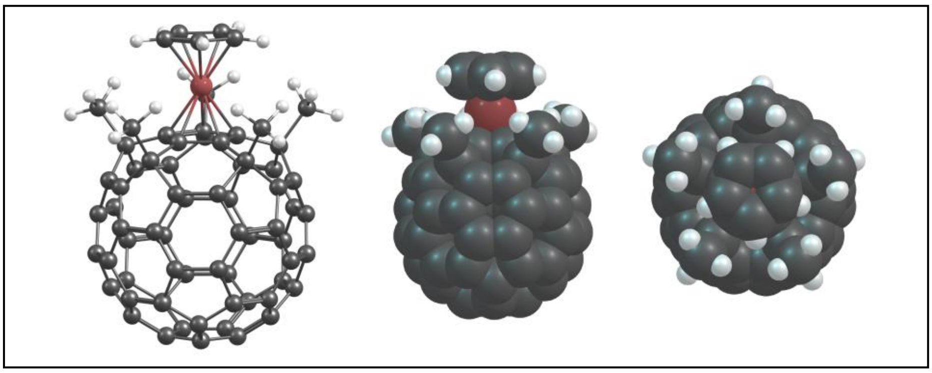

Figure 1. The optimized structure of $[Fe(Cp)(\eta^5\text{-}C_{60}Me_5)]$ at M06-L/def2-SVP level of theory.

Keywords: Fullerene, Ferrocene, Ruthenocene, Osmocene, Theoretical study

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DFT study of electronic structure and optical properties of a novel heteroleptic cationic Ir(III) complex with 2,4'-bipyridinium ligand

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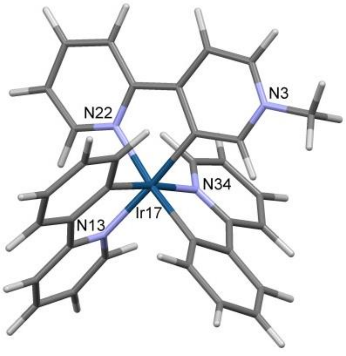
In the past few decades, many research efforts are devoted to synthesis of efficient light-emitting compounds [1]. Photoactive octahedral iridium(III) complexes are an important class of emissive molecular materials [2]. This complexes are well known to present rich photophysical and photochemical properties due to their triplet [d_{π}(M)$\rightarrow$ π*(ligand)] charge transfer excited states. Recently, cationic Ir(III) complexes have attracted a great deal of attention for application in the fabrication of light-emitting electrochemical cells (LEECs) [3,4]. In this research work, we present the electronic structure of a novel cationic Ir(III) complex with mixed 2-phenyl pyridine and 2,4'-bipyridinium ligands, studied at density functional level of theory (DFT). According to our calculations, the HOMO is located on 2-phenyl pyridine ligands with heavy contribution of the iridium d orbitals to it. However, the LUMO is mostly the π* orbital on 2,4'-bipyridinium ligand. Moreover, electronic spectrum of the compound is predicted by time dependent density functional theory (TD-DFT) method and is interpreted on the base of the calculated electronic structure.



Keywords: Cationic Ir(III) complex, Heteroleptic complex, 2,4'-bipyridinium ligand, Electronic structure, DFT study

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Electronic structure and optical properties of a novel charged Al(III) complex for high performance light emitting devices: a DFT study

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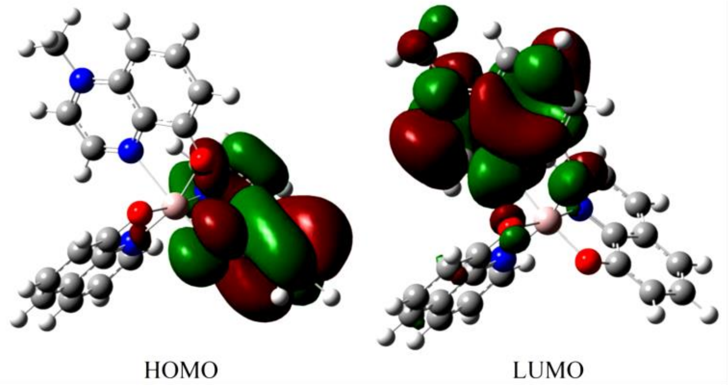
Recently, electroluminescent (EL) devices, based on ionic complexes have attracted attention of many investigations [1-3]. A large variety of Alq3 derivatives (q = 8-hydroxy quinolinate) have been synthesized with the aim of applications in organic light-emitting diodes [4]. In this research work, we report the electronic and optical properties of a new cationic Al (III) complex with mixed 8-hydroxy quinolinate and 5-Hydroxyquinoxalinium ligands calculated by DFT method. The ground-state geometry and molecular orbitals of the complex are calculated at B3LYP/6-31G(d,P) level of theory. According to our calculations, the HOMO is located on one 8-hydroxy quinolinate ligand, while, the LUMO is the π* orbital on 5-Hydroxyquinoxalinium ligand. Also, the electronic absorption spectrum of the complex is calculated by TD-DFT method.



Keywords: Al complex, Cationic Complex, OLED, DFT Calculations

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Theoretical study of the electronic band structure and linear optical properties of strontium pyroarsenate

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Pyrochlore $A_2B_2O_7$ materials have been widely studied. The compounds are of importance due to their ability to form substituted and defective structures, permitting interesting tunable physical properties [1]. Alkaline earth diarsenates have been the subject of several previous studies [2]. However, strontium pyroarsenate ($Sr_2As_2O_7$), which crystallizes in tetragonal $P4_1$ [3] and $P4_3$ [4] space groups, has scarcely been studied. Here, the electronic structure of the both polymorphs of the compound are calculated by density functional theory (DFT) method at GGA-PBE level of theory. Plane wave basis set ($E_{\text{cut off}}$ = 600.0 eV) for the valence electrons and normconserving pseudopotentials (NCP) for the ionic cores were used in the reciprocal space. DFT calculations indicate that the $P4_1$ and $P4_3$ polymorphs have an indirect band gap of 3.99 eV and 3.96 eV, respectively. The top of VBs mainly originates from the O-2p states. The CBs between 3.5 and 6.6 eV are mainly consisting of the As-4s atomic states with minor contributions from O-2p and As-4p states. Linear optical properties of the solid compound were calculated by DFT method. The calculated absorption and reflectivity spectra, show that $Sr_2As_2O_7$ is theoretically transmitting for frequencies of <7.25 eV.

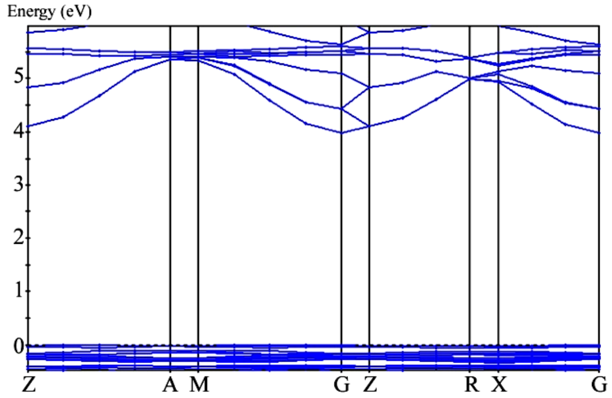

Fig. 1. The calculated band structure for $Sr_2As_2O_7$ (space group $P4_1$).

Keywords: Strontium pyroarsenate, Electronic band structure, Linear optical properties, DFT study

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Evaluation of Oxazole and Thiazole Ligand Effects on Hoveyda-Grubbs Catalysts

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The Hoveyda-Grubbs ruthenium carbene catalysts have attracted considerable attention, due to their improvement in the efficiency, selectivity and practicality of transition-metal-mediated reactions such as olefin metathesis. Furthermore, NHC-bearing ruthenium catalysts can support the formation of the C–C bond in medicine, biology, and material science compounds [1-3]. Hence, in this study, the electronic effects of various ruthenium-bearing carbene ligands including oxazole (**1**) and thiazole (**2**) were investigated. Therefore, equilibrium geometries and harmonic vibrational frequencies were carried out using the B3LYP and M06 methods with a DZP basis sets. On optimized structures, the natural bond orbital (NBO) and atoms in molecules (AIM) data were implemented at B3LYP/QZVP and M06/Def2-QZVP levels. The results of these calculations reveal that the lowest positive charge on ruthenium belongs to catalyst **1** in both levels (-0.146 and -0.247) (Table 1). The ruthenium in **2** has the highest positive charge in the both method (-0.124 and -0.226). Hence, the oxazole ligand is a powerful σ-donor compared to the thiazole ligand in which the ruthenium atom has less electron-deficient. The catalyst **1**, which has the oxazole ligand, induces more electrostatic nature of metal-carbene bond due to value of $\nabla^2\rho_b = 0.394$. The value of ρ_b in B3LYP method for catalysts **1** and **2** are 0.225 and 0.213 respectively, which indicates a stronger bond between Ru−C: bond. Based on the geometry calculation, the bond distance between carbene carbon and metal in **1** is shorter than **2**, which indicate that the **1** has the stronger Ru–C: bond than **2**.

Table 1. The results of the NBO analysis, AIM parameters, and bond length (R).

Catalyst	Partial Charge(B3LYP/M06)		Bond Critical Point (B3LYP)						R (Å)
	q_{Ru}	$q_{C:}$	BCP	ρ_b	λ_1	λ_2	λ_3	$\nabla^2\rho$	Ru–C:
1	-0.146/-0.247	0.586/0.605	Ru–C:	0.225	-0.376	-0.313	1.084	0.394	1.882
2	-0.124/-0.226	0.111/0.135	Ru–C:	0.213	-0.349	-0.281	0.975	0.346	1.888

Keywords: Grubbs' catalyst, DFT, N-heterocyclic carbene, olefin metathesis.

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A density functional theory study of [Pd(bpy) (non-dtc)] NO_3 complex

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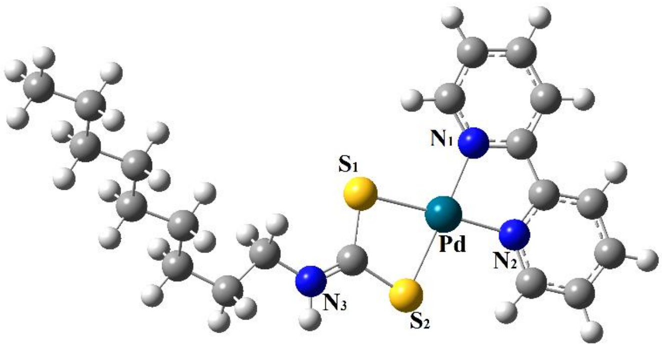
Nowadays, density functional theory (DFT) method, which include electron correlation effects, is commonly used to test transition metal complexes [1]. In the present study, the electronic structure of the [Pd(non-dtc) (bpy)]$^{+2}$ cation has been specified with DFT method, and time-dependent DFT (TDDFT) calculation has been utilized to better understand the electronic and spectroscopic properties in more detail. The DFT calculations have been carried out to determine the geometric preferences for mention compound using the 6-311G++(d,p) basis set for H, C, N and S atoms, and LANL2DZ pseudo-potential for Pd^{2+} atom. The optimized structure in gas phase was checked to be real global minima by vibrational frequencies.

With the help of Chemissian software a qualitative molecular orbital diagram was depicted on the basis of Mulliken molecular orbital percentage compositions in term of fragment orbitals. By comparing the experimental and calculated absorption spectra of the complex, one can notice that both sets of data are in good accordance with each other.



Optimized geometry of the [Pd(bpy)(non-dtc)]$^{+}$ complex in B3LYP level of theory

Keywords: Palladium (II) complex, DFT calculation, Molecular orbital diagram

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Density-Functional Theory calculation of redox potential of copper bis(thiosemicarbazone) complex in DMF

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Copper complexes of bis(thiosemicarbazone) ligands act as radiopharmaceuticals for the specific targeting of hypoxic tissue. This purpose is connected to redox properties of Cu complexes. So in current investigation, one-electron reduction potential of Cu(II)/Cu(I) of copper complex with a symmetric 2-[1-(2-{3-[2-({2-[(4-bromoanilino)carbothioyl]hydrazono}methyl) phenoxy]propoxy}-phenyl)methylidene]-N^1-(4-bromophenyl)-1-hydrazinecarbothiamide ligand (H_2L) was theoretically calculated by the density functional theory (DFT) B3LYP/6-31+G(d) level in solution phase. The effects of solvation in DMF solvent were incorporated as a self-consistent reaction field (SCRF) using the polarisable continuum model (PCM) and are found to be essential for quantitative agreement. The resulting estimate potential (E_{cal}) showed a good agreement with the experimental potential (E_{exp}) derived from cyclic voltammetry.

Keywords: Thiosemicarbazone, Cu, Redox potential calculation, Cyclic voltammetry

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Synthesis and photophysics of mono-cycloplatinated(II) phosphine complexes: an experimental study into the influence of aromatic thiolate ligands on tunning the excited state and rigidity

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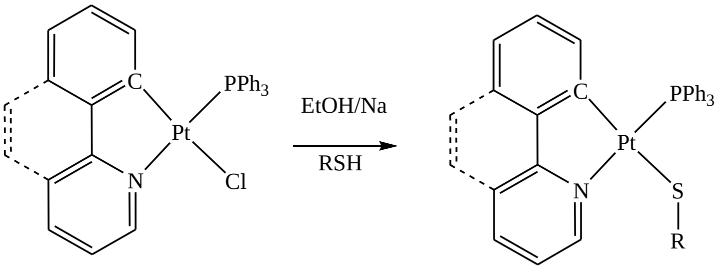
Thiolate ligands can behave as auxiliary ligands in transition metal complexes while it has been believed that they play important roles in the facility of tuning both steric and electronic properties of these complexes. [1-2] The present study extends the information on the structures and optical properties of cyclometalated platinum(II) complexes containing thiolate ligands (**1-3**). Reaction of cycloplatinated thiolate complexes by the salt metathesis reaction on the corresponding chloro precursors complexes (**A** and **B**) leads to a profound change in the nature of lowest-energy singlet and triplet excited states, to ones which feature charge transfer from the thiolate (mixed with some metal character) to the $C^{\wedge}N$ ligand, supported by TD-DFT calculations. In cases which the geometry changes because of lack of rigidity, the complexes show large deviation from square planar geometry and the emission quenches via non-radiative metal centered transition. Also, it seems that decreasing the rigidity of environment leads to flexibility of rotation of the –SR containing aryl ring about the axis of the Pt–S bond and failing of intramolecular π···π stacking in these complexes.

A bzq
B ppy



	R	$C^{\frown}N$
1a	Ph	bzq
1b	Ph	ppy
2a	py	bzq
2b	py	ppy
3a	pyN	bzq
3b	pyN	ppy

Keywords: cycloplatinated(II) complexes, thiolate ligands, excited state, TD-DFT

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Optical properties of Silver Nanoparticle interacted with Amino acids: Theoretical and experimental Investigations

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Silver nanoparticles and clusters have attracted much attention in chemistry and material science because of their unique optical and electronic properties. The affinity of noble metal clusters to interaction with the variety of bimolecular ligands, made them suitable for the use in biochemical sensing and detection. These interactions affected their electronic structures and more over the optical properties. Detections of different amino acids due to their structural similarity is a challengeable task in proteomics science. In current work, the bacterial cellulose nanopaper with their extraordinary mechanical and physicochemical features was chosen as an efficient substrate for silver nanoparticles and the effect of adsorption of different amino acids on their optical properties has been measured. Furthermore, theoretical density functional calculation on the interactions of amino acids with silver cluster has been carried out to find out the effect of different amino acids on tuning the optical properties of silver clusters. The binding energies of Alanine, Valine and Cysteine with Ag_6 cluster have been obtained and revealed the significant affinity of Cysteine in comparison to other amino acids. On the other hand, the time-dependent DFT calculation (in Fig. 1) displays the damping of theoretical UV excitation intensity for silver cluster after interaction with Cysteine.

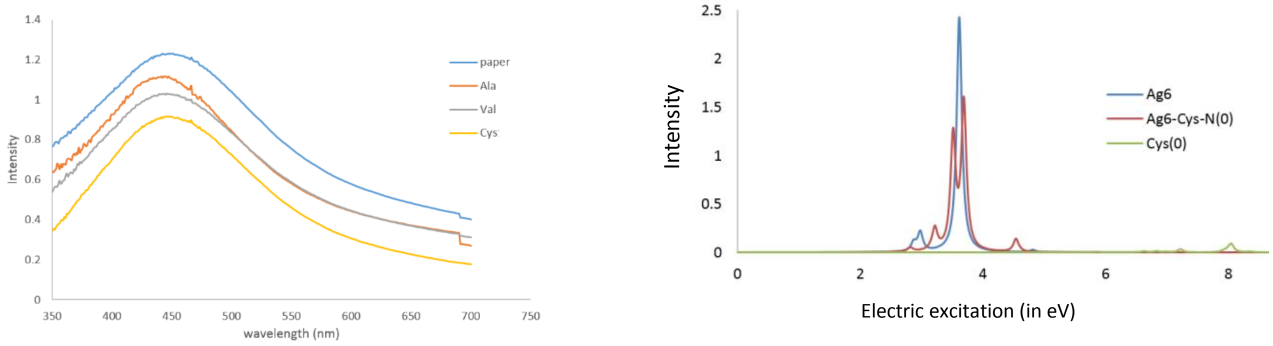

Fig. 1 The experimental absorption and theoretical UV spectra of Cysteine interacted with silver.

Keywords: Silver nanoparticles, Amino acid, Optical sensing

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Copper supported on modified magnetic nanoparticles as efficient and reusable nanocatalyst for the synthesis of 5-substituted 1H-tetrazoles

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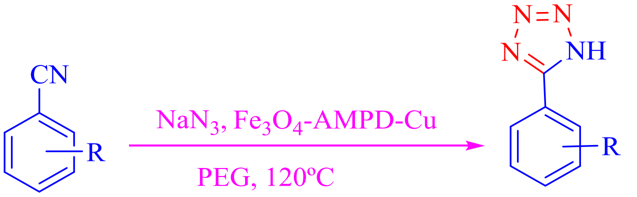
Separation nanoparticulate catalysts from the reaction mixture is often difficult, due to the need for conventional techniques such as filtration or centrifugation. In recent years, magnetite (Fe_3O_4) has been the focus of much attention as an interesting alternative to allow separation of the nanocatalyst from the reaction mixture by means of an external magnetic field [1–2].In this regard, a new magnetically reusable nanosolid (Fe_3O_4-AMPD-Cu) as a versatile and highly effective catalyst was fabricated and characterized using by FT-IR, XRD, VSM, TGA, TEM, SEM, EDX and ICP-OES techniques. This nanosolid shows great catalytic activity for the synthesis of 5-substituted tetrazoles in short reaction times and with high yields (Table 1).



Scheme 1. Fe_3O_4-AMPD-Cu catalyzed the one-pot synthesis of 5-substituted tetrazoles.

Table 1. Synthesis of 5-substituted 1H-tetrazole derivatives in the presence of Fe_3O_4-AMPD-Cu.

Entry	Substrate	Time (min)	Yield (%)[a]	M.p. (°C)
1	Phthalonitrile	55	86	214-215
2	3-Nitrobenzonitrile	80	93	152-154
3	2-Chlorobenzonitrile	10	89	177-180
4	4-Nitrobenzonitrile	60	94	222-224
5	Malononitrile	8	87	115-117

[a] Isolated yields

Keywords: Fe_3O_4 nanoparticles, Coppper(II), tetrazoles

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Synthesis of new zirconium complex supported on MCM-41 and its application as an efficient catalyst for the oxidation reactions

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Silica mesoporous molecular sieves have specific advantages, including ease of preparation, low cost, excellent thermal and chemical stability, large internal surface area and high concentration of surface Si–OH groups. MCM-41 is member of mesoporous molecular sieves with hierarchical structure and hexagonally packed arrays that can be used as catalyst supports [1–3]. In the present work, we report synthesis of new zirconium complex supported on mesoporous silica by anchoring of adenine on the wall of functionalized MCM-41, then reacted with $ZrOCl_2$. The resultant MCM-41-Adenine-Zr was characterized by FT-IR, XRD, TEM, SEM, TGA, EDS, ICP and BET techniques. It was exhibited that the MCM-41-Adenine-Zr can be used as an efficient and thermally stable nanocatalyst forthe oxidation of sulfides.

Table 3

Oxidation of sulfides to the sulfoxides in the presence of MCM-41-Adenine-Zr.

Entry	Substrate	Product	Time (min)	Yield (%)[a]	M.p.(°C)	
					Found	Reported
1	Dipropylsulfide	2a	55	98	Oil	Oil
2	Diethylsulfide	2b	45	96	Oil	Oil
3	Dibenzylsulfide	2c	35	95	130-133	127-129
4	Benzylphenylsulfide	2d	40	89	122	117-119
5	Tetrahydrothiophene	2e	5	93	Oil	Oil

[a]Isolated yields

Keywords: MCM-41, Sulfoxide, Zirconium complex

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Synthesis, Structure Characterization, DFT Studies and Catalytic Comparison of two Copper(II) Schiff base and diazo Complexes in Azide-alkyne Cycloaddition Reaction

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According to the high value triazole compounds in different fields such as pharmaceutical, polymer and agrochemicals, a great deal of attention is allocated to azide-alkyne cycloaddition (AAC) reaction [1-3], introduced by sharpless [4] and meldal [5]. At first it was thought that the (AAC) reaction can be catalyzed only by Cu(I) complexes and in this regard, it was common to use Cu(II) salts and reducing agents to reduce Cu(II) to the active type Cu(I). But lately, variant works have been published in click chemistry reactions area using Cu(II) complexes as catalysts without any reducing agents [6,7]. Due to the nature of circulating electrons in the structure of the applied ligands and π-conjugation, used ligands definitely affect the catalytic system [8].

In this study, Two Cu(II) complexes were synthesized through the reaction of $Cu(OAc)_2.H_2O$ with a Schiff-Base ligand (1-(((3,4- dichlorophenyl)imino)methyl)naphthalen-2-ol) and a diazo ligand (1-((3,4-dichlorophenyl)diazenyl)naphthalen-2-ol) in methanol. The complexes and ligands were characterized employing ^{1}H NMR, elemental analyze, electronic spectra and single crystal X-ray diffraction. Furthermore, Computational studies were performed on ligands and complexes. The catalytic potential of the complexes were compared together in one-pot azide-alkyne cycloaddition reaction in water due to finding out the effect of Schiff-Base and diazo ligands nature on the catalytic system.

Key words: Schiff-Base complex, diazo complex, AAC reaction, 1,2,3-triazoles, click chemistry

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Chemiluminescence study of luminol in presence of a new mixed chelate of copper (II) complex and ethylenediamine

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The quenching effect of ethylenediamine on strong chemiluminescence of luminol system in the presence of chelate of copper complex (N-(2-(2-aminoethylamino) ethyl)-1H-pyrrole-2-carboxamide-Cu (II)) was studied. Copper (II) complex with a tetradentate unsymmetrical ligand was prepared by one-pot condensation of methyl-2-pyrrole carboxylate, diethylenetriamine and copper (II) sulfate [1]. The chemiluminescence parameters were evaluated from computer fitting of the resulting intensity-time plots [2]. These systems resulted in Stern–Volmer plots in the quencher concentration range of 1.00×10^{-5} to 1.00×10^{-3}M with k_Q value of $1.7*10^4 M^{-1}$.

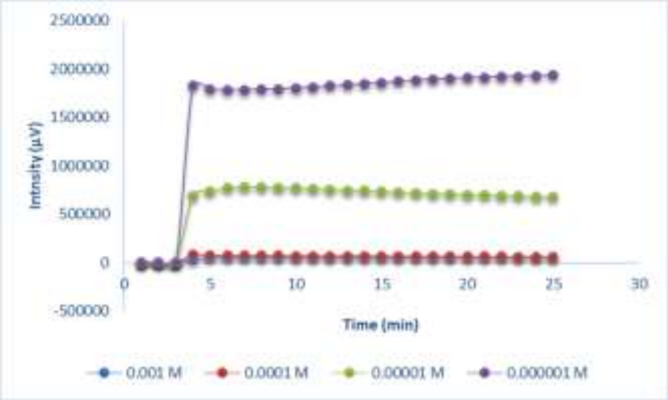

Figure 1: Chemiluminescence emission intensity as a function of time for luminol, H_2O_2, (N-(2-(2-aminoethylamino) ethyl)-1H-pyrrole-2-carboxamide-Cu (II)) and different concentration of ethylenediamine system with constant concentration of luminol (1.00×10^{-3} M), H_2O_2 (1.00×10^{-3} M), (N-(2-(2-aminoethylamino) ethyl)-1H-pyrrole-2-carboxamide-Cu (II)) (1.0×10^{-6} M).

Keywords: Chemiluminescence, Luminol , Quenching, Ethylenediamine

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Effect of spray drier parameters on size and morphology of the FCC catalyst

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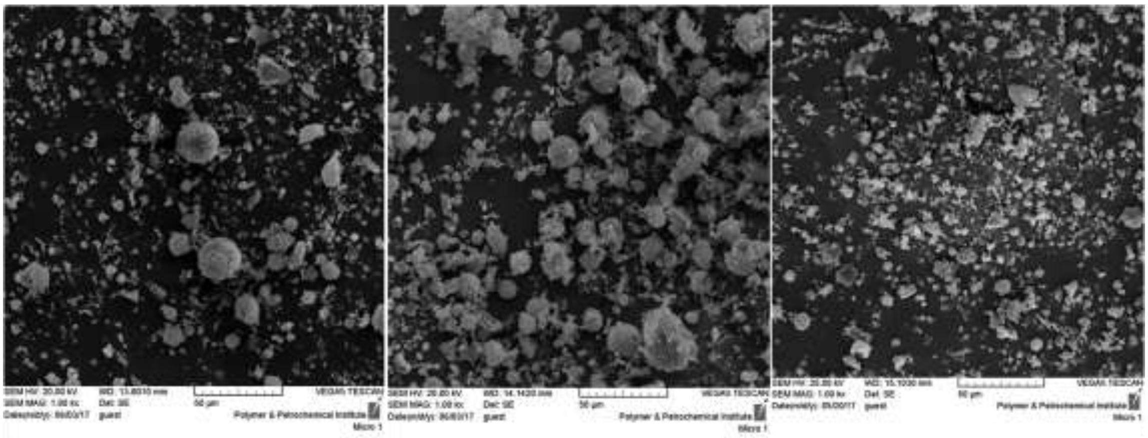
The most important and widely used process in heavy oil conversion in the modern refinery is fluid catalytic cracking (FCC) unit. It has been broadly adopted to transform high-boiling, high-molecular weight petroleum hydrocarbons into valuable distillates such as olefins, gasoline, and diesel in the last decades [1]. Modern FCC catalysts consist of two main components: (a) zeolites which provide the main active sites for the oil conversion and gasoline fraction and (b) matrix which offer the physical characteristics of the catalysts and extra acidic sites for pre-cracking of heavier fractions [2]. One of the key steps in preparation of an FCC catalyst is spray drying step which determine the size, shape and morphology of the final catalyst [3]. In the present study, slurry of FCC catalyst was prepared and introduced to spray drier. The influence of different spray drying parameters including inlet temperature, feed pump rate and air flow have been investigated on size and morphology of the resulted catalyst particles. The results showed that decreasing the pump rate and air flow increases the particle sizes as well as more spherical particles. Furthermore, lower inlet temperatures caused larger and spherical catalyst particles.



Keywords: Fluid catalytic cracking, FCC catalyst, Morphology, Spray drying.

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Pillared-bilayer porous coordination polymers of Co(II) with mixed ligands: synthesis and structure

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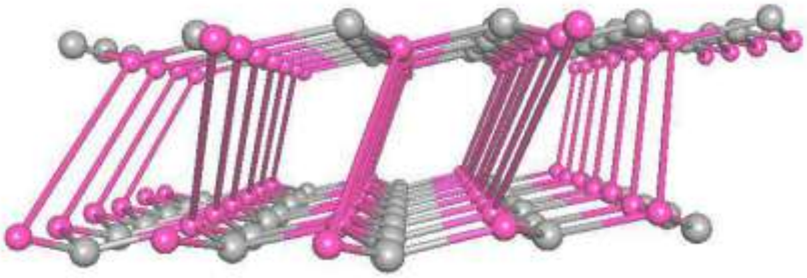
Porous coordination polymers (PCPs) have been recently highlighted because of their high synthetic designability in both structure and properties. These porous materials are generally constructed by metal ions or clusters (known as nodes) and bridging organic ligands (known as linkers). The structural features of such porous materials can easily be tuned by changing the organic linkers which are the integral part of their pore walls or by changing the metal nodes. In this work, we have used a mixed ligand system of a linear pyridyl-based linker and an amino functionalized trigonal dicarboxylate ligand in the presence of Co(II) ion to generate a porous coordination framework. The compound crystallizes in the monoclinic space group *P*-1 and show a 2D pillared-bilayer coordination framework. The compound has been characterized by FT-IR spectroscopy, PXRD, BET and single crystal X-ray diffraction.



Schematic representation of a simplified 2D net.

Keywords: Porous coordination polymer, Co(II), Pyridyl-based ligand, Amino functionalized carboxylate linker.

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Nature of metal-ligand bond in some derivatives of [(NHC(R))$_4$Re(O)(Y)] complexes (Y= OMe, Cl; R=H, CH$_3$, F, Cl, Br): A Theoretical Study

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N-heterocyclic carbenes are most accessible organic ligands in both organometallic and coordination chemistry, which is reflected by thousands of applications involving NHC-bearing metal complexes in areas ranging from homogeneous catalysis to material science [1]. The chemistry of N-heterocyclic carbenes (NHCs) and their metal complexes has advanced significantly over the last two decades in the field of organometallic catalysis and medicinal chemistry [2]. Herein we report a theoretical study on structure and nature of C→Re bonds in some derivatives of [(NHC(R))$_4$Re(O)(Y)] (Y= OMe, Cl R=H, CH$_3$, F, Cl, Br) complexes at PBE1PBE/def2-SVP level of theory.

The interaction energies between [NHC(R)]$_4$ and Re(O)Y in optimized structures of [(NHC(R))$_4$Re(O)(Y)] (Y= OMe, Cl R=H, CH$_3$, F, Cl, Br) complexes were calculated at PBE1PBE/def2-TZVP level of theory. The data showed that the C→Re bonds in the complexes especially with electron donating substituents are stronger than the other complexes. Also the results showed that the calculated interaction energies increase with changing R substituents in studied complexes, from F to Br atoms.

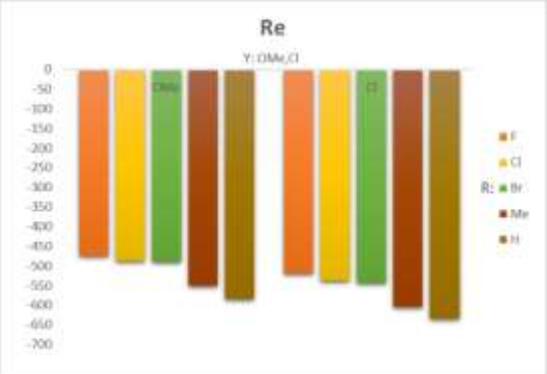

Fig. 1. The variation of calculated interaction energies in [(NHC(R))$_4$Re(O)(Y)] (Y= OMe, Cl R=H, CH$_3$, F, Cl, Br) complexes.

Keywords: Theoretical study; Nature of Metal-ligand Bond; NHC Ligand

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Density functional theory study on some transition metal complexes with bi dentate Lewis bases derived from 3-bromoacetyl-cumarine-2-one

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Transition metal complexes of cumarine ligands have been studied and attract many attention against the antitumor activity. In particular metal *cheaters* of cumarine have been known for some time to be antitumor agents [1,2]. Because of their biological activity and analytical application, the thiosemicarbazones, as well as their metal complexes have been the subject of many studies [3]. Density functional theory (DFT) calculations were employed to optimize the geometry of the new synthesized Schiff base ligand prepared with ω-bromo-8-3-acetylcoumarin and potassium thiocyanate and its transition metal complexes including Co^{2+}, Ni^{2+} and Cu^{2+} in the gas phase at B3LYP/6–31 + G(d,p) levels of theory (Figure 1). The results showed that the Schiff base L ligand behaves as a bidentate through both O atoms of carbonyl groups which can coordinated to metal ions. The optimized geometry revealed that all the metal complexes were formed in 2:1 molar ratio of ligand to metal with an octahedral geometry coordinating with two chlorine atoms. Also, natural bond orbital analysis (NBO) was carried out for the investigation of major stabilizing orbital interactions. The excited states of the electronic transition probabilities of the representative transition metal complexes were investigated in the framework TDDFT/PCM procedures.

Figure1. The optimized structure of Schiff base (left side) and its metal complexes (M(II)=Co, Ni, Cu)

Keywords: Cumarine ligand, DFT, Transitional metal, Schiff base

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Bidentate Schiff base as a photochoromic compound

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Bidentate *o*-hydroxysalicylidene-diisopropylphenylamine Schiff base ligand have been synthesized and characterized by FT-IR, ^{1}H NMR, UV-Vis spectroscopic methods and also single-crystal X-ray diffraction. The photochromic effect have been studied theoretically by using Gaussian09 program package at DFT / cc-pVDZ level. The calculations indicated that the photoexcitation causes a charge transfer from phenolic part to imine part. Then, intramolecular excited state proton transfer (ESIPT) from oxygen atom to nitrogen atom occurs and this leads to the reversible tautomeric equilibrium change within enol and keto forms. The potential energy profile calculation for H transfer and rotation of the N−C bond in excited and ground states obtained. As a results, in the ground state the enol−keto transformation is not favored by considering the energy changes, but in the excited state, this transformation will be favored by decreasing the internal energy of the system along the enol− keto transformation. From calculations the *trans*-keto form produced by UV excitation, and compared to enol form shows a 100 nm bathochromic shift as photochromic species.

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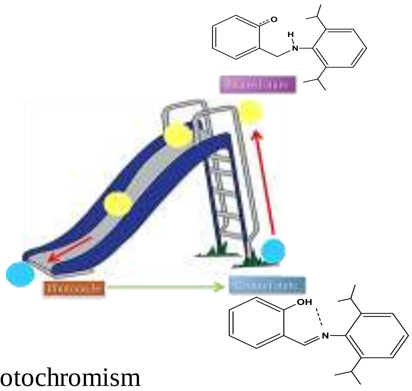

Keywords: Schiff Base, Proton Transfer, Photochromism

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Synthesis, characterization and theoretical study of a number of potentially tetradentate ligands containing Azo group and their Mn (III) complexes

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The interest in Schiff base ligands are due to their easy synthetic process. Tetradentate Schiff bases with a N_2O_2 donor atom set are well known to coordinate with various metal ions. Their metal complexes have been used for dioxygen uptake and as homogeneous catalysts for many organic conversions, such as oxidation of olefins, ring-opening of epoxides, and stereo selective polymerizations of lactides [1]. Azo substituent is an effective group that changes the properties (especially the photophysical properties) of different ligands and their complexes [2]. In this work, we report the synthesis and characterization of three new azo-substituted Schiff bases and their Mn(III) complexes. The synthesized Schiff bases and their complexes were characterized by IR and UV-Vis spectroscopies. Furthermore, DFT and TD-DFT calculations on complexes were done, at M06/def2-TZVP and BP86/def2-TZVP levels of theory using the Gaussian 09 set of programs. To investigate the nature of interactions in complexes, the EDA and NBO analyses were done. The energy and the intensity of electron transfers in complexes were calculated and their UV-Vis spectra were simulated using TD-DFT calculations. The data of TD-DFT calculations are in good agreement with the observed experimental ones.

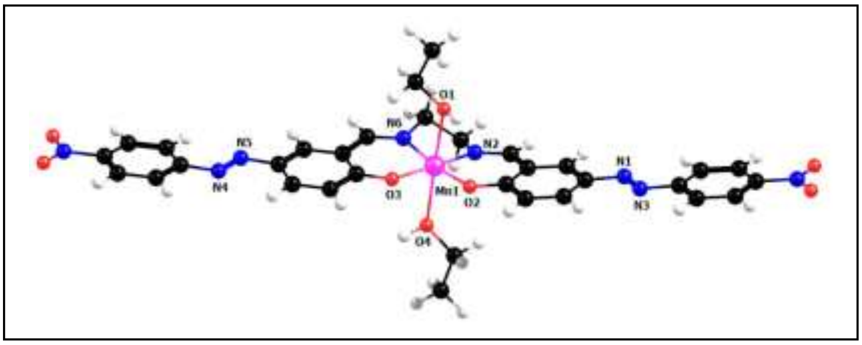

Figure 1. The optimized structure of [MnL^1(EtOH)2]$^+$ complex, at M06/def2-TZVP level of theory.

Keywords: Schiff base, Metal complexes, Computational study, TD-DFT, Energy decomposition analysis

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Azo-substituted Schiff base complexes of Cu(II): Synthesis, characterization, DFT and TD-DFT study

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Azo compounds and their metal complexes are known to be involved in a number of biological reactions, such as inhibition of DNA, RNA, and protein synthesis, nitrogen fixation, and carcinogenesis [1,2]. The properties and applications of Schiff base complexes vary with the electronic characters of substituents on the Schiff base. Azo substituent is an effective group that changes the properties (especially the photophysical properties) of different ligands and their complexes [3]. In this work, three potentially tetradentate azo-substituted Schiff base ligands N,N-bis(5-phenylazosalicylidene)ethylenediamine (H_2L^1), N,N-bis(5-Choloroazosalicylidene)ethylenediamine (H_2L^2) and N,N-bis(5-Nitroazosalicylidene)ethylenediamine (H_2L^3) were synthesized from the reaction of aldehydes with ethylenediamine and their Cu(II) complexes were also prepared. All synthesized ligands and complexes were characterized by IR and UV-Vis spectroscopies and also by elemental analysis. The theoretical studies on the synthesized ligands and complexes were performed at BP86/def2-TZVP and M06/def2-TZVP levels of theory using the Gaussian 09 set of programs. To investigate the nature of interactions in complexes, the EDA and NBO analyses were done. The energy and the intensity of electron transfers in ligands and complexes were calculated and their UV-Vis spectra were simulated using TD-DFT calculations. The data of TD-DFT calculations are in good agreement with the observed experimental ones.

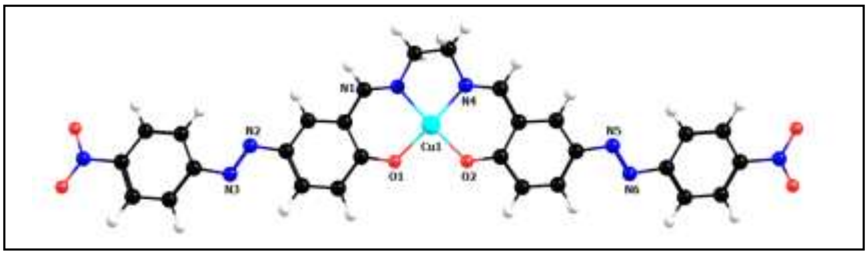

Figure 1. The optimized structure of [CuL^1] complex, at M06/def2-TZVP level of theory.

Keywords: Schiff base, Metal complexes, theoretical study, TD-DFT, NBO, Energy decomposition analysis.

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A computational study on group 5 metal complexes of the η^5-Pentamethyl[60]fullerene

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The transition metal η^5-fullerene complexes of type $[M(\eta^5\text{-}C_{60}R_5)L_n]$ (M = metal atoms, R = organic groups, L = ligands) belong to a new class of organometallic compounds that exhibit unique functions, such as an ability to form liquid crystalline materials, to form a photoinduced charge separation state, and to effect asymmetric organic transformations [1]. Rhenium pentamethyl[60]fullerene tricarbonyl, $[Re(\eta^5\text{-}C_{60}Me_5)(CO)_3]$, is an example of this class of complexes that has been recently synthesized and characterized by X-ray crystallography [2]. Herein, we report a computational study on group 5 metal complexes of the η^5-Pentamethyl[60]fullerene with formula $[M(\eta^5\text{-}C_{60}Me_5)(CO)_3]$; ($M=Mn^+$, Tc^+ and Re^+). The geometries of complexes in the gas-phase were fully optimized with def2-SVP basis set at M06-L and BP86 levels of theory using the Gaussian 09 set of programs. The interaction energies were calculated and corrected for the basis set superposition error (BSSE). EDA-NOCV and NBO calculations were also performed on complexes. The calculated interaction energies between $M(CO)_3$ and $C_{60}Me_5$ fragments show the following sequence: $[Re(\eta^5\text{-}C_{60}Me_5)(CO)_3] > [Tc(\eta^5\text{-}C_{60}Me_5)(CO)_3] > [Mn(\eta^5\text{-}C_{60}Me_5)(CO)_3]$.

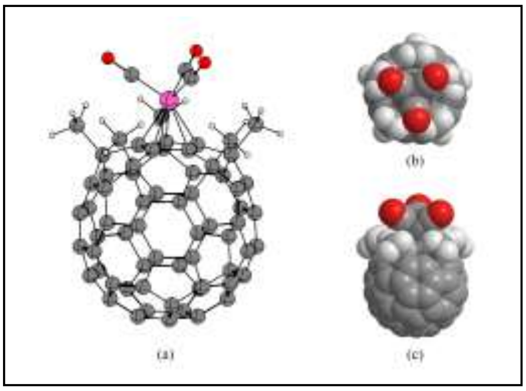

Figure 1. The optimized structure of $[Re(\eta^5\text{-}C_{60}Me_5)(CO)_3]$ at M06-L/def2-SVP level of theory.

Keywords: Fullerene (C_{60}), metal complexes, DFT, EDA-NOCV, NBO analysis.

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Synthesis, characterization and the QSAR study of bisphosphoramidate derivatives as acetylcholinesterase inhibitors

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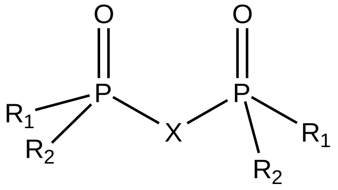
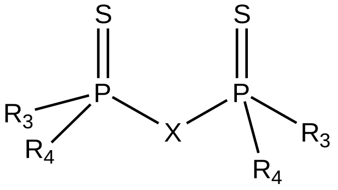
The extensive investigation on the phosphoramidates has indicated that they are human cholinesterase (CHE) enzyme inhibitor. Phosphoramidate compounds remain as one of the most interesting classes of pesticides from both the commercial and toxicological point of view. In this study, a series of phosphoramidate derivatives with the general structure of P (O) NH–X–NHP (O) were synthesized and characterized by 31P, 13C, 1H NMR and FT-IR spectral techniques. A quantitative structure–activity relationship (QSAR) model was used to predict the ACHE inhibitory activities. A data set consisted of 25compounds with known ACHE inhibitory activities was used. A suitable group of calculated molecular descriptors was selected by employing stepwise multiple linear regressions (SW-MLR) and genetic algorithm-multiple linear regressions (GA-MLR) as variable selection tools. The proposed MLR models were fully confirmed applying internal and external validation techniques.





R_3,R_4= OCH_3; X= NH-$(CH_2)_2$-NH,, NH-CH(CH_3)-CH_2-NH,,NH$(CH_2)_3$-NH....

R_1,R_2= OC_2H_5; X= NH-$(CH_2)_2$-NH,, NH-CH(CH_3)-CH_2-NH,,NH$(CH_2)_3$-NH....

Keywords: Phosphoramidate, Acetylcholinesterase, GA-MLR

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Theoretical study of DNA interaction with new amino acid Pd complex with phendione ligand by molecular docking method

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The aim of this work is the investigation of the structure effect of amino acid Pd complex on DNA interaction as an anticancer agent. The molecular docking can be an appropriate method for the prediction and confirmation of experimental data in pharmaceutical and biophysical studies [1]. Here, molecular docking calculation was performed by AutoDock 4.2 program package using the AutoDock empirical free energy function and the Lamarckian genetic algorithm with local search. The structure of the Pd complex was drawn and optimized using HyperChem 8 and AM1[2-3]. Docking energy, run and number of conformations in cluster for docking of [Pd(phendione)(isopentylglycine)]NO_3 complex to DNA as well as shows thermodynamic parameters resulting from the most negative cluster rank, The value of docking energy is -10.21 kcal/mol for the synthesized complex docked to DNA. The results retrieved from the docking study are in good agreement with those from experimental measurements, and the negative value indicates a spontaneous process. Both molecular docking and secondary structure studies in the circular dichromic spectrophotometry show the [Pd(phendione)(isopentylglycine)]NO_3 drug interacted via minor groove binding of DNA. This complex has branched and long hydrocarbon chains which causes to bind several nucleotide of DNA such as DA17, DA18, DT19, DC9, DG10 and DC11. In addition to VDW bonds, three hydrogen bonds have been formed between the nucleotides of DNA and ligand including DA17 (3.19 Å & 2.93 Å) and DC9 (2.74 Å).

Keywords: Molecular docking, Amino acid, Phendione, DNA interatction

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Viscometric studies on the interaction of Isoxsuprine hydrochloride with DNA

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Deoxyribonucleic acid (DNA) plays an essential role in life processes as it carries heritage data and instructs biological synthesis of proteins and enzymes through replication. Studies on the binding mechanism of small molecules with DNA have been deliberated as one of the essential topics during the past few decades [1]. In the present investigation, we studied the interaction of Isoxsuprine hydrochloride (ISX) with DNA.Viscosity of DNA is susceptible to changes in the length of its double helix. Accordingly the viscosity measurement is considered as one of the most critical tests for the binding mode of a drug molecule and DNA. The viscosity of the DNA solution has low changes when drug molecules bind to DNA through an electrostatic or groove binding mode. However, a classical intercalator will push the affected base pairs of DNA away from each other, resulting in elongation of the double helix of DNA and also increasing the relative viscosity of the solution. The relative viscosity of DNA solution upon the addition of ISX is shown in Fig. 1. As can be seen, there is a slight change in the viscosity value of DNA with increasing the ISX concentration, indicating that ISX mainly interacts with DNA through groove mode of binding or surface binding and not intercalation mode of binding [2].

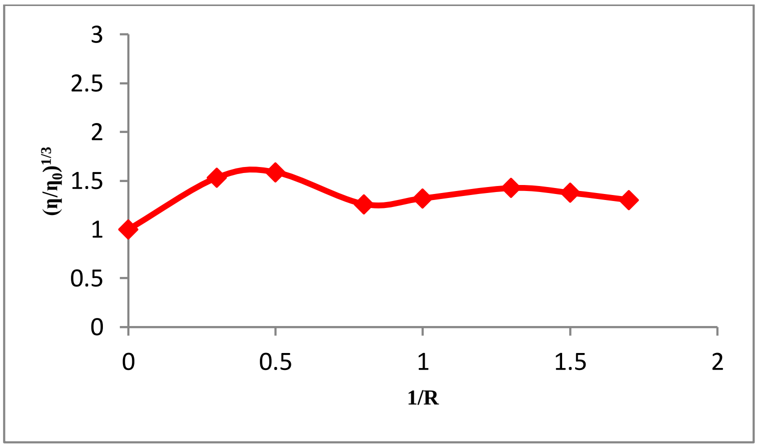

Fig. 1. Effect of ISX on the viscosity of DNA.

Keywords: DNA, Groove, ISX, Viscosity

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Electrochemical studies the interaction of Cu(II) complex contain isoxsuprine with DNA

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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 analogs [1]. In this work, we studied the interaction of Cu(II) complex of isoxsuprine, $[Cu(ISX)(Cl)_2]$, with DNA. The electrochemical methods enable us to appraise and auspicate DNA interactions and damage of DNA strand caused by binding of drug molecules to DNA as a means for further illustrating of the binding interaction between Cu(II) complex and DNA. The differential pulse voltammograms (DPV) were studied in Tris–HCl buffer (pH=7.4). Fig. 1 displays the differential pulse voltammograms of the Cu(II) complex at the absence and presence of different concentrations of DNA. The positive shift of peak potential confirms the effective interaction between Cu(II) complex and DNA. The apparent reduction in the peak currents of Cu(II) complex upon the addition of DNA to the solution was attributed to the diffusion of the Cu(II) complex bound to the large slowly diffusing DNA molecule [2]. The results suggest that this copper(II) complex interacts with DNA via intercalation binding mode [3].

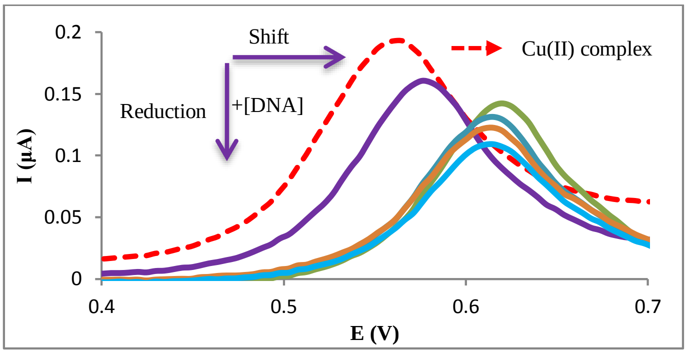

Fig. 1. Differential pulse voltammogram of Cu(II) complex in presence of DNA at different concentrations.

Keywords: DNA, Cu(II) complex, Interaction, Voltammograms.

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Interaction of cis-platin and its four analogues with guanine: a theoretical study

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Since discovery of cisplatin, many efforts have been devoted to understand the mechanisms associated with its antitumor activity, which are nowadays quite well established [1]. The primary target of cisplatin is genomic DNA, and more especially the N7 position of guanine bases. Although there is no doubt that a Pt−N7 bond forms during initial attack, the exact structure of the monofunctional adduct is not well known [2]. A better understanding at the molecular level of the interactions between the Pt and DNA building blocks can be helpful in establishing a new strategy to design cisplatin analogues. In this work we report a theoretical study on the interaction of cisplatin and its four analogues (see Figure 1) with guanine, at BP86/def2-TZVP level of theory. Since the guanine has three possible binding sites with the transition metal, all isomers and conformers of drug-guanine complexes were optimized. The calculated relative free energies as well as interaction energies between drugs and guanine showed that the preferred binding site of guanine to Pt atom in studied drugs is N7. To investigate the nature of interactions between drugs and guanine, the EDA-NOCV and NBO analyses were also performed on drug-guanine complexes. The results of energy decomposition analysis show that the interaction between drugs and guanine is more electrostatic (~64%) than covalent (~36%) and contribution of dispersion forces is ~5%.

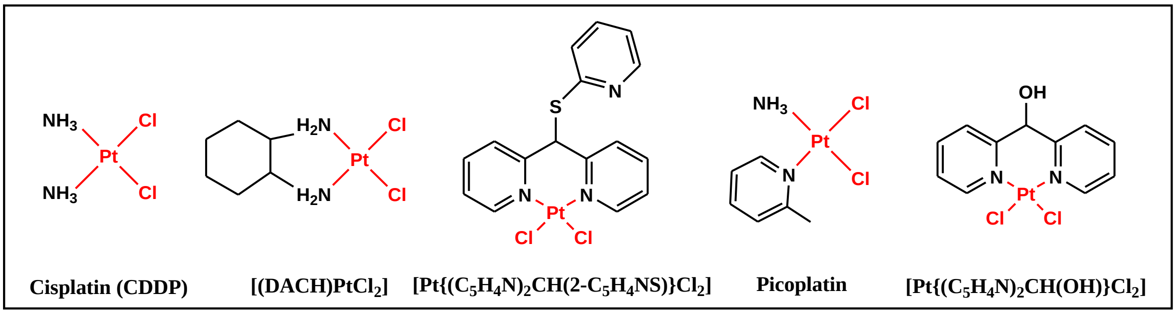

Figure 1. The molecular structure of cisplatin and its four analogues studied here.

Keywords: Cisplatin, Metal complexes, Guanine, EDA-NOCV, NBO analysis.

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A computational study on interaction of antitumor agent $[Pd\{(C_5H_4N)_2CH(2\text{-}C_5H_4NS)\}Cl_2]$ with guanine; EDA-NOCV and NBO analysis

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Palladium-based complexes are closely related to their platinum analogues, due to their structural similarities and significant overlap of coordination chemistry for the two metals. A series of novel palladium complexes have been synthesized which exhibit promising activity against tumor cell lines. In several cases the palladium complexes have exhibited better anti-tumor activity than their platinum counterparts [1]. One of the early synthesized palladium-based complexes is $[Pd\{(C_5H_4N)_2CH(2\text{-}C_5H_4NS)\}Cl_2]$ (**1**; see Figure 1) that has been characterized by X-ray crystallography [2]. In this work we report a theoretical study on the interaction of **1** (after removing one Cl^-) with guanine, at BP86/def2-TZVP level of theory. Since the guanine has three possible binding sites with the transition metal, all isomers and conformers of **1**-guanine complexes were optimized. The calculated relative free energies and interaction energies between **1** and guanine showed that the preferred binding site of guanine to Pd atom in complex **1** (similar to cisplatin) is N7. To investigate the nature of interaction between **1** and guanine, the EDA-NOCV and NBO analyses were also performed on **1**-guanine complex. The results of energy decomposition analysis show that the interaction between **1** and guanine is more electrostatic (~62%) than covalent (~33%) and contribution of dispersion forces is ~5%.

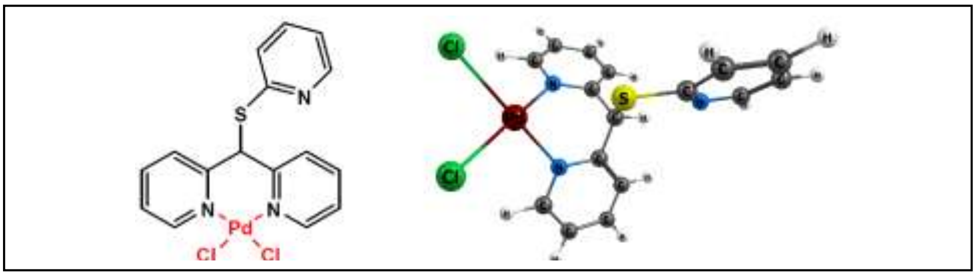

Figure 1. The molecular (left) and optimized (right) structure of complex **1**, at BP86/def2-TZVP level of theory.

Keywords: Antitumor agent, Palladium, Metal complexes, DFT, EDA-NOCV, NBO analysis.

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UV-vis studies the interaction of Propranolol hydrochloride with DNA

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The study of interaction of drug with DNA is very exciting and significant, not only in understanding the mechanism of interaction, but also for the design of new drugs. However, mechanism of interactions between drug molecules and DNA is still relatively little known. [1]. In the present work, we studied the interaction of propranolol hydrochloride with DNA. Electronic absorption spectroscopy is an effective technique to study the interaction between drug molecules and DNA by monitoring possible changes in absorption intensity and position of the bands [2]. The changes in UV–vis absorption of propranolol hydrochloride in the absence and in the presence of DNA (with increasing concentration) were examined in the Tris–HCl buffer solution (pH=7.4) (Fig. 1). As increasing concentration of DNA, the absorption band of the propranolol hydrochloride at 289 nm was influenced, resulting in hypochromicity and indicated that there is an attractive interaction between propranolol hydrochloride and DNA which is not consistent with the intercalation binding mode [3]

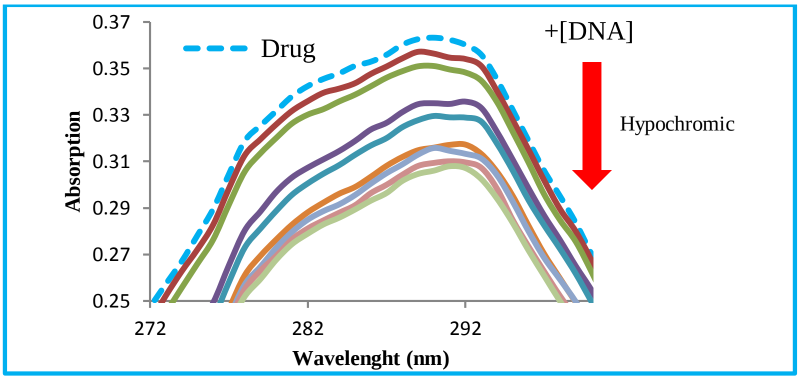

Fig. 1. Absorption spectra of propranolol hydrochloride in the presence of DNA at different concentrations of DNA.

Keywords: DNA, UV-vis, Hypochromicity, Propranolol hydrochloride

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A new Pd(II) complex containing the orthometallated C, C-chelating ligand C_6H_4- $PPh_2C(H)C(O)CH_2Cl$: Synthesis, Characterization, DNA/BSA interactions and *in-vitro* cytotoxic activity

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Phosphorous ylides are versatile ligands due to their ambidentate character, in addition to their applicability in organic synthesis [1, 2]. Carbonyl-stabilized phosphorus ylides are interesting ligands because they can behave as C or O donors owing to delocalization of the ylidic electron pair [3, 4]. Some recent contributions have shown that it is possible to obtain orthopalladated complexes derived from CH activation at Ph rings belonging to the R′ or R″substituents of the ylidic carbon and, more precisely, belonging to benzamide moieties [4]. A new mononuclear orthopalladated complex $[Pd(L_1)(pph_3)Cl]$ ($L_1 = C_6H_4\text{-}PPh_2C(H)C(O)CH_2Cl$ is obtained by the reaction of palladacyclic dimer with pph_3 and has been synthesized and characterized by using IR, NMR and elemental analysis. The crystal structure has been determined by single crystal X-ray diffractometry. The binding of the complex with native calf thymus DNA (CT-DNA) was monitored by UV-Vis absorption spectrophotometry and fluorescence spectroscopy. The results of site-competitive replacement experiments with specific site markers clearly helped us to conclude that complex bind to BSA. Finally, the molecular docking experiment effectively proved the binding of Pd (II) complex to DNA and BSA.

Keywords: Phosphorus ylide, DNA & BSA interaction, Crystal structure

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Polypyridyl Ni(II) Enantiomers; Synthesis, Characterization, and DNA Binding

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Some studies have recently found the efficiency of polypyridyl complexes as an electrochemical probe for nucleic acid sensing, particularly for CT-DNA, fluorescent probes for nuclear and protein components, DNA photocleavage agents [1,2]. Also, some polypyridyl Ni(II) complexes such as $[Ni(phen)_2(PHPIP)](ClO_4)_2$ [1], and $[Ni(bipy)_2(phen\text{-}dione)](OAc)_2$ [3] show good affinity in DNA binding to exert biological effects. First time, Nordén and Tjerneld observed enantioselective DNA binding for chiral complexes, in 1976 [4]. Initial studies indicated that the chiral tris(chelate) metal complexes bind to DNA with different modes of interaction and a certain degree of enantioselectivity [5]. For example, it has been reported for $[Fe(phen)_2(dppz)]^{2+}$that the Δ-enantiomer binds to CT-DNA about two times stronger than the Λ-enantiomer [6].

Herein, we report a general synthesis method for the preparation of pure Δ- and Λ-enantiomers. The DNA binding of enantiomers of $[Ni(dpyz)(phen)_2]^{2+}$ complex was studied by spectroscopic techniques including UV-Vis, circular dichroism (CD) and fluorescence spectroscopy. The results show the intercalation of the enantiomers into the base pairs of DNA due to the presence of planar aromatic moieties. The racemization rate of the Ni(II) enantiomers was also investigated in the presence and absence of DNA. The racemization rates are the same for the free enantiomers but the rates are significantly different in the presence of DNA. The racemization rate of the Δ- enantiomer is slower in low concentration of DNA due to the interaction between two neighboring Δ-enantiomers.

Keywords: Ni(II) complex, Enantiomer, Circular dichroism (CD), DNA binding, Fluorescence

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Palladium (II) Complexes Based on Schiff Base Ligands Derived from *ortho*-Vanillin and Study of Their Anti-cancer Properties

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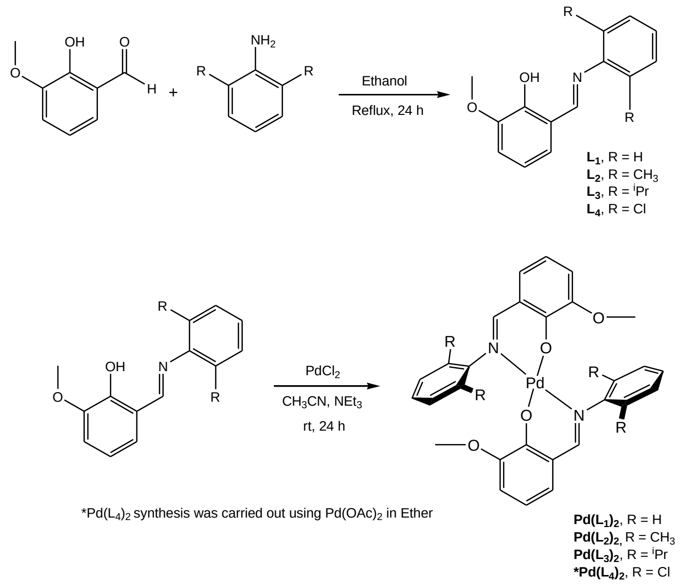
Medicinal inorganic chemistry has grown significantly in the last two decades following successes with platinum based metallodrugs in clinical tests against certain cancer cells [1]. However, side effects of *cis*-platin has prompted search for alternative metal based drugs in fight against various types of cancers with less side effects and better cytotoxic properties compared to *cis*-platin [2]. As our contribution to this field, we have developed L_{1-4} ligands, shown in Scheme below, and their corresponding palladium complexes $[Pd(L_{n)2}$, n=1-4]. The geometries of the $[Pd(L_n)_2]$ complexes were derived from single X-ray crystallography experiments. The central Pd(II) ion adopts a square planar geometry. FT-IR, ^{1}H, ^{13}C NMR and single X-ray crystal structures are reported. The cytotoxicity effect of four Pd(II) complexes was assessed on three cancerous cell lines and the results compared with that for *cis*-platin. One out of four metal complexes, **Pd(L$_1$)$_2$**, exhibited the highest anti-proliferative activity on three investigated cancerous cells lines which is even better than *cis*-platin.



Keywords*:* Metallodrug, cis-platin, ortho-vanillin, Apoptotic effect, Annexin V

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Spectral and theoretical study of coordination of oxazolidine-based ligand toward copper halides

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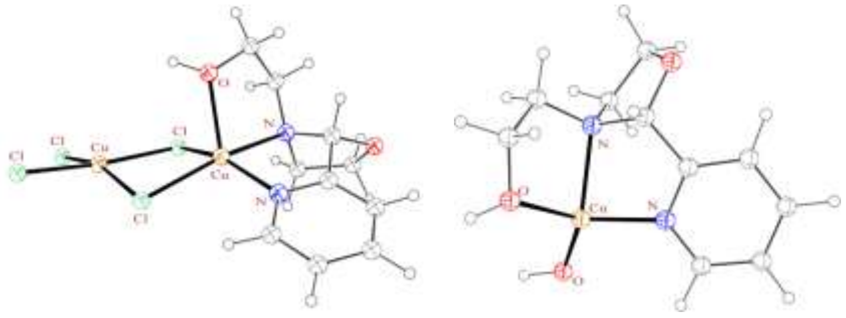
Oxazolidines are important class of compounds found in a variety of pharmacological active molecules [1]. Several substituted oxazolidines have been investigated extensively because of their importance as chain-protecting groups for amino alcohols [2], crosslinking agents [3] and optical probe applications [4]. For extending the chemistry of oxazolidines, in this paper, two new complexes of copper, $[(HL)Cu(\mu\text{-}Cl)_2CuCl_2]$ (**1**) and [CuL(OH)] (**2**) were as HL: 2-(2-(pyridin-2-yl)oxazolidin-3-yl)ethanol, from starting salts, $CuCl_2{\cdot}2H_2O$ and CuI, respectively, were prepared and identified by elemental analysis, molar conductivity, UV-Vis and FT-IR spectroscopies. Structures of two complexes were evaluated by density functional theory (DFT) at B3LYP/LANL2DZ level and shown in figure 1. The experimental data revealed that the alcoholic group of ligand can be deprotonated during the complexation process. Combination of spectral data and optimized structure of complexes shows that ligand acts as tridentate NN'O-donor. The optimized structure of **1** revealed a binuclear complexes containing chloride bridges in which two copper complexes have different geometries (square planar and square pyramidal). In the proposed structure of **2**, the copper atom coordinated by a tridentate deprotonated ligand and one hydroxyl ligand with square planar geometry. Molecular orbital energy diagrams of complexes and related HOMO and LUMO orbitals were performed and discussed.



Complex **1** Complex **2**

Figure1. Optimized structure of complexes **1** and **2**.

Keywords: Copper, Coordination chemistry, Theoretical studies, Binuclear complex, Oxazolidine

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Theoretical study of structure, charge and multiplicity spin of the Ferrous Verdoheme-Rat Heme Oxygenase Complex

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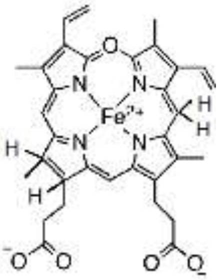
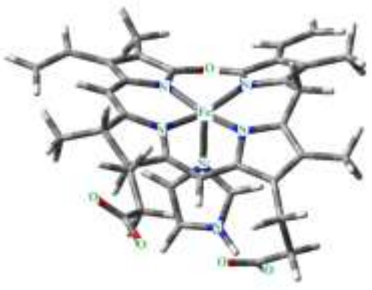
HO (hemeoxygenase) (EC 1.14.99.3) is a microsomal enzyme that catalysis the O_2-dependent degradation of heme to biliverdin IXα, carbon monoxide (CO) and free iron through a multi-step mechanism [1].HO employs heme as both the prosthetic group and substratecatalyses the degradation of heme to biliverdin IXα through three distinct intermediates, α-hydroxyheme, α-verdohemeand ferric biliverdin–iron chelate,at the expense of $O_2$and electrons [2].To investigate the chemistry of the verdoheme degradation, information on the three-dimensional structure of verdoheme– HO complex is indispensable.

Recently the three-dimensional structure of verdoheme–Rat HO complex was solved by the Sato et all [3] . Many parameters of verdoheme–Rat HO complexstructure and their role and function on Heme degradation were unknown. In this work the structure of ferrous verdoheme in complex with Rat HOaccording to the structure of verdoheme that was solved by Sato et all, was studied by density functional theory based B3LYP method and 6-31G basis set. Many parameters such as charge of verdoheme ring, electron distribution and ring multiplicity spin, proximal substituents on verdoheme ring and their arrangement were investigated. According to our study, in spite of the planar structure that had been proposed for verdoheme ring, we found that the structure of verdoheme rat hemoxygenase is not plannar and the carboxylic acids as proximal substituents are as carboxylate ion. There are three hydrogenson verdoheme ring those cause unplanarity.





Keywords: Rat-Hemoxygenase, ,verdoheme, Density functional theory.

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A computational study on maleonitriledithiolate metal complexes $[M(mnt)_2]^{2-}$ (M = Ni, Pd, Pt); EDA-NOCV and NBO analysis

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Since the superconductivity in synthetic organic conductors was first reported in 1980, chemistry and physics of molecular-based conductors have achieved remarkable progress and a number of exotic phenomena have been reported [1]. Metal complexes of bis-1,2-dithiolene, have been intensively studied as the component of molecular conductors and have provided a unique category of conducting materials [2]. In this work, we report a theoretical study on maleonitriledithiolate (mnt^{2-}) complexes with group 8 dications (Ni^{2+}, Pd^{2+} and Pt^{2+}). The geometries of complexes in the gas-phase were fully optimized with def2-TZVP basis set at BP86 levels of theory. Vibrational frequency analysis, calculated at the same level of theory, indicates that the optimized structures are at stationary points corresponding to local minima without any imaginary frequency. The interaction energies were calculated and corrected for the basis set superposition error (BSSE). To investigate the nature of interactions between metal and ligands in complexes, the EDA-NOCV and NBO analyses were also performed. The results of energy decomposition analysis for all complexes show that the interaction between metal and two ligands is more electrostatic (~64%) than covalent (~36%).

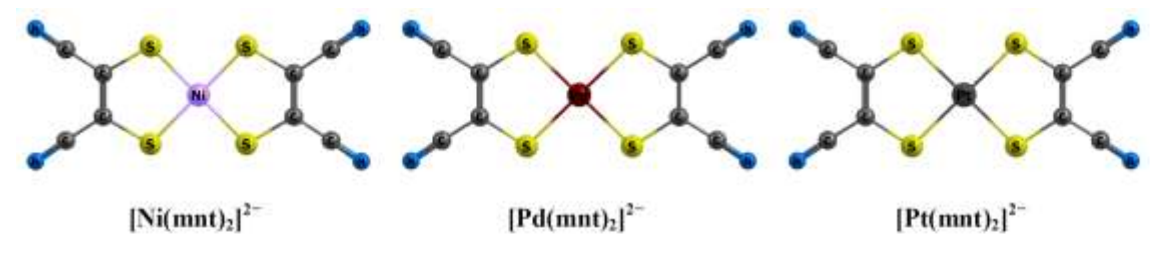

Figure 1. The optimized structures of $[Ni(mnt)_2]^{2-}$,$[Pd(mnt)_2]^{2-}$ and $[Pt(mnt)_2]^{2-}$ complexes at BP86/def2-TZVP level of theory.

Keywords: Maleonitriledithiolate, Metal complexes, DFT, EDA-NOCV, NBO analysis.

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Density Functional Theory Calculations of [2,2-ˈbipyridine]Ni[4,5-difluoropyridazine] Complex in Gas Phase

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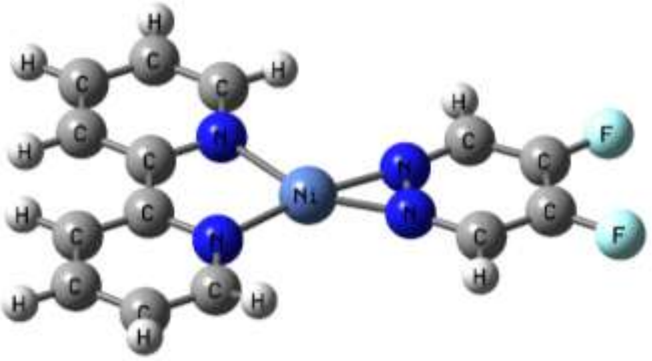
The structure parameters and ionization energies of [2,2-ˈbipyridine]Ni[4,5-difluoropyridazine] Complex were calculated by Density Functional Theories (DFT) using Becke's three-parameter hybrid functional with 6-31+G* basis set and LANL2DZ effecitive core potential using Gaussian 03 software [1]. Vibration frequencies were also calculated to the structure with optimized geometry and no imaginary frequency were obtained, so the stationary point correspond to the minima of the potential energy surface. Electronic structure studies were carried out in a DFT method with a B3LYP potential, which is the most complete potential actively used in modern research and showing the best agreement to experiment in the sequence of levels. Also, the restricted Hartree–Fock method was employed for electronic structure calculations of closed-shell complexes, and the unrestricted approximation was used for open-shell complexes. The contributions of atomic orbitals were evaluated from the squares of the diagonal elements of the density matrix. Also, the bond orders and the electronic properties of the complex were calculated. The relationship between the stability constants of the complexes and the electronic properties of the complex were examined. It was found that the stability constants of the complexes correlate with the calculated bond orders between metal and ligand, and also geometry of [2,2ˈbipyridine]Ni[4,5-difluoropyridazine] Complex.



[Scheme]

Keywords: [2,2ˈbipyridine]Ni[4,5-difluropyridazine] Complex, Electronic Properties, DFT

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Examination of thermodynamic and structural properties of transition metal complexes with Schiff base ligands using quantum chemical calculations

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Schiff bases played a key role in the development of coordination chemistry as they readily form stable complexes with most transition metals [1]. Metal complexes of Schiff bases are specifically of interest in bioinorganic chemistry because many of these complexes provide biological models for use in understanding the structure of biomolecules and biological processes [2]. In this project, Schiff base ligands derived from *O*-phenylenediamine and 5-bromo-salicylaldehyde were used to study the conformation analysis and metal ion affinity (MIA) of these ligands with transition metal by a chemical quantum approach. Structural properties of the Schiff bases before and after complex formation were also analyzed. All of the structure optimizations and frequency calculations were performed at the B3LYP level with 6-311++G(d,p) basis set by using Gaussian 09. Natural bond orbital theory (NBO) and quantum theory of atoms in molecules (QTAIM) were used to investigate the charge transfer process and the nature of interactions in the formed complex.

Keywords: Schiff base, *O*-phenylenediamine, 5-bromo-salicylaldehyde, Quantum chemical calculation

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Effect of particle sizes of absorbent on uptake and release properties of pyridacil drug

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Herein, we study uptake and release properties of pyridacil (**PY**) from bulk HKUST-1 metal–organic frameworks (Cu–MOFs) (mechanosynthesis) in comparison with nanostructure (ultrasonic synthesis). The **PY** content was estimated by thermal gravimetric analysis (TGA) and UV/vis spectroscopy. To explore the absorption ability of the MOF to **PY** molecules, fresh sample of Cu–MOF (50.0 mg) was immersed in an aqueous (4.0 mL) solution of **PY** (0.02 g L^{-1}) and were monitored in real time with UV/vis spectroscopy [1]. The sorption capacity of Cu–MOF increases with the increase of contact time. The change of intensity and width indicates that the resulting solid Cu–MOF retains the host framework crystallinity as **PY** molecules diffused in [2,3]. Results show that among the nano and bulk compounds, bulk compound has higher absorption activity. The increase in capacity for **PY** in bulk compound can be explained by two phenomena. First, higher sorption for bulk compound is attributed to the lengthy and deep channels. Second, based on the obtained results for the specific surface area of bulk and nano compounds, under ultrasound-assisted methods the surface area is decreased, since the amount of the **PY** adsorption decreased by this method. In the other hands, increasing the surface area leads to improvement in absorption activity. In comparison as long as 48 h, the uptake of **PY** (88.2%) on bulk compounds is remarkable and clearly exceeds that of nano compounds (23.3%) in the aqueous solution of **PY**. After loading of **PY**, there was a decrease in the volume of the cavity, and the specific surface area decreased from 1042.5 m^{2}g^{-1} (bulk compound) to 68.4 m^{2}g^{-1}. These results indicate that there remains almost no residual porosity after the **PY** adsorption. Therefore, the **PY** approximately filled up the pores and channels, and these frameworks have a remarkable **PY** absorption capacity.

Keywords: Metal–organic frameworks, Nano, Bulk, Pyridacil, Crystallinity.

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Synthesis and Structure Determination Some of Mono, Bis , Tris and tetrakis Phosphoramide Derivatives: Theoretical modeling Study, Investigation of Coordination Behavior and Structure-Activity Relationships

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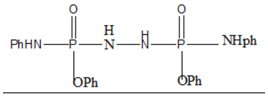
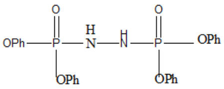
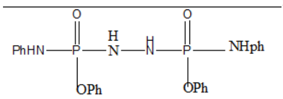
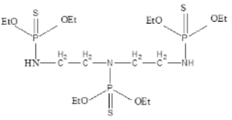
In this research, some new mono, bis ,three and tetra dentate including functional groups P=X (X=S,O) will be synthesized. Bis and tris and tetrakisphosphoramide with phosphorus as central nuclear, terminal substituent containing of isoelectronic groups, also bridge substituent including amine, diamine, dialcohol, diaminoalcohol of aliphatic and aromatic. Structural and spectroscopic studies of the ligands and synthetic complexes (especially rare metals with luninscence properties) will be performed by spectroscopy methods IR, Mass ، NMR و X-ray crystallography. Biological parameters (enzyme, bacteria,…) and physical chemistry parameters (electronic, steric, lipophilicity and…) compounds based on changing of bridge and terminal will be evaluated and will be investigated structure-activity relationships (SAR). Theoretical studies complex of ligand-protein (spatially AChE Enzyme) for investigation of affecting mechanism in central activity of enzyme using from the modeled ligands will be studied by DFT method and these performing will be used experimental data.









Keywords: Bisphosphoramide (amidotioate), Trisphosphoramide, Complex, Luminscence, AChE, Lipophlicity, X-ray crystallography, DFT Studies, Structure-Activity relationships

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Synthesis of new Zn (II) complex supported on Fe_3O_4 and its application as a green catalyst for the oxidation reactions

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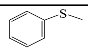
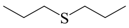
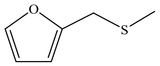
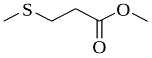
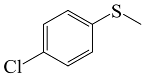
Magnetic nanoparticles MNPs are considered as ideal supports for the heterogenization of homogeneous catalysts support because of their easy preparation and high surface area, high dispersion resulting in high catalyst loading capacity, outstanding stability, easy separation of the catalyst through an external magnet, and simple and inexpensive procedure(1-4). In the present study, Fe_3O_4 nanoparticles were prepared via simple and versatile procedure. Then, a novel and green catalyst was synthesized by the immobilization of Zn on Fe_3O_4 nanoparticles coated with adenine. The activity of this nanostructure compound was examined for the oxidation of sulfides. The final nanohybrid compound was characterized by FT-IR spectroscopy, XRD, ICP-OES, TGA, EDS and SEM techniques.

Table 1. Oxidation of sulfides to the sulfoxides in the presence of Fe_3O_4-Adenine-Zn.

Entry	Substrate	Product	Time (min)	Yield (%)[a]	Melting point (°C) [Ref.]
1		2a	75	98	Oil
2		2b	65	94	Oil
3		2c	35	97	Oil
4		2d	35	89	Oil
5		2j	130	98	Oil

[a]Isolated yield.

Keywords: Magnetic nanoparticles , Sulfoxide, Zn (II)

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Synthesis of Silicon Carbide and investigating its biosensor applications

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Carbide compounds are generally known as very hard ceramics with outstanding chemical properties on account of strong bonds between carbon atoms and cations such as Si, B, Ti, etc. Among these compounds, silicon carbide is one of the non-oxide ceramics which has various industrial applications [1]. High melting point, high thermal conductivity, high oxidation resistance, high mechanical strength and good chemical properties are some of its most important characteristics[2]. In the recent studies silicon carbide's electrochemical properties as well as its biological inertness and biocompability has been of much interest for using in biosensor fabrication [3]. In this study SiC nanotubes were synthesized using carbon nanotubes (CNTs) as template through sol-gel and magnesiothermic methods. The resulting samples were doped with other elements such as N, S and P to achieve optimum electrochemical properties. The samples' structures were tested using conventional methods such as SEM, EDS, FTIR, XRD, etc.

Keywords: SiC, Nanotube, Silicone Carbide, Biosensor

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DFT study on the adsorption of diethyl, ethyl methyl, and dimethyl ethers on the surface of gallium doped graphene

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In this study, we used density functional theory (DFT) to search on the adsorption properties of three important compounds of ether family; diethyl ether (DEE), ethyl methyl ether (EME), and dimethyl ether (DME) on the surface of Gallium doped graphene (GaG). We used three functionals (B3LYP, wb97xd, and MPW1PW91) for optimization and calculation of adsorption energy. After fully optimization, we scruti- nized on the charge allocations on the adsorbed ethers as well as GaG (at the area of interaction) based on natural bond orbitals (NBO). Besides, we have calculated the amount of charge transfer upon adsorption of each analyte. We revel that GaG is an ideal adsorbent for chemisorption of all above-mentioned ethers. There is a little difference between the values of adsorption; −123.5, −120, and −118.3 kJ/mol (based on wb97xd) for DEE, EME, and DME, respectively. We found significant changes in the electronic structure of both adsorbent and adsorbate upon adsorption. Moreover, results of charge analyses confirm GaG is a p-type semiconductor.

Keywords: Gallium doped graphene , Density functional theory , Ether , Semiconductor , Nanostructure adsorbent

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The effect of reaction times on Fe-Mg oxide nanoparticles prepared by wet impregnation method

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In this paper, wet impregnation method was employed to prepare bimetallic Ferrite-Magnesium oxide nanoparticles and the effects of reaction time was investigated as an important factor in this research with the purpose of using them as a catalyst in industrial process. The reaction of precursors were done in various times (30-150 min) to obtain the best product in the water steam therm. Wet impregnation is a commonly used technique for the synthesis of heterogeneous catalysts. Typically, the active metal precursor is dissolved in an aqueous or organic solution. Then the metal-containing solution is added to a catalyst support containing the same pore volume as the volume of the solution that was added. Different analysis such as FE-SEM, XRD and EDX were used to determine the physical and chemical properties of synthesized nanoparticles. The XRD results confirm the formation of Fe-Mg compounds (Fe_2O_3-Fe_3O_4-$MgFe_2O_4$-$MgFeAlO_4$) and crystals size lied between 5-25 nm. In addition, according to the FE-SEM images, the particles have spherical morphologies with average size of 50 nm in the optimum sample. The FE-SEM image and the XRD pattern below show the investigation of a sample in 2 hours reaction time.

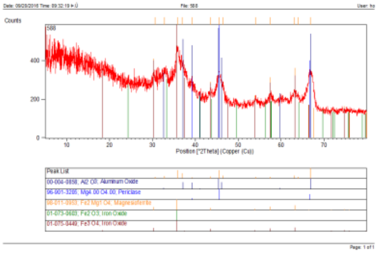

Fig1. XRD pattern

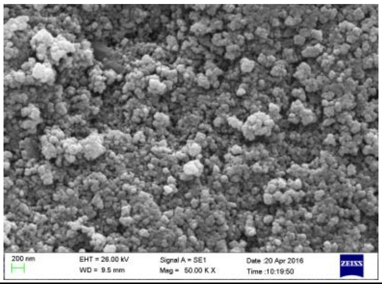

Fig2. FESEM

Keywords: wet impregnation, bimetallic, Fe-Mg oxide, reaction time

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Preparation of copper nanoparticles by chemical reduction of copper(II) complexes in the solid state

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Copper nanoparticle are used in different areas such as optoelectronic, catalysis and biological applications [1,2]. Transition metal complexes, especially the metal compounds of group IB, such as copper(II) varying the morphology of the nanoparticles, due to chemical reaction method, can alter their catalytic activity [3]. These nanoparticles can be generated in a variety of ways. The methods are included molecular beams, chemical reduction, thermal decomposition of transition-metal complexes and electrochemical synthesis [4]. In this work, Cu nanoparicles have been prepared by reduction of copper(II) complexes. Here hydrazinium sulfate has been used as a reducing agent in chemical reduction of metal complexes. These nanoparticles were characterized by X-ray diffractometer (XRD), IR spectroscopy, scanning electron microscopy (SEM), and EDX analysis.

Keywords*:* Chemical reduction, Nanoparticles**,** solid state reaction, Copper

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Preparation of magnetic nickel nanoparticles from their coordination compounds in amorphous silica

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Nickel nanoparticles have received a lot of attention because of their unique magnetic properties [1-3]. Magnetic materials are used in a broad range of applications, including the production of magnetic fluids, stealth technology, refrigeration, optoelectronic, catalysis and biological applications. These materials have also been used as catalysts for hydrogenation of organic synthesis [4]. In this work, nickel nanocrystallites have been prepared by reduction of nickel complexes. In a mechanochemical method, nickel complexes were reacted with hydrazinium sulfate as a reducing agent. Nickel nanoparticles were formed due to the silica substrate and the reduction potential of Ni^{II} complexes. These nanoparticles were characterized by X-ray diffractometer (XRD), scanning electron microscopy (SEM), vibrating sample magnetometer (VSM), EDX analysis and IR spectroscopy.

Keywords*:* Amorphous silica, Chemical reduction, Nickel complexes, Nanoparticles, Magnetic particles size.

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Synthesis of substituted pyranopyrazole derivatives in solvent free media with molybdenum complex supported on magnetic nanoparticles as recyclable catalyst

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Metal complexes immobilized onto metal nanoparticles are a category of relatively new promising materials for catalysis and analytical chemistry [1-3]. A magnetically recoverable catalyst consisting of molybdenum complex was prepared. This heterogeneous catalyst was characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray (EDX), vibrating sample magnetometry (VSM), inductively coupled plasma atomic emission spectroscopy (ICP-AES) and Fourier transform infrared (FT-IR). Pyranopyrazoles are very desirable as a type of heterocycles due to their potential uses in pharmaceutical field. They display a varied range of biological activities like anti-inflammatory, anticancer and antimicrobial [4]. The immobilized catalyst was shown to be an efficient heterogeneous catalyst for the synthesis of pyranopyrazole derivatives. The catalyst could be easily and efficiently isolated from the final product solution by magnetic decantation and be reused for 6 consecutive reactions without showing any significant activity degradation.

Fig 1. Mo complex@MNPs mediated synthesis of substituted pyranopyrazole under solvent-free and room tempreture condition.

Keywords: Pyranopyrazole derivatives, Recyclable catalyst

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Organic-Inorganic hybride Tungsten Oxide as Supercapacitor

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In this paper, we have synthesized new organic-inorganic tungsten oxide hybrids using three amino-hydroxy ligands as supercapacitors that were briefly named as W_1, W_2, and W_3. The physicochemical properties and the structures of obtained compounds were characterized by various techniques such as XRD, FT-IR, TGA and SEM. Then the supercapacitor properties of obtained compounds was investigated at different tempretures 100, 200, 300, 600 ℃. Cyclic voltametry and galvanostatic charge-discharge tests were carried out to estimate the capacitance of three synthesised electrodes. The best results were obtained from W_{1-100},W_{2-100}, and W_{3-300} samples. The discharge curve of W_{3-300} electrode presents the longest discharge time of 23.0s at 2 A/gr which corresponds to a high C_F value of 207.27 F g^{-1}, indicating the outstanding charge/discharge performance for this case, while the W_1 and W_2 based SC electrode shows relatively shorter discharging time of 20.2 and 6.6 s corresponding to the C_F value of 193.48 F g^{-1} and 61.81 , respectively.

Keywords: organic,inorganic hybrid, tungsten oxide, supercapacitor

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Synthesis of Porous Bio-inspired Silicon Carbides as the Green absorbent

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In this paper, nanostructured silicon carbides were prepared via green route at low temperature. In this method, natural materials were used as the sources of silicon and carbon to synthesis the bio-inspired porous silicon carbides. Also, nitrogen-doped and nitrogen, sulfur-doped SiC was prepared using natural sources too. In this approach, Si natural source was placed in carbohydrate solution, and then it was calcined for 1 hour in N_2 atmosphere. After calcination, nanoporous silicon carbides were synthesized by heating in furnace for 5 hours at low temperature. The produced SiCs showed mesoporous structures with high surface area and identical structures due to their initial precursors. The products were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Brunauer-Emmett-Teller (BET) method. The obtained porous SiC, N-doped SiC, and N,S-doped SiC was investigated as absorbent in removal of organic polutants. The results illustrated that bio-inspired SiC, especially N,S-doped SiC are the promising candidates for absorbent due to present of sulfur and nitrogen in it structure.

Keywords: Porous Bio-inspired nanostructures, Silicon carbide, Absorbent

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Preparation, characterization of colloidal friendly fluid hydroxyapatite nanocompsite using natural milk casein

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Biodegradable polymer/hydroxyapatite nanocomposites are a novel class of materials which has been attracted interest as biomaterials vehicles carriers in drug delivery. The objective of the present work was to study preparation and characterization of Fluidal HA nanocomposites based on biodegradable polymer casein, for evaluation of its potential in ocular drug delivery purposes. Characterization of the samples was carried out by means of Fourier Transform Infrared (FT-IR), X-ray powder diffraction patterns (XRD), Field Emission Scanning and Transmission Microscopy (SEM & TEM) and Dynamic light scattering (DLS) technics. The results revealed successful formation of HA nanocomposites with average particles size 20 nm. Synthetic nano hydroxyapatite (nHA) is one of the most suitable materials for drug delivery. It is possible to create composite materials based on nHA with an inorganic and organic biologically active substance[1-3]. In this study, Needle like hydroxyapatite nanoparticles (HA), was successfully prepared in the micro emulsion template phase and Modified Inverse micro emulsion process is a very suitable and interesting method for preparation of colloidal needle like HA in a highly ordered size for using in drug delivery purposes

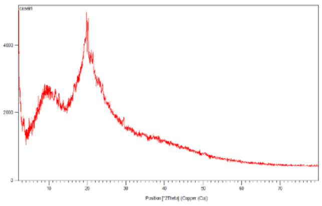

Fig.1. The XRD patterns of Casein extracted

Keywords: Casein, Hydroxyapatite, nanocomposite, Microemulsion template; Biodegradable, Dynamic light scattering

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Catalyst Enhancement and Recyclability by Immobilization of Metal Complexe onto Graphene Surface by Noncovalent Interactions

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The immobilization of a homogeneous catalyst onto a solid surface is one of the major challenges in catalysis, because it may facilitate the separation of the catalyst and the reaction products and may also give rise to the reutilization of the catalyst in multiple subsequent cycles. Noncovalent interactions between the catalyst and the support are arising as interesting alternatives to the more widely used covalent interactions, because they avoid the functionalization of both the catalyst and the surface, which may in turn lead to the modification of the inherent properties of the catalyst. However, some other problems may arise, such as leaching. In this work, we have obtained new complex containing an N-heterocyclic carbene ligand with a pyrene tag, which we immobilized onto the surface of reduced graphene oxide (rGO), by π- stacking.this complex obtained by reaction of palladacyle and imidazolium salt. The catalytic properties of the molecular complex and hybrid material have been studied in the palladium catalyzed suzuki-miyara The results show that the catalytic properties are improved in the hybrid materials, compared to the catalytic outcomes provided by the homogeneous analogues. Although the palladium-catalyzed reactions may be due to the formation of Pd nanoparticles. hybrid material characterized by XRD, TEM, BET, ICP-OES. The work constitutes a clear improvement over other known immobilization methodologies and offers a practical methodology which may inspire future developments of efficient heterogenized catalysts.

Keywords: Suzuki-Miyara, graphene, palladium, N- heterocyclic carbenes

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Nanoparticle supported, magnetically separable vanadium and molybdenum complexes as catalyst for selective oxidation of sulfides

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A novel organic–inorganic hybrid heterogeneous catalyst system was obtained from the reaction of the molybdenum(VI) complex [$MoO_2Cl_2(DMSO)_2$] and vanadium(V) with silica-coated Fe_3O_4 nanoparticles containing 3-aminopropyl triethoxysilane (APTS) groups. This straightforward preparation yields magnetically separable molybdenum(VI) and vanadium(V) nanoparticles with high molybdenum and vanadium loading respectively. These nanoparticles were efficient catalysts for selective oxidation of sulfides to corresponding sulfoxides with urea hydrogen peroxide in excellent yields. Leaching and recycling experiments revealed that the nanocatalyst can be applied for nearly complete oxidation of sulfides for at least five successive cycles. The particle morphology and textural properties of nanoparticles molybdenum and vanadium were studied by SEM and representative images are shown respectively in Fig. a and b. In the SEM image, nanoparticles with spherical shapes are observed with particle diameter in the range of 70-100 nm.

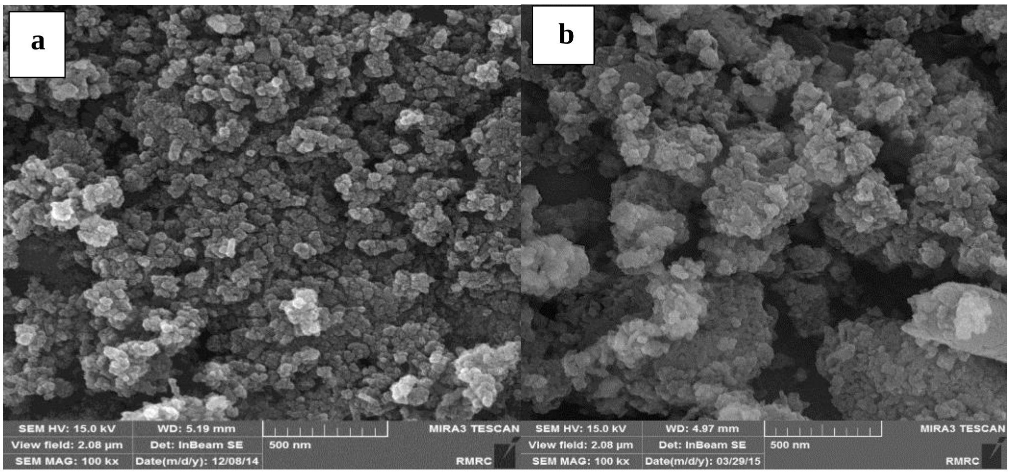

Fig. a). SEM images of molybdenum nanocatalyst and b). SEM images of vanadium nanocatalyst

Keywords: Magnetic separation; Nanocatalyst; Oxidation of sulfides; Surface functionalization

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Mo(VI) complex supported on the magnetic nanoparticles: Magnetically separable nanocatalysts for selective oxidation of sulfides to sulfoxides

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A molybdenum(VI) Schiff base complex as an efficient and highly heterogeneous catalyst was developed by immobilization of a molybdenum complex on the surface of modified Fe_3O_4 magnetite nanoparticles, The complete characterization of catalysts was carried out by means of thermogravimetric analysis (TGA), Energy-dispersive X-ray spectroscopy (EDX) analysis, FT-IR. The obtained nanoparticles were employed as catalysts for the selective oxidation of sulfides to corresponding sulfoxides using urea hydrogen peroxide as the oxidant. Furthermore, the obtained catalysts showed not only high catalytic activity in oxidation reactions but also high degree of chemical stability in various organic solvents. The immobilized molybdenum complex on silica coated magnetic nanoparticles can easily be recovered from the reaction system using an external magnet and reused several times with high yields. The thermogravimetric analysis (TGA) curve of the nanocatalyst shows the multistep mass loss of the organic materials between 50 and 600 °C (Fig. 1). EDX analysis of the nanocatalyst showed expected elements such as oxygen, silicon, carbon, nitrogen, chlorine and molybdenum (Fig. 2).

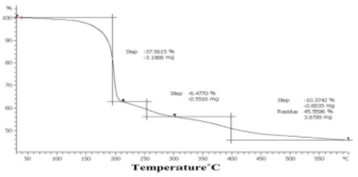

Fig.1. The TGA curve of nanocatalyst

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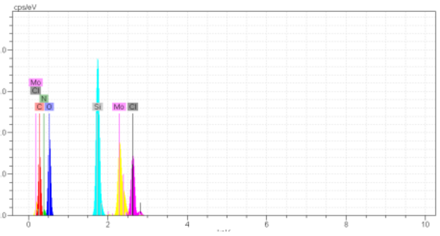

Fig. 2. Energy-dispersive X-ray spectroscopy (EDX) of the nanocatalyst

Keywords: Oxidation of sulfides, Magnetic nanoparticles, Complex of molybdenum.

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Preparation and characterization of $BaMg_xZr_xFe_{12-2x}O_{19}$ and Polyaniline/$BaFe_{12}O_{19}$ composites and investigation of their microwave absorptions

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$BaMg_xZr_xFe_{12-2x}O_{19}$ (with x=0, 0.25, 0.5, 0.75, 1, 1.25, 1.5) synthesized by Sol-gel method[1] and characterized by X-ray diffraction (XRD), FTIR spectrophotometer, Field emission scanning electron microscope (FE-SEM), vibrating sample magnetometer,(VSM). The vector network analyzer (VNA) applied for microwave absorption properties . The FT-IR spectra show Fe-O-Fe band in region of 432-576 cm^{-1}, X-ray diffraction shows a single magnetoplumbite phase for the magnetic powders with Mg-Zr content(x=0.25-1.5) For the magnetic powder with Mg-Zr content (x) of 0 or 0.5, magnetic impurities appear in the structure, and the crystalline size of the particles varies from 21.31 to 28.40 nm. In the electromagnetic measurements, it was found that the saturation magnetization remanence, and coercivity decreased with Mg-Zr doping. The maximum reflection loss of $BaMg_{0.25}Zr_{0.25}Fe_{11.5}O_{19}$/PANI ferrite composites was -38 dB at 9.6 GHz.

Keywords: Saturation magnetization; Composite

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Synthesis a new Pt(II) comlex containing valganciclovir drug with calf thymus DNA using multispectroscopic and computational methods

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A new complex, [Pt(valcyte)(DMSO)Cl], in which valcyte served as a valganciclovir drug, was synthesized and characterized by different physicochemical methods. Binding interaction of this complex with calf thymus DNA (ct-DNA) has been investigated by multi spectroscopic techniques. The complex displays significant binding properties with ct-DNA. The results of fluorescence and UV–Vis absorption spectroscopy indicated that this complex interacted with ct-DNA in a groove-binding mode, and the binding constant was $(0.38\times10^{4}\ M^{-1})$. Furthermore, the complex induced detectable changes in the CD spectrum of ct-DNA and slightly changed its viscosity which verified the groove-binding mode. Finally, all results indicated that Pt(II) complex interact with DNA via groove binding mode.

Keywords: [PtCl(dmso)((valcyte)], Valganciclovir, ct-DNA , Minor groove .

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Ultrasound-assisted fabrication and characterization of a novel Co(II) mixed-ligand coordination polymer and evaluation of catalytic properties

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A novel Co(II) mixed-ligand coordination supramolecular polymer with composition $[Co_2(ppda)(4\text{-}bpdh)_2(NO_3)_2]_n$ (1) (where, ppda =p-phenylenediacrylic acid, 4-bpdh = 2,5-bis(4-pyridyl)-3,4-diaza-2,4-hexadiene) was prepared using solvothermal and sonochemical methods. Compound 1 and the new nanostructure have been characterized by single-crystal X-ray, infrared spectroscopy (IR), powder X-ray diffraction (PXRD) analysis and scanning electron microscopy (SEM). The thermal stability of compound 1 was also studied by thermal gravimetric analysis (TGA). The surface area of these compounds was determined by BET. The single-crystal X-ray data shows a new interesting two-dimensional coordination polymer (CP). In addition, the effect of various sonication concentrations of initial reagents, power of ultrasound irradiation and also the time on the size and morphology of nano-structured coordination polymer 1 were evaluated. Moreover, it has been demonstrated that the nanostructure of the CP1 can be used as a catalyst in Knoevenagel condensation reaction.

Keywords: Solvothermal synthesis; Sonochemical synthesis; Coordination polymer; Catalysis; Knoevenagel condensation reaction

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Hydroxyapatie and Calcium Hydroxide Nanocomposites in Preservation of Paper-Art-Works

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Paper-Art-Works are the large part of archives, libraries, and museums. Various factors can damage these historical papers. Oxidation and acidic hydrolysis of cellulose are the most important chemical damages in paper works. One of the most effective method for reducing these chemical damages is the use of nanomaterials. In this project, we used some polymeric nanocomposites that are compatible with historical papers and can decrease the rate of oxidation and hydrolysis via two mechanisms. For this purpose, calcium hydroxide and hydroxyapatite nanoparticles and different biopolymers were used to prepare these nanocomposites. Various methods such as infrared spectroscopy, electronic microscopy, and tensile strength measurement were used before and after accelerated aging to examine the effects of these nanocomposites to stop the oxidation and hydrolysis reactions. The results showed that the calcium hydroxide nanoparticles are more effective than hydroxyapatite nanoparticles in deacidification of papers, but the composites that are prepared with HA nanoparticles showed the better effects to decrease the oxidation and hydrolysis simultaneously. Also, the selected biopolymers can be very effective in these protective coatings. They can increase the protective effects of nanoparticles and also consolidate the paper works.

Keywords: Paper-Art-Works, Nanocomposites, Calcium hydroxide, Hydroxyapatite, Oxidation, Hydrolysis.

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Synthesis of 2,4,6-Trichloroborazine ($B_3N_3H_3Cl_3$) for preparation of borazine derivatives

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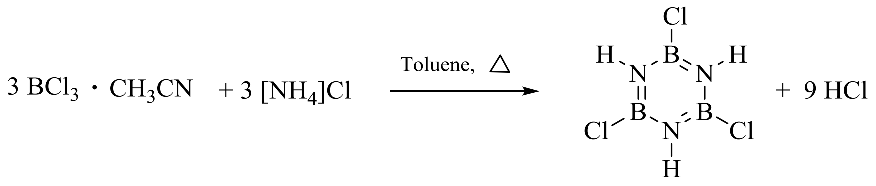
The borazine molecule consists of a six-membered Heterocyclic ring of alternate boron and nitrogen atoms in which one hydrogen atom bonds to each boron and nitrogen atom. Borazine ($B_3H_6N_3$) is an inorganic compound and isoelectronic and isostructural with benzene, consequently borazine is named as "inorganic benzene". Here we report on the synthesis of 2,4,6-Trichloroborazine (TCB) as the precursor for preparation of borazine derivatives. Borazine and its derivatives are the effective precursor for preparation of variety species of Boron nitride (BN) and multinary ceramic systems containing B, N, Si and C elements. Synthesis of TCB was carried out by reference method of Brown and Laubengayer with some modifications and crude product was purified by sublimation in vacuum. In this research, boron trichloride (BCl_3) solution in n-hexane and ammonium chloride (NH_4Cl), toluene and acetonitrile (CH_3CN) were utilized as starting materials. All experiments were performed under Argon atmosphere and anhydrous conditions using standard Schlenk technique. The synthesis of white powder of TCB was confirmed by ^{11}B- and ^{1}H-NMR-spectroscopy, δ (^{11}B) = 30.3 ppm and $\delta(^{1}H)$ = 5.32 ppm. The compound TCB is a very expensive substance and this is the first report of successful preparation of TCB in Iran which is done under conventional condition in appropriate yield of 80%.



Synthesis of 2,4,6,-trichloroborazine (TCB)

Keywords: 2,4,6-Trichloroborazine, Boron nitride, Borazine derivatives, Schlenk technique

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Theoretical investigation of oxidative mechanism of action for a new Platinum(IV) compound toward DNA

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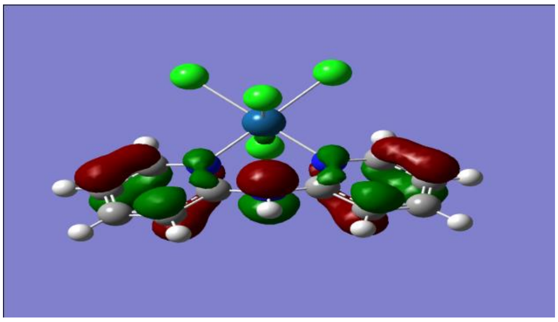
Many transition metal complexes mediate DNA oxidation in the presence of oxidizing radiation, photosynthesizers, or oxidants. Oxidative damage of DNA plays a critical role in mutagenesis, carcinogenesis, aging and lethality. It is well established that many metals are capable of promoting catalyzing the oxidative transformations of nucleobases. Platinum complex is currently in clinical use for about three decades. In this regard, Choi and co-workers investigated the oxidative behavior of some Platinum(IV) complexes toward DNA and showed that these complexes are able to oxidize guanine (G) nucleotides such as 5'-dGMP, 3'-dGMP and 5'-[GTTTT]-3' through a consecutive two-step inner-sphere mechanism .Density functional theory (DFT) has been used to investigate the oxidation of guanine nucleotided by platinum(IV) , a process that can be important in the degradation of DNA. Here we have investigated a mechanism of oxidation of a nucleotide (5'-dGMP) by [Pt (2, 2'-dipyridylamine) Cl_4].We have provided a comprehensive mechanism for all of the step in this process. A number of intermediates are predicted to occur but with short lifetimes that would make them difficult to observe experimentally. A key step in the mechanism is electron transfer from guanine to Platinum (IV), and we show that this is driven by the loss of a chloride ligand from the Platinum complex after nucleophilic attack of 5'-phosphate to C_8 of guanine. We have investigated several different initial Platinum (IV) guanine adducts and shown that the adduct formed from replacement of an axial chlorine ligand in the Platinum (IV) complex underground oxidation more easily.



Keywords: Platinum(IV), Anticancer, Cytotoxicity, Oxidative transformations, DFT

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5-7 September 2017

A new Methodology in Drug Delivery

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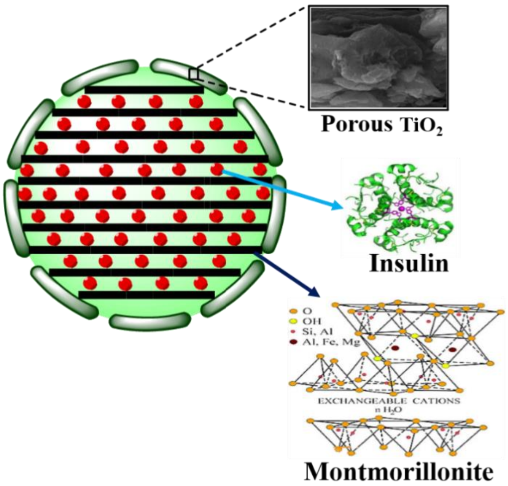
Our main goal in presenting this methodology was to modify the conventional systemic delivery of drugs because such procedures may cause toxicity; for example, polymeric coatings may present some disadvantages such as limited chemical stability, local inflammatory reactions and so on. As a result, we thought that it could be interesting to embed bioactive compounds and biomolecules within inorganic coating such as TiO_2, ZrO_2, and SiO_2. This type of coating increases drug passage time through its small and long pores forward intended fluid (whether *in vitro* or *in vivo*) and eliminates different stimuli such as (temperature, pH, ultrasonic irradiation,...) to remove the coating on the surface of drug carrier system. This could be very effective economically and time spent. Moreover, if such inorganic coatings have nanostructure properties, they improve cellular adhesion, enhances osteoblast proliferation, and increase biomineralization. In this talk, emphasis is placed on presenting the technique, and would like to explore it as a new methodology in drug delivery.



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Preparation and investigation of nanotublar halloysite phenolic resin nanocomposites

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A novel generation of nanocomposites consisted of phenol formaldehyde (PF) resin and surface modified halloysite nanotubes (HNT)s had been prepared by sonochemical assisted synthesis.[1]. The surface modifications of HNTs were achieved by using polydopamine. In this process dopamine could self-polymerize to adhere to the surface of HNTs and form a thin active bio-coating. The phenol-formaldehyde was prepared by polymerization of phenol and formalin in alkaline condition. The PF nanocomposites had been synthesized by solution process using surface modified HNTs. The structure of the modified HNT was studied by spectroscopic methods. Results of FT-IR analysis demonstrated that the polydopamine derived species have been covalently attached to the surface of the HNTs. PF/HNT NCs with different contents including 2, 4, 6 and 8 wt% of HNTs were prepared by using sonochemical method.Characterization with FT-IR, powder X-ray diffraction, field emission scanning electron microscopy (FE-SEM), differential scanning calorimetry (DSC) and atomic force microscopy (AFM) confirmed the success in synthesis of NCs with well dispersion properties. XRD analysis results showed that the obtained NCs displayed the amorphous nature. The size of HNTs in NCs are about 50-70 nm as characterized by FE-SEM and AFM analyses[2].

Keywords: Nanocomposites, Phenol formaldehyde, Halloysite nanotubes

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Electronic Structures of [3-(pyridine-2-yl)pyridazine]Ni[4,5-dichloropyridazine] Complex, a Theoretical Investigation

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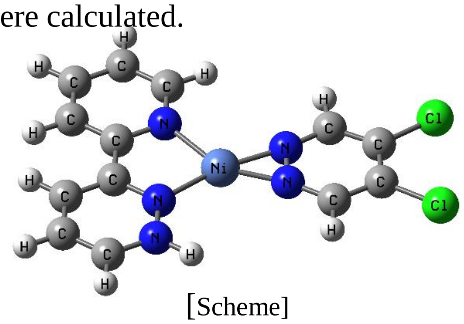
Organometallic complexes [1] consisting of metal atoms, metal clusters, and metal surfaces interacting with organic molecules have been carried out for a long time using conventional chemical synthesis procedure. A fundamental understanding of this interaction, however, is hampered by the fact that one must incorporate the effects of the solvent [2]. The electrostatic potential is widely used in studies on biological systems to predict the reactivity of numerous chemical systems in electro- and nucleophilic reactions [3]. The quantum chemical calculations of [3-(pyridine-2-yl)pyridazine]Ni[4,5-dichloropyridazine] complex were made by Density Functional Theories (DFT) using Becke's three-parameter hybrid functional with 6-31+G* and 6-311+G basis sets and LANL2DZ effecitive core potential [4]. Vibration frequencies were also calculated to the structure with optimized geometry and no imaginary frequency were obtained, so the stationary point correspond to the minima of the potential energy surface. Electronic structure studies were carried out in a DFT method with a B3LYP potential, which is the most complete potential actively used in modern research and showing the best agreement to experiment in the sequence of levels. The restricted Hartree–Fock method was employed for electronic structure calculations of closed-shell complexes, and the unrestricted approximation was used for open-shell complexes. The contributions of atomic orbitals were evaluated from the squares of the diagonal elements of the density matrix. Also, the bond orders and the electronic properties of the [3-(pyridine-2-yl)pyridazine]Ni[4,5-dichloropyridazine] complex were calculated.



[Scheme]

Keywords: [3-(pyridine-2-yl)pyridazine]Ni[4,5-dichloropyridazine] Complex, Quantum Chemical Calculations

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Synthesis and characterization of a Schiff base ligand functinalized Fe_3O_4 magnetic nano-particles

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Magnetic core shell nano-composites are composed of the nano-magnetic core such as magnetite nano-particles(MNPs) and polymeric shells. These nano-composites have the high surface area. furthermore by the chemical modification of polymeric shells, the surface can be functionalized and used for various applications such as drug delivery, magnetic resonance imaging, removal of heavy metals, etc [1-3]. In this work, a novel magnetic core–shell, Fe_3O_4@SiO_2/Schiff base, with Fe_3O_4 spheres as the core and silica Schiff base as the shell, was prepared. Schiff base in this work is a Salen type Schiff base. The surfaces of nano-particles were successfully modified by the suitable deposition of silica onto the nano-particle surface by the ammonia-catalyzed hydrolysis of tetraethylorthosilicate (TEOS). Next, the nano-composite surface was functionalized by 3-amino propyl triethoxy silane (APTES). In the next step, an aldehyde, salicylaldehyde-5-sulfonic acid, was synthesized from salicylaldehyde. Fe_3O_4@SiO_2/Schiff base, was synthesized by condensation reaction between the -NH_2 groups of functionalized MNPs and carbonyl group of the aldehyde. The nano-composite characterized by FT-IR, X-ray diffraction (XRD), scanning electron microscopy (SEM), vibrating sample magnetometer (VSM) and TG analysis.

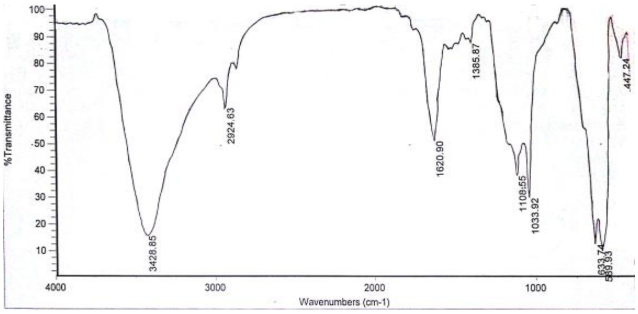

Fig.1 FT–IR spectrum for Fe_3O_4@SiO_2/Schiff base

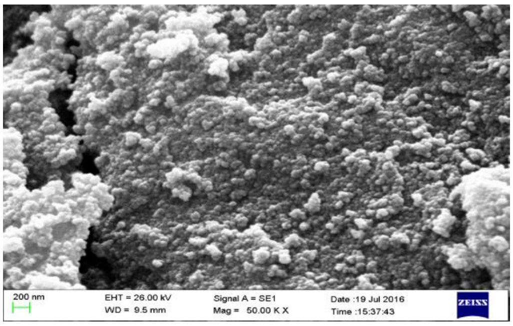

Fig.2 SEM image for Fe_3O_4@SiO_2/Schiff base

Keywords: core shell, nano-composite, Schiff base, magnetite.

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The influence of molar ratio of starting materials on the morphology of CuO nanostructures synthesized by mechanochemical method

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Copper (II) oxide is an important p-type semiconductor oxide with electrical and optical properties. CuO with different morphologies has been successfully synthesized by various techniques [1]. One of the approaches to prepare copper oxide nanostructures is the ball milling or mechanochemical method [2]. In this work, we synthesized CuO in nano scale by utilizing mechanochemical reaction and then calcination procedure. Copper acetate monohydrate and diammonium oxalate monohydrate were used as reagents and the resulting precursor was calcinated at 400 ℃ for 2h in air. Also, we investigated the influence of the molar ratio of starting materials on morphology of obtained CuO. These morphologies of nanorod (Fig. 1-a) and nanowire (Fig. 1-b) were obtained via copper acetate monohydrate and diammonium oxalate monohydrate as the precursor with ratios of 1:1 and 2:3, respectively. The product was characterized using FT–IR, XRD and SEM techniques.

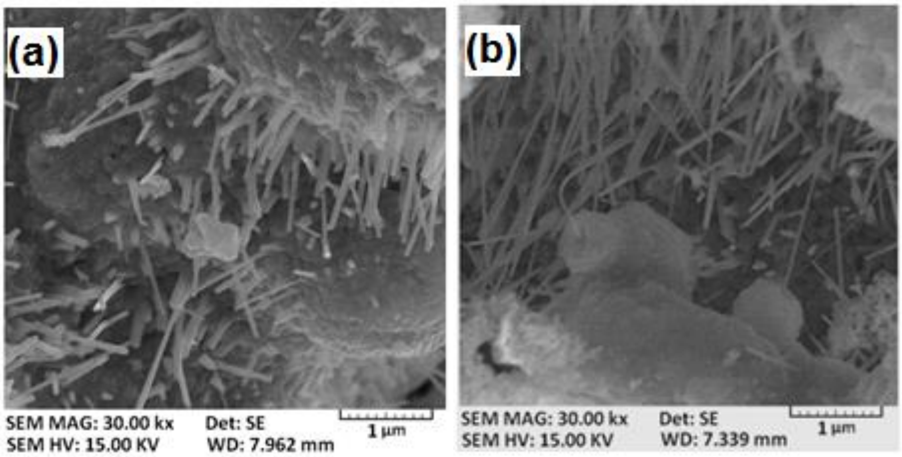

Fig. 1. SEM images of CuO nanrod (a) and nanowire (b).

Keywords: Copper (II) oxide, Mechanochemical method, Nanorod, Nanowire

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Silver-based heterostructured photocatalysts for the degradation of industrial wastewaters

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Ag[1-butyl 3-methyl imidazolium]Br nanospheres were prepared by a coprecipitation method at ambient temperature. The obtained products were characterized by X-ray diffraction (XRD) (Fig. 1), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Diffusion Reflectance Spectra (DRS), the Brunauer−Emmett−Teller (BET) nitrogen adsorption-desorption isotherms, and Fourier Transform Infrared spectroscopy (FTIR) analysis methods. Their photocatalytic properties were evaluated by degradation of Acid Blue 92 (AB92) and rhodamine B (RB) dye solutions under visible irradiation and the results compared with the earlier works [1, 2]. According to the recycling experiments, the samples were able to minimize the concentration of the pollutant after four times of repeated using. To assure the practical capacity, photodegradation of a real wastewater related to the textile industry was studied under same conditions and the results indicated that the concentration of the wastewater decreased efficiently after photocatalytic treatment.

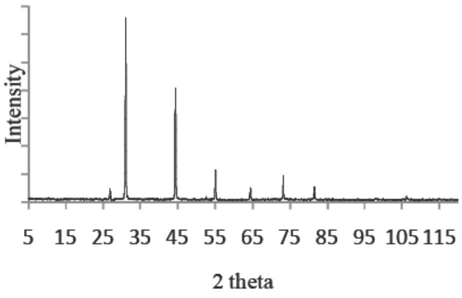

Fig. 1 XRD pattern of the prepared photocatalys

Keywords: Photodegradation, Nanosphere, Ionic liquid, Wastewater, Bacteria

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Silver-based heterostructured photocatalysts for the degradation of industrial wastewaters

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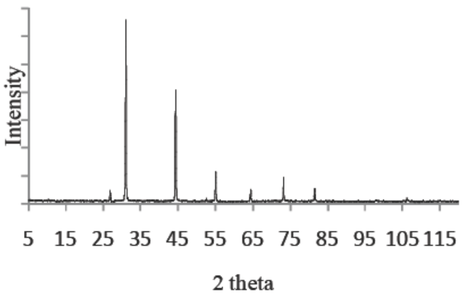
Ag[1-butyl 3-methyl imidazolium]Br nanospheres were prepared by a coprecipitation method at ambient temperature. The obtained products were characterized by X-ray diffraction (XRD) (Fig. 1), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Diffusion Reflectance Spectra (DRS), the Brunauer−Emmett−Teller (BET) nitrogen adsorption-desorption isotherms, and Fourier Transform Infrared spectroscopy (FTIR) analysis methods. Their photocatalytic properties were evaluated by degradation of Acid Blue 92 (AB92) and rhodamine B (RB) dye solutions under visible irradiation and the results compared with the earlier works [1, 2]. According to the recycling experiments, the samples were able to minimize the concentration of the pollutant after four times of repeated using. To assure the practical capacity, photodegradation of a real wastewater related to the textile industry was studied under same conditions and the results indicated that the concentration of the wastewater decreased efficiently after photocatalytic treatment.



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Synthesis and study of structural and photocatalytic properties of pure cerium oxide and Co-doped nanocatalysts

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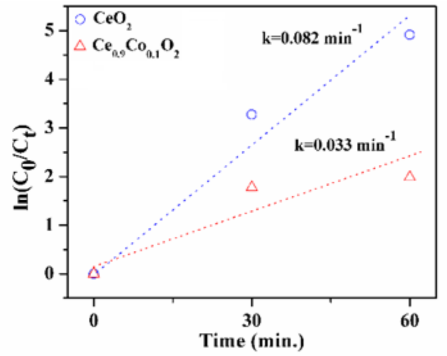
In this research pure cerium oxide and Co-doped nanocatalysts were successfully synthesized by coprecipitation method. Cerium nitrate and cobalt nitrate were used as the starting materials and deionized water as the solvent. The structural properties and morphology of the prepared samples were investigated using X-ray diffraction (XRD) and scanning electron microscopy (SEM) technique. The XRD patterns showed that all the samples had cubic structures without any unwanted phases. The average crystallized size and lattice strain were estimated and calculated using scherrer formula and size-strain plot (SSP) method. The SEM image showed that the particle size is almost spherical with the average size of about 30 nm. Methylene blue was used to investigate the degradation activity of the synthesized samples. Our photocatalytic results indicated that the pure cerium oxide had better degradation activity compared to the Co-doped samples.



Keywords: Nanocatalyst, Cerium oxide, Degradation activity.

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Sonosynthesis and Characterization of TiO_2@ZrO_2 Core-Shell NPs by Sol- Gel Method

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Nano TiO_2@ZrO_2 core-shell was synthesized by two steps method. First, TiO_2core was prepared via hydrothermal method and then ZrO_2shell layer was covered on core via sol – gel by ultrasonic irradiation. The precursor of TiO_2 and ZrO_2 are Titanium tetra isopropoxide TTP and zirconium terta chloride. The magnitude and time of ultrasonic radiation were affected on size and morphology of nanoparticles ZrO_2 .In this research, we were investigated application of ultrasonic irradiation is important and optimum time is 30 min.

The synthesized TiO_2@ZrO_2 core-shell NPs was characterized by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Field emission scanning electron microscopy (FESEM) and Emission X-ray dispersive analysis (EDX) . Structural characterization by XRD confirmed the formation of the anatase phase of TiO_2 and high crystalline tetragonal zirconia. The crystallite size of TiO_2@ZrO_2 core-shell NPs was estimated to be 17 nm, by using the Deby-Scherrer equation. The FT-IR analyses indicated that the positions of peaks related to Ti-O and Zr-O absorption bands. In addition, FESEM images indicated the uniform morphology of the NPs and the average particle size of NPs is 33 nm. . EDX analysis exhibited the elemental percentage of nanostructure.[1-3]

Keywords: Core-Shell, Hydrothermal, Sol- gel, TiO_{22}, ZrO_2

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Green synthesis of CuO nanoparticles using Cystoceira and Padina brown algae

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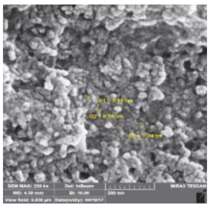
CuO nanoparticles have found some applications as catalyst, semiconductor, superconductor and lubricant [1, 2]. They have also found some application in electronic and optical devices. CuO nanoparticles have been prepared by various methods. Green synthesis is one of the uncommon methods, introduced recently for the preparation of nanaparticles. Many of biological systems, including algae and microorganisms have been used for the preparation of nanoparticles. Green synthesis has many advantages including lower price, environmental friendly, renewable, pharmaceutical adaptation, biomedical application and easy to use in large scale synthesis**.** In this work, green synthesis of CuO nanoparticles have been performed using Cystoseira and Padina brown algae,that are abundant at Persian Gulf off-shores. Chemical compounds in these algae could be used as stabilizer against the aggregation of CuO nanoparticles. CuSO4 and Cystoseira or Padina brown algae extract were used for the preparation of CuO nanoparticles at basic condition**.** CuO nanoparticles were characterized by XRD and FESEM methods. XRD pattern showed that CuO is pure, single phase with monoclinic crystal structure. The crystal size was 5.2 and 4.2 nm for the nanoparticles produced by Cystoseira and Padina extracts respectively. Both are in the domain of quantum dot. CuO nanoparticles were black and FESEM images show that they are spherical particles. CuO nanoparticles were insoluble in water and ammonium hydroxide solution. The prepared CuO nanoparticles showed good photocatalytic activity for degradation of malachite green dye in water at sun light.



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Keywords: CuO nanoparticles, Algae, Green synthesis

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Metal oxide/Zeolite composites as the active catalysts for dehydrogenation of ethylbenzene to styrene process

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Zeolites are crystalline aluminosilicates with regular and uniform porous structures. In these materials, Si/Al molar ratio can be varied from 1 to ∞; so highly hydrophobic aluminum-free synthetic zeolites can also be attainable .Thanks to the development of the synthetic techniques, there are grated many synthetic zeolites with different compositional elements and frameworks. Other elements, especially transition metals, can incorporate into the zeolite framework such as Fe,Cr,Mn&etc. In this speech, synthesis and characterization of Nano Fe_2O_3/Zeolite composites are presented. Styrene (ST) is one of the most essential materials in the petrochemical industry for production of synthetic polymers and plastics. The most conventional process for the commercial production of styrene is ethylbenzene (EB) dehydrogenation by the K−Fe-based catalysts with high iron loading in the presence of a large amount of superheated steam at a high temperature of 600−650 °C. However, this traditional process has many disadvantages such as high energy consumption and thermodynamic equilibrium limitations. Hence, a worldwide investigation of the alternative process is being considered. Recently, as a substitute for steam, CO_2 gas has received great attention as a co-feed gas for dehydrogenation of ethylbenzene. The presence of CO_2 in the ethylbenzene dehydrogenation reaction suppresses coke formation and also helps remove the carbonaceous deposits.

This investigation introduces novel composites of Fe_2O_3/ K-metalosilicate with high performance in oxidative dehydrogenation (ODH) of ethylbenzene to produce styrene with CO_2. Regarding K-metalosilicate as catalyst support, various amounts of iron oxide nanoparticles (γ-Fe_2O_3) were introduced into porous support by different methods such as solid-stated dispersion (SSD),hydrothermal,sol gel and… in order to enhance catalytic activity. The prepared samples were characterized by

X-ray diffraction (XRD), scanning electron microscopy (SEM) coupled with the energy dispersive analysis–EDX, and N_2 physical adsorption analysis.The high performance of catalytic activity of the composites in ethylebenzene dehydrogenation process can be attributed to the synergistic effect of transition metal oxide ,K^+ and Fe^{3+} ions in the structure of catalysts.

Synthesis and characterization of iron oxide magnetic nanoparticles coated with curcumin and DNA binding studies

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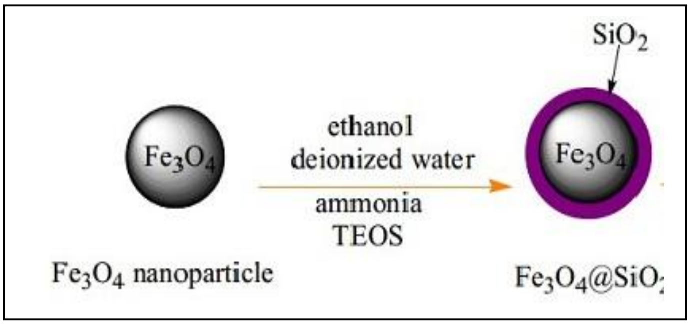
Curcumin (CUR), a natural polyphenol component extracted from the underground rhizome of tumeric, has gained a considerable attention recently because of its multiple pharmacological activities, including anti-inflammatory, antioxidant, anti-bacterial, antiviral activities and especially wide spectrum of actions against tumors [1,2]. In the present work, the synthesis, characterization and DNA binding study of Fe_3O_4@SiO_2-Curcumin magnetic nanoparticles (MNPs) were undertaken.The Fe_3O_4 nanoparticles were synthesized via chemical co-precipitation and coated by silica according to sol-gel method [3]. Then, the surface of the Fe_3O_4@SiO_2 MNPs, was modified by an antioxidant agent, curcumin, to obtain new magnetic nanoparticles for biological applications.The MNPs were subsequently characterized by fourier transform infrared (FT-IR) spectroscopy, According to FT-IR data, the MNPs were successfully coated with SiO_2 and Curcumin drug. Transmission electron microscopy (TEM) was used to verify particle size and morphology of the Fe_3O_4@SiO_2-Curcumin MNPs. Finally, biological applications of the Fe_3O_4@SiO_2-Curcumin MNPs were investigated in vitro (DNA-binding study). The interactions between the Fe_3O_4@SiO_2-Curcumin MNPs with calf-thymus DNA (ct-DNA) were studied by uv-vis spectroscopy.



Keywords: Curcumin, Fe_3O_4@SiO_2, DNA

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Fluorometric studies of DNA interaction with iron oxide magnetic nanoparticles coated with riboflavin and zidovudine drug

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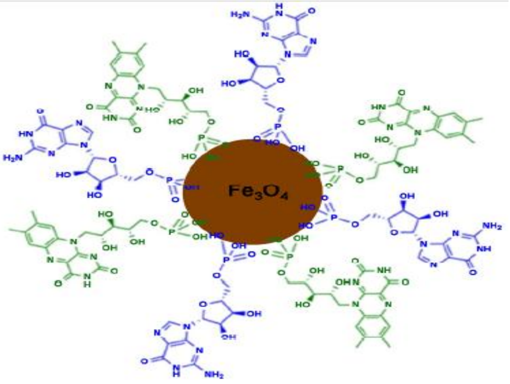
Riboflavin is an essential vitamin for cellular metabolism and is highly upregulated in metabolically active cells. Consequently, targeting the riboflavin carrier protein (RCP) may be a promising strategy for labeling cancer and activated endothelial cells. Therefore, ultrasmall super paramagnetic iron oxide nanoparticles (USPIO) coated with SiO_2 were adsorptively coated with the endogenous RCP ligand Riboflavin and Zidovudine as an antiviral drug, which renders them target-specific and fluorescent. The core diameter, surface morphology and surface coverage of the resulting Riboflavin-coated USPIO (Fe_3o_4@sio2-ribo-zido MNPs) were evaluated using a variety of physicochemical characterization techniques (TEM, IR, and fluorescence spectroscopy) [1]. Zeta potential measurements revealed particulate morphology approximately 180-182 nm in size in water. According to FT-IR data, riboflavin and Zidovudine were successfully loaded on the MNPs. The interactions between Fe_3O_4@SiO_2-ribo-zido MNPs) and calf-thymus DNA(ct-DNA) were studied by using uv-vis absorption methods.



Keywords: Riboflavin, Fe_3O_4@SO_2, Zidovudine, DNA interaction, Nnoparticles.

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بعد از دریافت ایمیل فعالسازی با کلیک روی لینک ارسال مقاله وارد بخش اعضا شده و با وارد کردن نام کاربری و رمز عبور وارد صفحه کابری خود می شوید. گزینه سامانه ارسال مقاله را انتخاب کرده و نوشتار(مقاله) جدید را کلیک می کنید. به ترتیب گزینه های اطلاعات مقاله، مولفین، پیشنهاد داور را تکمیل کرده و وارد مرحله فایل ها می شوید در این قسمت در قسمت نوع فایل با توجه به اینکه فایل ارسالی word یا pdf است را انتخاب می کنید سپس عنوان را وارد کرده و فایل مورد نظر را بارگذاری می کنید. با توجه به اینکه هر دو فرمت word و pdf را باید ارسال کنید هر دو مرحله باید اجرا شود و در انتها ثبت مقاله را کامل می کنید.

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Green synthesis of copper oxide nanoparticles using extracts of Garlic

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In recently, Researchers have been interested to find a safe and environment friendly method to reduce metal ions into metallic nanoparticles (NPs) due to the damaging effects of the chemicals on human health and the environment. The preparation of NPs is using extracts of various parts of plants such as roots, peels, leaves and fruit is a clear and nontoxic method [1]. Garlic is composed of carbohydrates, sulfur and phenolic compounds, and amino acids [2]. Garlic also has antibacterial properties and high biocompatibility. Copper oxide Nps are very good catalysts. They also have electrical properties, nano-fluid, and anti-bacterial activities [3].

In this work, dried powder of garlic was soaked in ethanol-water (50%) with ratio 5:1 for two days in absent of sunlight. After separation of the extract solution by centrifuge is stored at 4 ºC in refrigerator.

The CuO NPs was obtained from the reaction of $CuSO_4.5H_2O$ and garlic extract at 80 ºC for 3h. These NPs was characterized by common methods such as FT-IR spectra, XRD patterns, UV-Visible spectroscopy.

A band observed at 383 nm in UV-Vis. spectra of solution is due to surface plasma resonance of CuO NPs [4]. The XRD patterns of CuO NPs are shown ten peaks at 32.6, 35.6, 38.7, 48.4, 58.3, 61.5, 65.2, 67.8 72.4 and 75.1 º that was corresponded with JCPDS: 80-1916 [5]. The average size of CuO nanoparticles are calculated 40-50 nm by Deby-Scherrer equation from XRD patterns. The FT-IR spectra as-synthesized CuO NPs are shown a band at 525 cm^{-1} is due to stretching vibration of Cu-O bond [6].

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Green synthesis and characterization of CuO nanoparticles using extracts of Pomegranate peel

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A new method has been introduced, known as green synthesis due to the damaging effects of chemical materials on human health and environment. This method use plant extracts to synthesis of nanoparticles (NPs). Moreover, plant extracts have antioxidant property, and they can reduce metal ions into metal NPs [1]. Green synthesis of metal oxide NPs by microorganisms is one of the most important branches in nano-biotechnology [2]. Green synthesis can eliminate dangerous chemicals reagent from products that are more acceptable than traditional methods [3]. Different parts of pomegranate have high antioxidant which acts as reducing agent and stabilizer operate copper oxide NPs [4]. These NPs that are produced in this method have high antibacterial property.

In this work, the pomegranate extract was obtained by heating the pomegranate peel in hot water at 80 ºC for 6 h. In the next step, CuO NPs was obtained by adding an extract into the $CuSO_4.5H_2O$ solution and heating up the mixture at 90 ºC for 3 h. These Nps were characterized by common methods such as UV-Visible spectroscopy, XRD patterns and FT-IR spectra. The FT-IR spectra as-synthesized CuO NPs are shown a band at 540 cm^{-1} is due to stretching vibration of Cu-O bond [6]. The XRD patterns of CuO NPs were corresponded with JCPDS card: 80-1916 [7]. The average size of CuO NPs are calculated 38-55 nm by Deby-sherrer equation from XRD patterns [5]. A band observed at 398 nm in UV-Vis. spectra of solution is due to surface plasma resonance of CuO NPs [5].

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Cu (I) Complexes of Dihydrobis(2-mercapto-benzimidazolyl)borate and Dihydrobis(2-mercapto-benzothiazolyl)borate Ligands: Structural, Photophysical and Computational Studies

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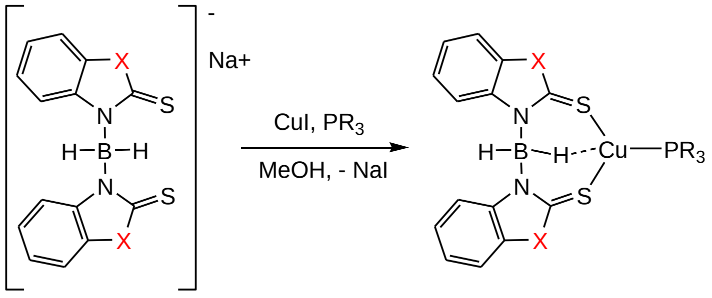
Since the discovery of Trofimenko's "scorpionate" ligands in 1966 [1], known as [hydrotris(pyrazolyl)borate], there has been great interest in their chemistry and application. These ligands could influence the properties of the transition metal center without getting directly involved in metal complex's reactivity. This view of the scorpionate ligands changed following the introduction of a new more flexible scorpionate ligand, [hydrotris(methylimidazolyl)-borate] or Tm, which is based upon a *N*-methyl-2-mercaptoimidazol-1-yl ring system. Newer scorpionate ligands have major differences compared to the Trofimenko's original ligand set [2]. They are more flexible and they are based on soft sulfur donor atoms. The flexibility of these ligands allow for B-H activation and in some instances formation of metalloboratranes. As our contribution to this field, we have developed some copper (I) complexes, supported with these ligands and phosphine donor ligands. Due to affinity of soft copper (I) ions to sulphur and phosphine ligands, the resulting complexes are highly stable and show interesting photophysical properties. We have synthesized eight copper (I) complexes with this ligand set and they are characterized fully with ^{1}H& ^{13}C NMR spectroscopy and single X-ray crystallography, whenever possible. Photophysical properties of these complexes, which is highly dependent on the nature of the phosphine ligands, will also be discussed.



NaBB; X = N-H

NaBB-2; X = S

PR_3 = Alkyl Phosphines

Keywords: Trofimenko, Scorpionate, pyrazolyl borate, metalloboratrane

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Palladium (II) Complexes Based on Schiff Base Ligands Derived from *ortho*-Vanillin and Study of Their Anti-cancer Properties

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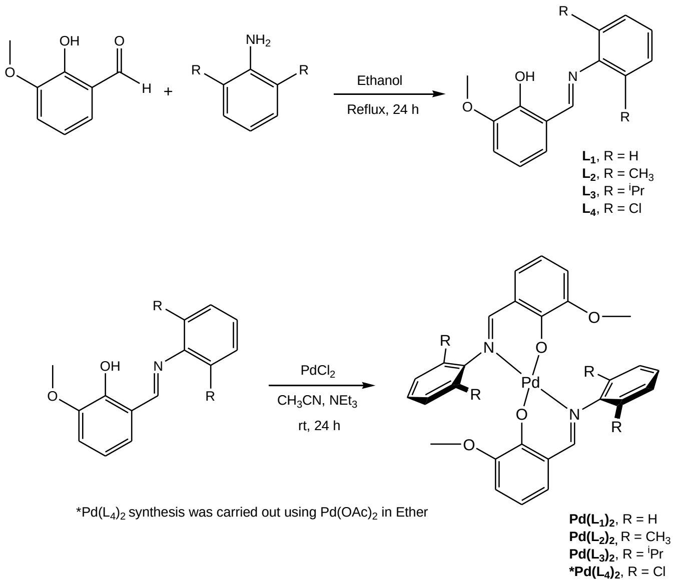
Medicinal inorganic chemistry has grown significantly in the last two decades following successes with platinum based metallodrugs in clinical tests against certain cancer cells [1]. However, side effects of *cis*-platin has prompted search for alternative metal based drugs in fight against various types of cancers with less side effects and better cytotoxic properties compared to *cis*-platin [2]. As our contribution to this field, we have developed L_{1-4} ligands, shown in Scheme below, and their corresponding palladium complexes [$Pd(L_{n)2}$, n=1-4]. The geometries of the [$Pd(L_n)_2$] complexes were derived from single X-ray crystallography experiments. The central Pd(II) ion adopts a square planar geometry. FT-IR, ^1H, ^{13}C NMR and single X-ray crystal structures are reported. The cytotoxicity effect of four Pd(II) complexes was assessed on three cancerous cell lines and the results compared with that for *cis*-platin. One out of four metal complexes, **$Pd(L_1)_2$**, exhibited the highest anti-proliferative activity on three investigated cancerous cells lines which is even better than *cis*-platin.



*$Pd(L_4)_2$ synthesis was carried out using $Pd(OAc)_2$ in Ether

Keywords: Metallodrug, *cis*-platin, *ortho*-vanillin, apoptotic effect, Annexin V

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The Investigation of the Reactivity of a Platinum Complex Precursor with a Borate Based Ligand

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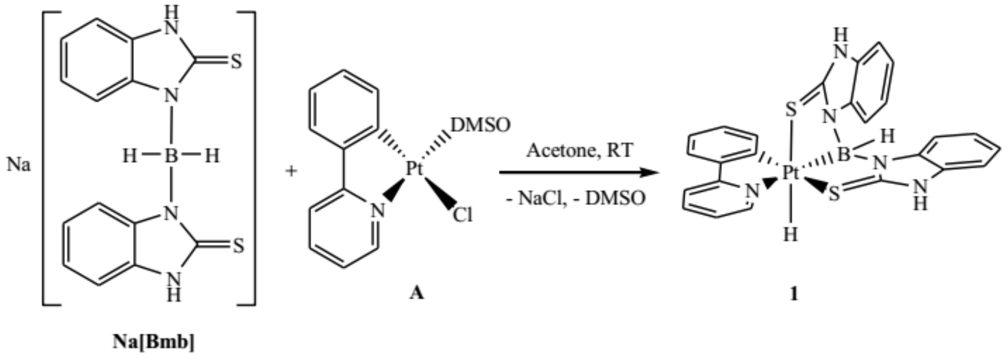
Trofimenko’s poly(pyrazolyl)borates recognized as "Scorpionate ligands" have undergone numerous modifications since their discovery decades ago [1]. Notable among these changes have been the addition of an extra atom or atoms between boron bridgehead and scorpionate's donor atom as well as changes in the nature of the donor atom such as the use of softer sulfur or phosphorous electron donors in place of nitrogen. These structural alterations have introduced more flexible scorpionates, thus allowing closer proximity of B–H or BH_2 units of the scorpionate ligand to the metal center with an increased likelihood of an intramolecular metal–boron interaction [2]. Recently, we discovered the unexpected and facile formation of a platinum hydride complex {[(κ^3-S,B,S-HB(mb)$_2$]Pt(ppy)H}, **1**, ppy = 2-phenylpyridine and mb = 2-mercapto-benzimidazole, from the acetone mediated reaction of [Pt(ppy)(DMSO)Cl], **A**, with sodium dihydrobis(2-mercapto-benzimidazolyl)borate Na[H_2B(mb)$_2$]. The aerobic hydrolysis of complex **1** led to the formation of a dimeric half-lantern platinum(II,II) complex [{Pt(ppy)(μ_2-mb)}$_2$], with simultaneous release of 2-mercaptobenzimidazole boronic acid.



Keywords: Hydride complex; Platinum; Borate ligand; Structural analysis; Metallaboratrane.

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$ZrCl_4$ Mediated Synthesis of Some 3,3'- Bisindolyl(aryl)methanes and Study of Their Photophysical Properties

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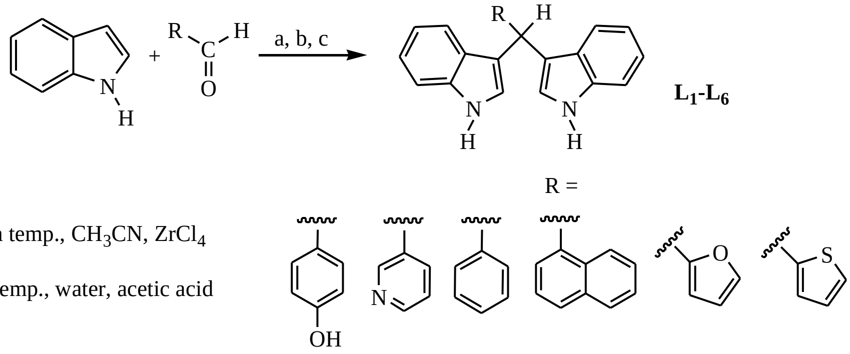
3,3'-bisindolylmethane (R = H, scheme shown below), the simplest form of a bisindol, is known to have diverse biological activities such as anti-cancer, anti-bacterial, and anti-inflammation [1]. Besides, this compound and its derivatives are used as intermediates in the synthesis of many organic compounds with pharmaceutical importance [2]. On the other hand, derivatives of 3,3'-bisindolylmethane with an aryl group on tetrahedral carbon atom bridging between two indole rings, commonly referred to as 3,3'-bisindolyl(aryl)methane, due to their affinity to a variety of metals and anions such as copper (II) and fluoride ions have found applications as colorimetric sensors.[7-10] Similar binding capability of these compounds to common protic and non-protic organic solvents and their dramatic color changes due to solvation of their ground or excited states have led to the development of simple and highly efficient solvatochromic combinations [3]. In this study, successful synthesis of a series of 3,3'-bisindolyl(aryl)methanes by modification of a previously reported synthetic method in the literature is reported. Main research goals included a detailed structural characterization of the products by means of NMR spectroscopy and X-Ray crystallography, and understanding the role of aryl substituent on the photophysical properties of these compounds.



a, b, c (except L_4) = room temp., CH_3CN, $ZrCl_4$

a, b, c (L4 only) = room temp., water, acetic acid

Keywords: Bisindolylmethane, anti-inflammation, solvatochromic, photophysical

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Enhancing acidic properties of supported solid acid catalysts: A new method for anchoring two acidic sites on the surface of $Fe_3O_4@SiO_2$

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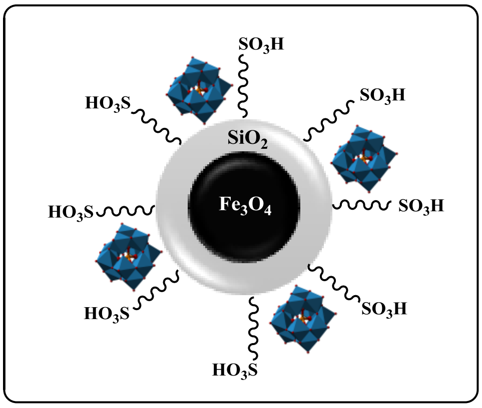
In recent years, different types of solid acid catalysts have been developed, and each type of these catalysts exhibited their unique catalytic activity. Among these synthesized catalysts, a catalyst with two distinct acidic sites which could be separated easily from the reaction mixture is promising. In order to reach this purpose, we prepared a solid acid catalyst based on silica coated magnetite nanoparticles with two kinds of bronsted acidic sites, sulfonic acid groups and phosphotungestic acid species. These functional groups were characterized by FT-IR spectroscopy and CHNS elemental analysis. Vibrating sample magnetometry (VSM) and X-ray diffraction (XRD) analyses were used to identify its magnetic properties and crystal phase, respectively. Also shape and size determination of these nanoparticles were performed by transmission electron microscopy (TEM). The prepared catalyst showed very good activity in the esterification of acetic acid with butanol. Conversions up to 70% of butanol and 100% selectivity toward the ester were reached after 8 h. The results exhibited that this catalyst with double acidic groups is promising solid acid catalyst to be used in the esterification of carboxylic acids with alcohols.



Keywords: Magnetite nanoparticles, Sulfonic acid, Phosphotungestic acid, Esterification.

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Hydrophobic and hydrophilic effects in different heterogeneous acid catalysts for the esterification of acetic acid with butanol

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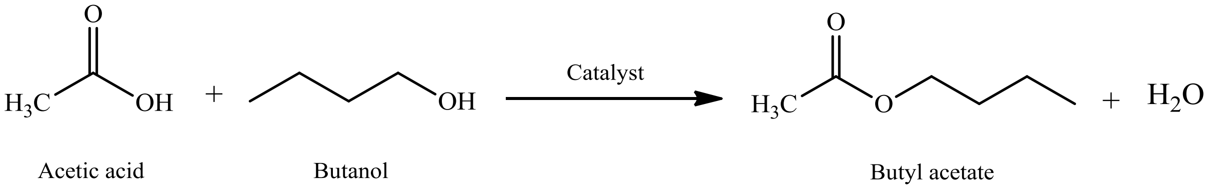
The catalysts used for the esterification reactions require hydrophobicity to avoid strong adsorption of water. Since the reaction involves highly polar reactants (or products) such as acids, alcohols, and water, leaching of the active components to the liquid phase is an important factor for designing the proper catalysts. For this aim, we used three kinds of supports with different surface characteristics such as silica coated magnetite nanoparticles (SCMNPs), MCM-41 and activated carbon (AC) for immobilizing sulfonic acid groups. These solid acid catalysts were characterized by various physicochemical methods such as FT-IR spectroscopy, SEM analysis and CHNS elemental analysis which showed that the sulfonic acid groups have been attached successfully to the surface of these supports. Then, they were utilized in the esterification reaction between acetic acid and butanol in order to investigate the hydrophobicity and hydrophilicity effects on their efficiency. It has been found that among these solid acid catalysts, the catalyst with hydrophobic support (AC) exhibits more than 99 percent of butyl acetate production whereas the other two hydrophilic catalysts show less efficiency. The reusability of these catalysts was also investigated and showed three cycle stability for acetic acid esterification without significant loss of activity.



Keywords: Solid acid catalyst, Sulfonic acid, Hydrophobicity, Hydrophilicity, Esterification.

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Highly efficient removal Methylene blue from waste water by Magnetic Nanoparticle Fe-Ce-Mn-O adsorption

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Dyes usually have a synthetic origin and complex aromatic molecular structures which make them more stable and more difficult to biodegrade [1]. There are many dye waste water treatment methods available, Adsorption has attracted our attention owe to its many advantages [2]. As part of our research program, we now focus on removal of Methylene blue (MB) in waste water by magnetic Nanoparticles Fe–Ce–Mn–O were prepared by co-precipitation high temperature method. In Fig.1 was shown that the majority of MB was removed in the first 15 min. the adsorbent showed good ability of removing the cationic dyes from waste water.

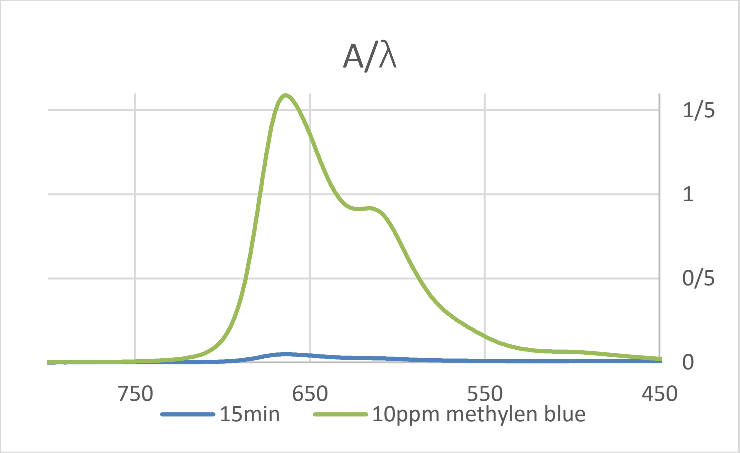

Fig. 1. UV-Vis spectra of Fe-Ce-Mn-O

Keyword: Nanoparticles, Adsorption, Methylene blue, water treatment

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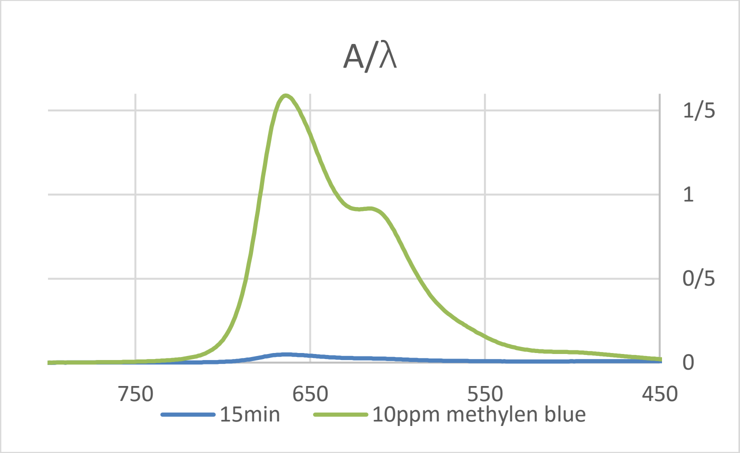

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Synthesis and characterization of Ni-Cr-Al LDH and its sensing behavior

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In recent years, layered double hydroxides (LDH), also known as anionic or hydrotalcite-like clays, have growing interest for using in the wide fields owing to their attracted desirable properties, which include good biocompatibility, intense adsorbaility, high catalytic activity, low cost, and high chemical stability. Ni–Cr-Al layered double hydroxide was synthesized by the co-precipitation method in constant pH, at various temperatures and various Ni^{2+}/Cr^{3+} / Al^{3+} molar ratios in H_2O [1]. The samples (LDHs) characterized [2-3] by powder X-ray diffraction and TEM. Then its sensing properties were investigated at room temperature. Desirable properties for a sensor include high sensitivity, low detection limit, good reproducibility, long-term stability, fast current response, and low interference.

Keywords: : LDH, Layered double hydroxide, coprecipitation, sensor

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Preparation and characterization of Fe-Ni oxide Nanoparticles based on Nano Alumina prepared by Co-precipitation method and the study of the effect of Aging condition on the structures

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Ferrit nickel is one of attracting materials due to their properties such as low melting point, high specific heating, large expansion coefficient and low saturation magnetic moment [1,2].It has many technical applications such as in photoelectric devices, catalysis, sensors, nano devices, microwave devices and biomedical applications like drug delivery and hyperthermia [3,4]. In this research nan crystalline ferrit nickel was prepared via co-precipitation method.0.16M solution of sodium carbonate (as precipitating agent)was slowly added to salt solution of 0.02M ferric nitrate and 0.017M nickel nitrate and 0.02M nano alumina as substrate. Consider aging condition at different times (2, 4, 6, 8, 10, 12 hours), dried at 120^{0}c for 4 hours and calcinated at 550^{0}c for 4 hours. X-ray diffraction (XRD) indicated that Fe_3O_4 (cubic), Fe_2O_3 (cubic), NiO (monoclinic), $NiFe_2O_4$ (cubic) and Al2O3(Rhombohedral) have grown respectively in the pages (311), (110), (111^{-}), (311) and (104). The particles size in the SEM were between 27.51-45.76nm.The result of (EDX) analysis showed the present of Fe, Al, O, Ni in the samples. All of the products were superpara magnetic. The result showed that the 4 hours aging is the best time.

EDX analysis	FE-SEM information		XRD information		Aging conditions	samples
Elements	morphology	Average nano particles size	Average crystal size	Phases		
O,Fe,Ni,Al	spherical	41.3	35.38	NiO,Fe_3O_4,$NiFe_2O_4$,Al_2O_3, Al_2FeO_4,Fe_2O_3	2	S1
O,Fe,Ni,Al	spherical	31.41	7.26	NiO,Fe_3O_4,$NiFe_2O_4$,Al_2O_3, Al_2FeO_4,Fe_2O_3	4	S2
O,Fe,Ni,Al	spherical	40.54	8.2	NiO,Fe_3O_4,Al_2O_3,$Al_3Fe_5O_{12}$	6	S3
O,Fe,Ni,Al	Layer-layer	27.51	9.85	NiO,$NiFe_2O_4$,Fe_3O_4,Al_2O_3, Al_2FeO_4	8	S4
O,Fe,Ni,Al	spherical	45.76	43.67	NiO,Fe_3O_4,Al_2O_3,FeO,$FeNi_2O_4$,Fe_2O_3	10	S5
O,Fe,Ni,Al	spherical	34.97	34.5	NiO,$NiFe_2O_4$,Fe_3O_4,Fe_2O_3,Al_2O_3	12	S6

Keyword: Co-precipitation, Nanoparticles, X-ray diffraction

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Co-Precipitation method for synthesis of Fe-Ni oxide Nanoparticles supported by Nano Alumina and Investigation of the Calcination conditions on their Structures

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In this study, Nano particles Fe-Ni oxide was synthesized with Co-precipitation method. The nanoparticles synthesis in various time and different temperatures of calcination conditions. The synthesized particles were characterized by X-ray Diffraction (XRD), Field Emission Scanning Electron Spectroscopy (FESEM), Energy-dispersive X-ray Spectroscopy (EDS). According to the XRD pattern, products were crystallized and structure was cubic. The crystal size ranged from 10-30 nm. Because of the obtained Fe_3O_4, NiO and $NiFe_2O_4$ compounds and the smaller particles the best time and temperature of calcination was 6 hours and $550C^0$.

Keywords: Co-precipitation; Calcination; Alumina; Fe-Ni Nanoparticles

Post-Synthesis Functionalization of Hollow Mesoporous Silica Nanospheres for an Anticancer Drug Delivery system

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Recently, hollow mesoporous silica nanospheres (HMSNs) have been studied as potential drug carrier materials as a result of their unique properties, such as large internal void space and well-ordered mesoporous shell pore channel. In this study, glycine functionalized hollow mesoporous silica nanospheres (gly-HMSNs) were successfully synthesized by a post-synthesis process. The prepared samples were characterized by FTIR, SAXS, N_2 adsorption-desorption, SEM, TEM and thermograviametric analysis techniques. The effect of the surface functionalization on the adsorption capacity and release profile of cisplatin (as an anticancer drug) was investigated. We found that the surface functionalization of HMSNs increases the loading capacity of drug. Moreover, release tests performed at two times in phosphate buffered saline (PBS, pH of 7.4) media showed a sustained and controlled release of cisplatin from the synthesized gly-HMSNs. The cytotoxicity effect of the as-synthesized gly-HMSNs was carried out in MCF-7 cell lines by MTT assay and the data proved that this material have a negligible toxicity. This results indicated that this support could be effective carrier for anticancer drug delivery systems.

Keywords: hollow mesoporous silica nanospheres (HMSNs), drug release, cytotoxicity, cisplatin

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Novel Nanocomposites of Graphene & Graphene Oxide: Synthesis, Spectral Properties and Microbial Studies

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Abstract

4 novel Graphene oxide(GO) and Graphene (Gr) based hybrid nanocomposites; graphene oxide/silver(GO/Ag) (1), Graphene oxide/pyrazole (GO/PYZ), Graphene oxide/3,5-dimethylpyrazole (GO/DMP), Graphene oxide/pyrrole (GO/PYR) (2), graphene/silver (Gr/Ag) (3)and Graphene/Silver – pyrazole (Gr/Ag – PYZ), Graphene/Silver – 3,5-dimethylpyrazole (Gr/Ag–DMP), Graphene/Silver–pyrrole (Gr/Ag–PYR) (4) were synthesized via Staudenmaier method. Graphene oxide composites were synthesized by using sodium citrate as a green reducing agent *via* the hydrothermal method. The synthesized composites were characterized by FT-IR, X-ray powder diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM) and Energy dispersive X- ray analyzer (EDXA). The antibacterial and antifungal studies of the compounds against Gram-positive, Gram-negative bacteria and fungi were carried out using the filter paper disk method. Imipinem, clindamycin, cefixime, nystatin and miconazole were used as standards for comparison.

1. Introduction

Graphene (Gr) is a two-dimensional extended honeycomb network of sp^2 hybridized carbon atoms [1].Many methods have been developed to produce large quantities of graphene sheets precisely[2-4]. One of the most promising methods is to use graphene oxide (GO) synthesized by the oxidation of graphite. Most of the properties of graphene are reportedly recovered by reduction of GO. Furthermore, GO itself is considered as a good candidate for use in the composite materials that exhibiting good electrical and gas-adsorbing properties [5-7].

GO has various oxygenated functional groups (hydroxyl, epoxide, and carbonyl groups) on its basal plane and edge [8-11]. The oxygen functional groups of GO can interact with many different functional groups or particles [12-14]. GO-based composite materials have been introduced for various applications such as electrochemistry, optoelectronic devices and lithium ion batteries [15,16]. In addition, GO and GO-based composites have been considered as new hydrogen storage media due to their large surface-to-volume ratio and intrinsically lightweight. For example, it was proposed that GO has the potential to become an ideal substrate for hydrogen storage [17] and that GO layers can be used as the building blocks for potentially useful hydrogen storage materials [18]. The functionalization of metal nanoparticles on the graphene based surfaces produces new hybrid materials which have potential importance in the areas such as optics, electronics, catalysis and sensors [19]. The biological studies of graphene and its composite materials are relatively limited. However, recent attention has been drawn towards the antimicrobial activities of graphene and its composites materials [20-22]. Shen et al. reported the Ag-chemically converted graphene (CCG) nanocomposite shows very good antibacterial activity against Colibacillus, S. aureus and C. albicans [20]. Ag-CCG shows a high asepsis ability and completely destroys the bacterial cultures. Silver (Ag) is a marvelous material for its distinctive properties, such as good conductivity, chemical stability, catalytic activity and antimicrobial activity [23]. Here, we report the syntheses of some GO-based hybrid nanocomposites and characterization of them by FT-IR, XRD, SEM, AFM and EDXA. Some compounds were also screened for their biological activities.

2. Experimental

2.1. *Materials and Instrumentation*

Graphite flakes were purchased from Sigma-Aldrich with a particle size of 150 µm (99.9% purity). All of the solvents and materials were analytical grades, commercially available and used without further purification. Infrared spectra were recorded as KBr disks on Tensor 27 Bruker spectrophotometer. The evaluation of GO and synthesized nanocomposites were monitored by powder X-ray diffraction Philips PW 1800 diffractometer with Cu Kα radiation. Atomic force microscopy was carried out on a Denmark Dualscope/RasterscopeC26 DME microscope. Scanning electron microscopy measurements was performed on a VEGA\\TESCAN at an accelerating voltage of 15 kV.

2.2. Preparation of GO nanosheets

Graphene oxide (GO) was prepared according to the staudenmaier method [24]. Concisely, a mixture of concentrated sulfuric acid and nitric acid (3:1, v/v) was mixed with graphite flakes at room temperature and stirred continuously for 4 days. The acid-treated natural graphite was filtered and the collected powder was washed thoroughly with water until the solution became neutral. The powder was dried at 60˚C in oven to remove the remaining moisture. Accordingly, the black powder graphite oxide was obtained [25]. The graphite oxide powder was immersed in an aqueous solution of alcohol inside an ultrasonic bath for 2 h. Finally, a homogeneous GO aqueous dispersion was obtained and used for the further preparation of GO/Ag and GO/Pyrazole, GO/3,5-dimethylpyrazole and GO/Pyrrole nanocomposites.

2.3. Preparation of GO/Ag (1)

The GO/Ag was prepared in one step reaction. In a typical procedure, 2×10^{-3} and 4×10^{-3} mol/dcm^3 $AgNO_3$ was added to 10 ml of GO in ethanol solution. The mixture was stirred for 30 min and 1 ml $NaBH_4$ was added dropwise to a mixture with continuous stirring for 5 h. Finally the products were washed with ethanol and the resulting GO–Ag was dried in a vacuum oven and named GO/Ag-1, GO/Ag-2 respectively.

2.4. Preparation of X- doped GO nanocomposite (2)

GO (0.06 g) and X (0.03 g) (X =pyrazole^1, dimethylepyrazole^2, pyrrole^3) were added to a 1:1 solution of ethanol/water at room temperature. The mixture was stirred for an hour; then ammonium persulfate (APS) (0.024 g) was added to the mixture and stirring was continued for two days. Eventually, the products were washed with ethanol and water and resulting GO–X were dried in a vacuum oven and named GO/PYZ, GO/DMP, GO/PYR respectively. The products were characterized by SEM, XRD and EDXA.

2.5. Preparation of Gr/Ag (3)

The Gr–AgNPs were synthesized by different dosage of $AgNO_3$. Briefly, citric acid (0.48 g) and $AgNO_3$ (0.44, 0.22 and 0.15 g) were added to graphene in water mixture (0.5 g). The mixture was stirred at 100℃ for 30 min. The pH of the mixture was adjusted to 8 by addition of ammonia solution. The mixture was then dried at 100℃ in a vacuum oven for 3 hours. The products were characterized by AFM method.

2.6. Preparation of X- doped Gr/Ag nanocomposite (4)

GO (0.06 g) and X (0.03 g) (X =pyrazole^1, dimethyle pyrazole^2, pyrrole^3) were added to a solution of ethanol and water in 1:1 volume ratio and stirred for an hour. Then APS (0.024 g) was added to the mixture. A The mixture was stirred for 2 days and then the product was washed with ethanol and water. The resulting powders of Gr/Ag–X(Gr/Ag–PYZ, Gr/Ag–DMP, Gr/Ag–PYR) were dried in a vacuum oven at 65℃. The products were characterized by SEM, XRD and EDXA.

3. Biological study

The in vitro antibacterial and antifungal activities of GO and the two novel synthesized composites (GO/Ag, Gr/Ag) were tested by using the filter paper disk method according to the US Pharmacopeia [26]. Imipinem (I), clindamycin (C), cefixime (CX) as the antibacterial, nystatin (N) and miconazole (M) as the antifungal references drug were used simultaneously. The bacteria were cultured in a nutrient agar medium and used as inoculation. Whitman filter paper disks (diameter 7 mm) were dried and stabilized with the suspension of the test compound (25 μL) under aspect condition. These disks were then placed on the surface of a sterilized agar nutrient medium that was inoculated with test bacteria and fungi, and then air-dried to remove the surface moisture. A control disk without the nanoparticles was similarly treated. Thence, the disks were incubated at 37 ± 1, 30 ± 1°C for 2 and 4 days for bacteria and fungi respectively. The zone of inhibition of growth was measured, which demonstrates the inhibitory activity of the compounds on the growth of the bacteria and fungi.

4. Results and Discussion

4.1. Spectral studies

The Fourier transform infrared (FTIR) spectra of GO is shown in Fig.1. The presence of the absorption band at 1629 cm^{-1} is assigned to the C=C bonding of the unoxidized GO carbon skeleton structure. The presence of other oxygenated functional groups are also detected, including OH at approximately 3443 cm^{-1}, C=O at 1735 cm^{-1}, C–OH around 1401 cm^{-1}, and C–O around 1055 cm^{-1}. Furthermore, the absorption peak at 1207 cm^{-1} is assigned to the C–O–C of epoxy group. The XRD patterns of the GO and the **1**, **2** and **4** groups of the synthesized compounds are shown in Fig.2. The high intensity peaks at 2θ of 12.20° in Fig.2a and 26.53° in Fig.2b are assigned to GO and Gr/Ag respectively. The broad peak in both Fig.2a and Fig.2b at 26.5° shows the presence of some amount of unoxidized graphite in the compound.

The corresponding d-spacing values of the Ag/GO-1 and Ag/GO-2 are 7.22 Å and 3.35 Å respectively. Also the increase of interlayer spacing from 3.35 Å to 7.22 Å is indicative of oxygen functional groups which increase the thickness of the carbon plates. The XRD patterns of the fourth group are exhibited a peak with high intensity for graphene at 26.53 and 3.35 Å interlayer spacing and a weak peak at a 2θ value of 54.67 ° with d-spacing 7.3 Å (d002). Generally, the oxidation results in increasing of the interlayer spacing of graphite nanosheets in GO relative to natural graphite, which can be attributed to the intercalation of oxygen-based groups or ions between layers. Hence, the interlayer distance of graphite can be increased from 3.35 Å to 6-10 Å, depending on water content and the extent of the intercalation process [27].

Fig.3 shows the SEM images of compounds. The results obtained from SEM showed the structures of graphene and GO are uniform and flaky. The morphology of silver nanoparticles was found by SEM to be spherical at 500 nm magnification (Fig3e and Fig.3f).

Atomic force microscope was used to investigate the morphology of the graphene surface with silver nanoparticles. Topography of AFM (Fig.4) represents the roughness of the surface. The thickness of silver nanoparticles of the fourth group are 60.3, 99.8, 187 nm respectively and also the height of the last two are 58.9 and 301 nm. The EDXA for **2** and **4** groups proved polymerized doped compound on GO and graphene surfaces respectively. The weight percentage of nitrogen of doped compounds on GO and graphene are given in Table 1.

4.2. Antibacterial study

The antibacterial tests are shown in Table 2. It is previously shown that graphene, GO and silver nanoparticles are biocompatible materials [28,29]. Thus, the *in vitro* antibacterial and antifungal activities of GO, three compounds of Gr–AgNPs and two GO/Ag-1, GO/Ag-2 with concentration range of 200-600 μg/mL were performed against four bacteria: two Gram-positive (*bacillus subtilis*and *staphylococcus aureus*) and two Gram-negative (*escherichia coli* and *pseudomonas aeruginosa*) and three fungi (*candida albicans*, *aspergillusniger* and *mycobacterium terrae*). The antibacterial studies demonstrated that Gr/Ag with 0.44 g dosage of silver is active against Gram-negative bacteria especially Pseudomonas aeruginosa. Also this compound shows a comparable antibacterial effect to reference drug cefalexin, only at higher concentration. Furthermore, three compounds of Gr/Ag had good antifungal activities against candida albicans and aspergillusniger at the highest tested concentration of 600 μg/mL. Whereas GO and Ag/GO showed no activity at the same concentrations.

5. Conclusions

In summary, we successfully synthesized nanocomposites of GO and graphene by staudenmaier method. The XRD is one of the best methods to confirm the formation of graphene nanocomposites and doped compound such as pyrazole, 3,5-dimethylpyrazole and pyrrole on GO and graphene surfaces. Also this spectral study shows the oxidation processes of graphite. Accordingly, after oxidation, the intensity diffraction line (d002) of the graphite at 26.5° with *d*-spacing 3.35 Å disappeared and a peak at 12.2° appeared. The interlayer spacing between neighboring graphene layers in GO has increased with oxidation (they are ≈7.22 Å apart), because of the intercalation by oxygen-containing groups and moisture.

Ag/Gr nanocomposite with 0.44 g dosage of silver showed stronger antibacterial activity against Gram-negative bacteria (Pseudomonas aeruginosa) than Gram-positive and antifungal activity. The results showed that GO, itself, did not show any biological activities and as the concentration of Ag is increased, the biological activity increases.

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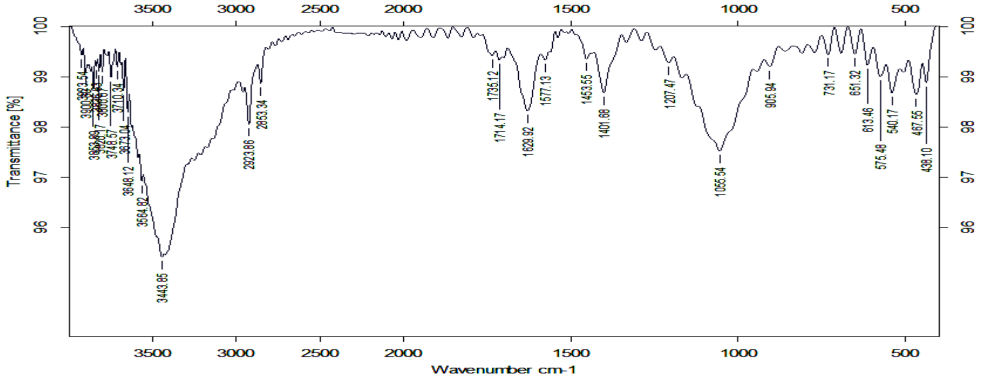
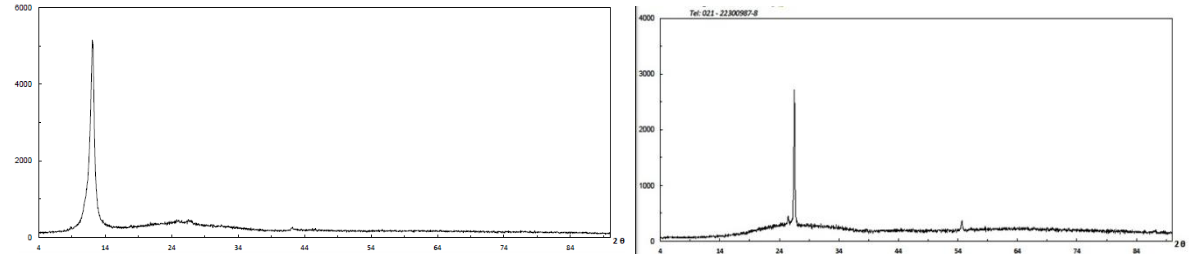
Fig.1. FTIR spectra of GO

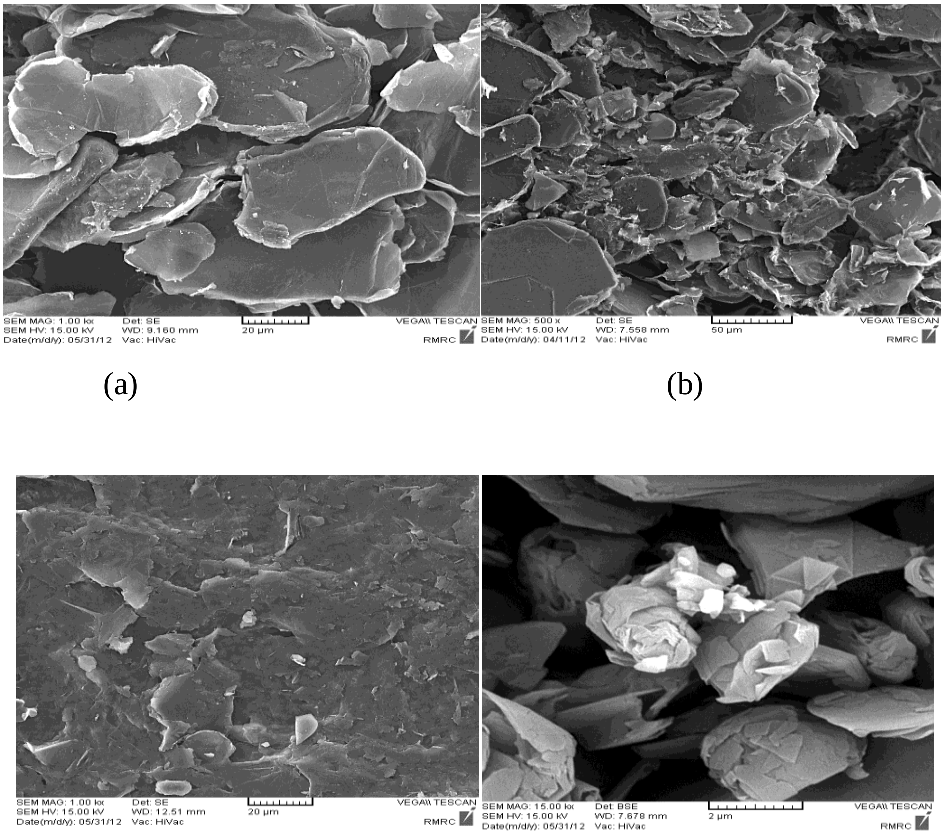




(a) (b)

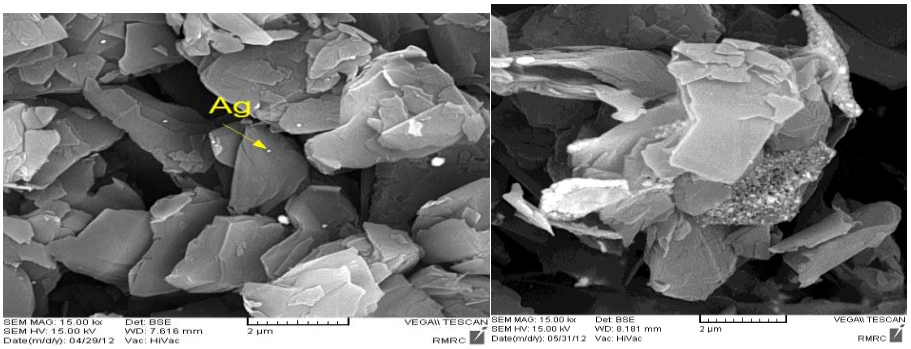
Fig.2. XRD pattern of graphene oxide (a) Gr/Ag-X(b)

Fig.3. SEM images; GO/PYZ(a), GO/DMP(b), GO/PYR(c), Gr/Ag-PYZ(d), Gr/Ag-DMP(e), Gr/Ag-PYR(f)



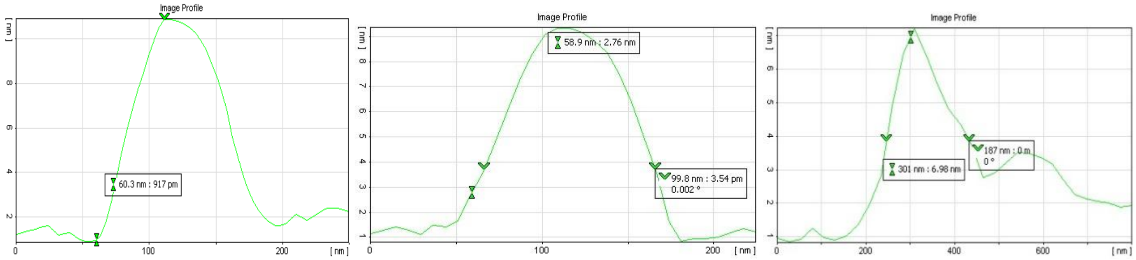
(a) (b)

(c) (d)



(e) (f)

Fig.4.AFM spectra of Gr–AgNPs with different dosage of Ag; 0.44g (a), 0.22g (b), 0.15g (c)



(a) (b) (c)

Table.1. Wt% of nitrogen of doped composites on GO and Gr

Comp.	GO/PYZ	GO/DMP	GO/PYR	Gr/Ag-PYZ	Gr/Ag-DMP	Gr/Ag-PYR
Wt%	4.16	6.44	5.28	5.28	6.92	6.69

Table.2. Inhibition zone (mean diameter of inhibition in mm) as a criterion of antibacterial and antifungal activities of the synthesized compounds

Strain	ATTC	Antimicrobial activity																
		Standard drug					**GO (µg)**	**GO/Ag-1 (µg)**	**GO/Ag-2 (µg)**	**Gr/Ag 0.44g (µg)**			**Gr/Ag 0.22g (µg)**			**Gr/Ag 0.15g (µg)**		
		I	C	N	M	CX	**200-600**	**200-600**	**200-600**	**200**	**400**	**600**	**200**	**400**	**600**	**200**	**400**	**600**
E.coli	11229	17	0	0	0	15	N	N	N	4	5	5	3	3	4	2	3	4
P.aureginosa	15442	18	0	0	0	4	N	N	N	1	3	4	1	1	3	1	1	2

S.aureus	6538	18	9	0	0	4	N	N	N	N	N	N	N	N	N	N	N	N
B.subtilis	6633	10	1	0	0	0	N	N	N	N	N	N	N	N	N	N	N	N
C.albicans	10231	0	0	9	10	0	N	N	N	8	10	18	7	8	16	9	12	13
A.niger	16404	0	0	6	5	0	N	N	N	3	7	11	2	5	7	6	7	8
M.terrae	1575	12	0	0	0	4	N	N	N	N	N	N	N	N	N	N	N	N

N= No activity

I:IMIPENEM, C: CLINDAMYCIN, N:NYSTATIN, M: MICONAZOLE,CX: CEFALEXIN

Crystal Structure, Application photo-catalytic properties of PdO nanoparticles, DNA Binding studies and Cytotoxicity of a New Hydroxyl-Quinolinato-Palladium Complex

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Abstract

The development of palladium anticancer drugs has been promising and their design has been based mainly on the structure-activity relationship used for platinum anticancer drugs as well as good models for the analogous Pt(II) complexes in solution[1-3].Thus our research in this area is focused on the interaction of Calf Thymus DNA (CT-DNA with a new palladium(II) anticancer complex of $[Pd(8Q)(Phen)]NO_3$ (where 8Q = 8-hydroxyquinolin and Phen = 1,10 phenanthroline).There is a set of 4 binding sits(g) for the complex on the DNA with positive cooperativity in binding. n,the Hill coefficient find out to be 2.59 at 300 and 2.34 at 310K respectively. K_{app} the apparent equilibrium constant are 76.52 and 83.03 mM^{-1} respectively. The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.057 at 300 to 0.054 mmol/L at 310K. (ΔG^0_{H2O}) determined to be 47.63 and 46.68 kJ/mol at 300K and 310K respectively. values for m, are 846.8 and 881.3 at 300K and 310K respectively. $\Delta H^0_{conformation}$ in the range of 300K and 310K is find out to be 75.44 kJ/mol. ΔS^0_{H2O} of DNA denaturation by complex is 0.092 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The cytotoxicity assay of the complex has been performed on human breast adenocarcinoma MCF7 cell line, at micromolar concentration.

Keywords: Crystal Structure, spectroscopic techniques,anti-tumor, Palladium (II) complex

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Crystal Structure, photo-catalytic properties of PdO nanoparticles, DNA binding studies and cytotoxicity of a new hydroxyl-quinolinato-palladium complex

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The development of palladium anticancer drugs has been promising and their design has been based mainly on the structure-activity relationship used for platinum anticancer drugs as well as good models for the analogous Pt(II) complexes in solution[1-3].Thus our research in this area is focused on the interaction of Calf Thymus DNA (CT-DNA with a new palladium(II) anticancer complex of [Pd(8Q)(Phen)]NO_3 (where 8Q = 8-hydroxyquinolin and Phen = 1,10 phenanthroline).There is a set of 4 binding sits(g) for the complex on the DNA with positive cooperativity in binding. The Hill coefficient find out to be 2.59 at 300 and 2.34 at 310K respectively. K_{app} the apparent equilibrium constant are 76.52 and 83.03 mM^{-1} respectively. The above compound can denature the DNA and the concentration of this ligand in the midpoint of transition ($[L]_{1/2}$), is decreased by improving temperature, from 0.057 at 300 to 0.054 mmol/L at 310K. (ΔG^0_{H2O}) determined to be 47.63 and 46.68 kJ/mol at 300K and 310K respectively. values for m, are 846.8 and 881.3 at 300K and 310K respectively. $\Delta H^0_{conformation}$ in the range of 300K and 310K is find out to be 75.44 kJ/mol. ΔS^0_{H2O} of DNA denaturation by complex is 0.092 kJ/mol at 300K. Fluorescence titration spectra and fluorescence Scatchard plots suggest that the Pd(II) complex intercalate in DNA. The cytotoxicity assay of the complex has been performed on human breast adenocarcinoma MCF7 cell line, at micromolar concentration.

Keywords: Crystal structure, Spectroscopic techniques, Anti-tumor, Palladium (II) complex

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Palladium Schiff base metal complexes immobilized on GO- $MnFe_2O_4$ for reduction of para-nitro phenol

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Palladium Schiff base metal complexes have been covalently grafted on to GO- $MnFe_2O_4$ previously functionalized with 3-aminopropyltriethoxysilane. Potential catalytic behavior was tested in the reduction of para-nitro phenol to para Amino Phenol by an excess of $NaBH_4$ in an aqueous medium at room temperature. The reduction of para nitro phenol was monitored using UV-Vis absorption spectroscopy. The catalyst was characterized using infrared (IR) , thermogravimetric analyses, inductively coupled plasma atomic emission spectrometry (ICP-AES), X-ray diffraction and transmission electron microscopy (TEM). IR spectroscopy, thermogravimetric analyses and ICP-AES confirmed the successful incorporation of the metal Schiff base complexes onto GO- $MnFe_2O_4$. X-ray diffraction and TEM showed the intact structure of the GO- $MnFe_2O_4$. palladium Schiff base complex on the Go-$MnFe_2O_4$ showed high catalytic activity in reduction of para nitro phenol . The recycling results of these heterogeneous catalysts showed good recoverability without significant loss of activity and selectivity within four successive runs.

Keywords: Schiff base metal complexes; graphene oxide, reduction of para-nitro phenol

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Metal Organic Framework with formula $Zn_2(bdc)_2(dabco)$ as a drug delivery

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Metal organic frameworks (MOFs), also known as coordinationpolymers or coordination networks, are the unique of crystallinematerials formed by connecting metal centers and organic ligandsinto infinite arrays through dative bonds [1]. As one types ofporous materials, MOFs exhibited potential advantages over conventionalmaterials, such as tunable pore size and shape, adjustablecomposition and structure, biodegradability, excellent loadingcapacity and controllable drug release, and versatile functionalities,which enable MOFs to perform as promising platforms for variousmedical applications, including drug delivery[2], molecularsensing and bioimaging, and theranostics[3].In this respect, MOFs could be advantageous over other classical porous materials owing to their diverse architecturesand tunable porosity, along with modifiable framework functionality.Moreover, in a MOF-based DDS, the drug payload and release could be controlled by changing the ligand lengthor the connectivity and functionality.

In this study, $Zn_2(bdc)_2(dabco)$ was synthesized and Then characterized by x-ray powder diffraction(XRD) and IR spectroscopy and effects of $Zn_2(bdc)_2(dabco)$ on the loading and release of drugs are investigated.

Keywords: Metal- Organic Framework , Drug Delivery, dabco, bdc

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Synthesis and Characterization of $Ag_3PO_4/Fe_3O_4/C_{60}$ Nanocomposite and Study of Their Antibacterial and Catalytic Activities

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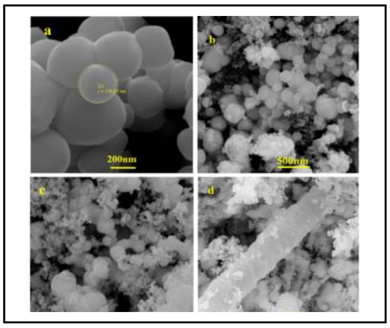
The $Ag_3PO_4/Fe_3O_4/C_{60}$ nanocomposite has been synthesized by a facile and effective hydrothermal method. This new nanocomposite was characterized by FT-IR, Raman spectroscopy, X-ray diffraction (XRD), UV–vis spectroscopy, Brunauer–Emmett–Teller (BET) specific surface area, and vibration sample magnetometry (VSM). Morphology of nanocomposites was investigated by scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The $Ag_3PO_4/Fe_3O_4/C_{60}$ nanocomposite showed good antibacterial activity against a few human pathogenic bacteria. The catalytic activity of the $Ag_3PO_4/Fe_3O_4/C_{60}$ nanocomposite for rapid and efficient reduction of toxic nitro compounds into less toxic corresponding amines by using NaBH4 as the hydrogen donor was also investigated. Our results show that $Ag_3PO_4/Fe_3O_4/C_{60}$ magnetic nanocomposite has exhibited higher catalytic activity better than Ag_3PO_4/Fe_3O_4 and Ag_3PO_4 respectively.



Keywords: C_{60}; Silver phosphate; Magnetic; Antibacterial Activity; Catalyst; reduction of phenols

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Synthesis and Characterization of $BiVO_4/Fe_3O_4/C_{60}$ Nanocomposite and Study of Catalytic Activity

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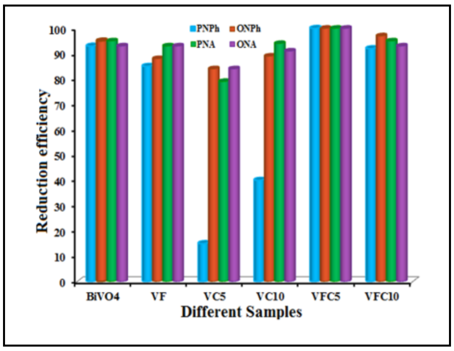
The $BiVO_4/Fe_3O_4/C_{60}$ nanocomposite has been synthesized by a facile and effective hydrothermal method. This new nanocomposite was characterized by X-ray diffraction (XRD), FT-IR spectra, Raman spectroscopy, vibration sample magnetometry (VSM), Brunauer–Emmett–Teller (BET) specific surface area and UV–vis spectroscopy. Morphology of nanocomposites was investigated by scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM). In this study, reduction of phenols and anilines on $BiVO_4/Fe_3O_4/C_{60}$ catalyst has been investigated. The catalytic activity of the $BiVO_4/Fe_3O_4/C_{60}$ nanocomposite for speedy and efficient reduction of toxic nitro compounds into less toxic resultant amines by NaBH4 as the hydrogen donor was also investigated. Our consequences show that $BiVO_4/Fe_3O_4/C_{60}$ magnetic nanocomposite has exhibited higher catalytic activity better than pure $BiVO_4$ and $BiVO_4/Fe_3O_4$.



Keywords: C_{60}; BiVO4; Magnetic; Catalytic activity; reduction of phenols; anilines

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complex tolanophanes and $HgCl_2$ and their application in the synthesis of the related cyclic vinylsulfonates

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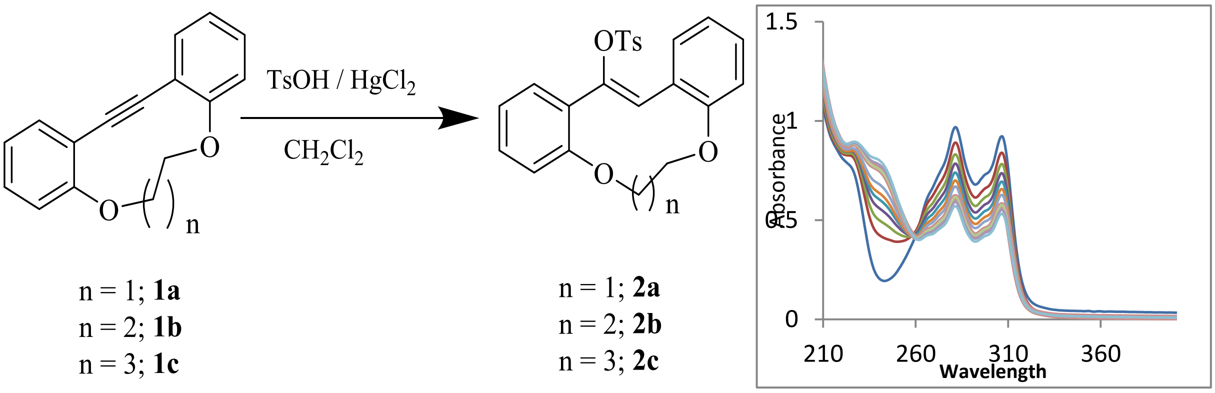
The basic principles of organometallic chemistry are the basis of the discovery of catalysts and catalytic processes.[1] The unsaturated alkyne triple bond can undergo a variety of metal-catalysed reactions, including the inter- or intramolecular addition of carbon or heteroatom nucleophiles; This reactivity is associated with a diverse coordination chemistry of organometallic alkyne species.[2,3] In continuous of our work on tolanopahnes **1**,[4] herein, we report their selective response towards $HgCl_2$ among various metal chloride ions by UV-Vis spectroscopy titration.(Scheme1) In order to evaluate the complex performance, the stoichiometric reactions of **1a-c** with p-toluenesulfonic acid in the presence and absence of $HgCl_2$ in CH_2Cl_2 were carried out which gave the corresponding cyclic vinylsulfonates **2a-c**. (Scheme1) The results revealed that *ortho* position of methoxy groups on the ring has a definite role on the tosylation. Despite the poor effect of $HgCl_2$ on acyclic tolans, a cooperative effect between $HgCl_2$ and cyclic **1a-c** was observed leading to significant increase of the yields of **2a-c**. The products are new which well characterized.



Scheme1. Synthesis of **2a-c** (left) UV-Vis spectrum of 1b with $HgCl_2$(right)

Keywords: *Organometallic, $HgCl_2$, Tolanophane , vinylsulfonates*

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Synthesis and characterization of some water soluble metal Schiff base complexes functinalized Fe_3O_4 magnetic nano-particles

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Schiff base transition metal complexes have been extensively studied because of their potential use as catalysts[1]. Recently, magnetic core–shell nano-structures have attracted more attention due to their unique magnetic properties. Therefore reparation of functionalized magnetic nano-particles, $Fe_3O_4@SiO_2$, with Schiff base complexes have attracted interest to provide magnetically reusable heterogeneous catalysts[2,3].

In this work, firstly the magnetite nano-particles synthesized by co-precipitation method from iron(II) chloride tetrahydrate and iron(III) chloride hexa-hydrate in alkaline condition. Then the surfaces of the nano-particles were coated with SiO_2. The surface of core-shell structures functionalized with NH_2 groups by reacting with 3-amino propyl triethoxy silane. In the next step, a water-soluble aldehyde (sodium salicylaldehyde-5-sulfonate) was synthesized and characterized. Condensation reaction between the NH_2 group and carbonyl group leads to a water-soluble Schiff base that is supported on the coated magnetite. Then the supported water-soluble Schiff base converted to the corresponding metal complexes of Cu(II), Co(II) and Mn(II) by reaction with acetate salts of these metals. In this way three water-soluble Schiff-base complexes supported on core-shell magnetite silica nano-particles were synthesized and characterized by FT-IR, XRD, SEM, EDX, TEM and TG analysis.

Keywords: core shell, nano-composite, Schiff base, magnetite,

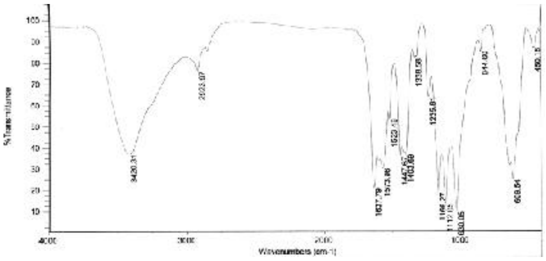

Fig.1 FT–IR spectrum for $Fe_3O_4@SiO_2$/Schiff base of Mn(II)

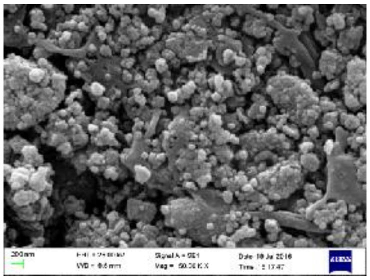

Fig.2 EM image for $Fe_3O_4@SiO_2$/Schiff base of Mn(II)

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Enhancing acidic properties of supported solid acid catalysts: A new method for anchoring two acidic sites on the surface of Fe_3O_4@SiO_2

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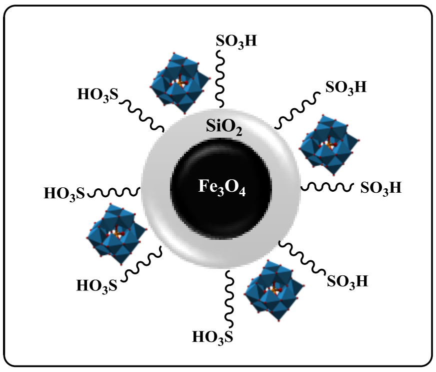
In recent years, different types of solid acid catalysts have been developed, and each type of these catalysts exhibited their unique catalytic activity. Among these synthesized catalysts, a catalyst with two distinct acidic sites which could be separated easily from the reaction mixture is promising. In order to reach this purpose, we prepared a solid acid catalyst based on silica coated magnetite nanoparticles with two kinds of bronsted acidic sites, sulfonic acid groups and phosphotungestic acid species. These functional groups were characterized by FT-IR spectroscopy and CHNS elemental analysis. Vibrating sample magnetometry (VSM) and X-ray diffraction (XRD) analyses were used to identify its magnetic properties and crystal phase, respectively. Also shape and size determination of these nanoparticles were performed by transmission electron microscopy (TEM). The prepared catalyst showed very good activity in the esterification of acetic acid with butanol. Conversions up to 70% of butanol and 100% selectivity toward the ester were reached after 8 h. The results exhibited that this catalyst with double acidic groups is promising solid acid catalyst to be used in the esterification of carboxylic acids with alcohols.



Keywords: Magnetite nanoparticles, Sulfonic acid, Phosphotungestic acid, Esterification.

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سنتز و شناسایی کمپلکس های مس (II) با استفاده از نمک فسفونیوم .حاصل از ترکیب تری فنیل فسفین با اتیل برمو استات, با استفاده از روش های استروسکوپی

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چکیده

نمک های فسفونیم دارای فرمول کلی $R_4 P^+ X^-$ بوده مانند $[P(CH_3)^+{}_4]^-$. بطور کلی فسفونیوم به یک مشتق آلی گفته می شود که از یون فرعی فسفونیوم چهارضلعی (PH^+) مشتق شده اند. ..مانند تترا متیل فسفونیوم کلرید و تترا متیل فسفونیوم یدید.

در این پروژه ترکیبات فسفونیوم $[C_2H_5COO\ (CH_2PPh_3Br)]$ و کمپلکس مس (II) آن $[Cu_2Cl_6]\ [C_2H_5COO\ (CH_2PPh_3Br)]$ تهیه و مشخص گردیدند.نمک فسفونیوم از واکنش اتیل برمو استات با تری فنیل فسفین تهیه و مشخص گردیدند.آنگاه با استفاده از واکنش بین ترکیب فسفونیوم با $Na_2[Cu_2Cl_6]$ ترکیب های نهایی تهیه شدند. سپس با استفاده از روش های طیف سنجی تهیه ی این ترکیب ها مورد بررسی قرار گرفت.

واژگان کلیدی : *فسفونیوم , ترکیب های مس (II) , تری فنیل فسفین , اتیل برمو استات*

مقدمه :

نمک های آلکیل تری فنیل فسفوینم برای تهیه واکنشگر wittig در واکنش wittig به طور گسترده استفاده شد. این نمک ها به آسانی توسط واکنش تری فنیل فسفین با یک الکید آلدهید ساخته می شوند. اگر الکیل، متیل یا الکیل گروه اصلی بازداری فضایی نشده باشند، واکنش بخوبی انجام می شود. اما معمولاً واکنش با الکیل هالید ثانویه یک واکنش ضعیف است. گروههای الکیل سه گانه نمی توانند ایلید را تولید کنند. نمک فسفونیم ترکیب پایداری است که غالباً از اتانول و از طریق تبلور مجدد بدست می آید [1] . در سالهای اخیر، نمک های فسفونیم به دلیل ساختار، ویژگیها و واکنش پذیری خود بسیار مورد پسند قرار گرفته اند.

واکنش آیلید با آلدهیدها یا کتون ها، که یکی از رایج ترین روشها برای تولید آلکن هایی در یک طیف خاص است، اولین باز توسط جورج ویتیگ معرفی شد. این واکنش مرحله اصلی تولید تعداد زیادی از فراورده های طبیعی و بیولوژیکی است. مزیت اصلی واکنش

ویتیگ انتخاب فضایی آن است. انتخاب فضایی به چند عامل بستگی دارد. ساختار نمک فسفونیم وجود کاتیون های فلزی و شرایط آزمایشگاهی است [2].

واکنش ویتیگ علاوه بر تحقیقات کاربردی استفاده های گسترده ای در تولید مواد دارویی و صنعتی دارد. برای آغاز واکنش، ابتدا الکیل هالید با یک فسفین وارد واکنش می شود تا فسفین کاتیون چهار وجهی بدست آید. برای تولید یک ترکیب خنثی، که آیلید فسفونیم نامیده می شود، این کاتیون با یک باز قوی مانند بوتیل لیتیم پروتون زدایی می شود.

آیلید کربن را با بار منفی باردار می کند، به عنوان یک نوکلئوفیل عمل کرده و به گروه کربونیل آلدهید یا کتون حمله می کند. فلزهای حفاظتی و مهارکننده خوردگی نقش مهمی در صنعت ایفا می کنند. اغلب محافظت کننده ها و مهارکننده ها ترکیب های آلی هستند که دارای هترو اتم هایی مانند فسفر، نیتروژن، سولفور و اکسیژن هستند. این ترکیب ها و مشتقات آنها آهن و فولاد را در مقابل خوردگی بازداری می کنند. بسیاری از این مهارکننده های خوردگی و حفاظتی اثرات زیان باری بر محیط زیست دارند. بنابراین دستیابی به مهارکننده های آلی موثر و غیر سمی برای آهن و فولاد موضوعی حائز اهمیت است. مهارکننده مناسب برای محیط زیست می بایست دارای ویژگی های زیست تخریب پذیری بوده و برای محیط زیست مخرب نباشد. ترکیب های فسفونیم در محلول های اسیدی به عنوان محافظ برای اغلب فلزات استفاده می شوند [3].

ترکیب های چهار وجهی فسفونیم در بسیاری از سیستم ها به عنوان عوامل مهارکننده رشد باکتری شناخته شده اند، که به طور گسترده در محیط زیست استفاده می شود [4]. مزایای این ترکیب ها شامل این موارد است: سمیت بسیار پایین، فرسایش سریع در محیط زیست (از طریق هیدرولیز، اکسیداسیون، تجزیه نوری و تجزیه بیولوژیکی)، و اثرات غیر تخریبی بر محیط زیست [5].

برای مثال، تری فنیل فسفونیم بروميد در محلول اسی سولفوریک 0/5 مول به عنوان یک بازدارنده خوردگی برای آهن و فولاد شناخته شده است و توسط ارزیابی های گالوانوستات و پوتنتیو استاتیک و با استفاده از اسپکتروسکوپی FT-IR و تصاویر حاصل از میکرویکوپ الکترونی و محاسبه کوانتوم تایید شده است [6]. همچنین برخی گزارشات در مورد تهیه پلیمرهای فعال بیولوژیکی با استفاده از گروههای آمونیوم و فسفونیم چهار وجهی، که دارای استفاده دارویی است، ارائه شده اند [7].

تولید مایعات یونی کاربرد دیگری از نمک های فسفونیم است که این مایعات نمک های آلی می باشند که در دماهای پایین (کمتر از 100 درجه سناتیگراد) دارای حالت مایع بوده [8] و دارای مزیت هایی چون طیف دمایی گسترده خروجی مایع، پایداری حرارتی و شیمیایی بالا، حلال های قوی و فشار بخار بسیار پایین در ترکیب با ترکیب های آلی، کاتالیست های شیمیایی، روشهای مختلف

جداسازی و نقش در الکترولیت های جدید در ساخت سلول های خورشیدی و سوختی هستند [9]. در سالهای اخیر مطالعات زیادی روی سیستم های فسفونیم چهار وجهی و ترکیب های جدید فسفونیم به نام مایعات یونی صورت گرفته است و استفاده از نمک های فسفونیم بیشتر از هر زمان دیگری است [10].

در سالهای اخیر حسگرهای رطوبتی پلیمر مهمی ساخته شده اند. انواع مختلفی از مونومرهای حساس به رطوبت در ساخت سنسورهای رطوبتی مورد استفاده قرار گرفته اند، از جمله نمک کاتیونی و آنیونی. نمک های فسفونیم به دلیل سادگی و تهیه آسان و پایداری بالا تحت شرایط مختلف در مقادیر بسیار زیاد برای ساخت سنسورهای پلیمری رطوبت مورد استفاده قرار می گیرند. اخیراً نمک های تری فنیل فسفونیم کلرید تهیه و در تولید سنسورهای رطوبتی ضدآب استفاده شده اند. می توان از تری بوتیل فسفونیم کلرید به عنوان یک مونومر در تولید این سنسورها استفاده نمود [11]. نمک های فسفونیم به طور موفقیت آمیزی به عنوان کاتالیست در انواع بسیاری از واکنش های آلی استفاده شده اند بطوریکه می توان گفت که این فعالیت کاتالیزوری نمک نمک ساده فسفونیم به عنوان واکنش بنزیل کلرید فسفونیم آلکوکسیسیل سیانو کتون ها و استفاده از نمک فسفونیم به عنوان کاتالیزور اسید لوئیس بدون فلز است که رشد در زمینه کاتالیزورهای آلی را سرعت بخشیده است [13].

روش آزمایش :

فرآیند تهیه ترکیب [$C_2H_5COO(CH_2PPh_3Br)$]

در این مطالعه 10 m mol اتیل برمو استات (1.1 ml)و 10 m mol تری فنیل فسفین (2.62 gr) را بصورت جداگانه در 50 ml بنزن حل کرده و سپس به یک بالن 100 ml اضافه می کنیم. که پس از 2 الی 3 دقیقه شروع به رسوب می کند. و تا 24 ساعت در دمای اتاق هم زده شد.سپس محلول را پس از شستشو با دی اتیل اتر . صاف کرده و سپس در دسیکاتور خشک گردید. وزن رسوب بدست آمده 2.98 gr و بازدهی واکنش 69٪ بود. که این رسوب در دمای 165 ^0c ذوب شد.

تهیه کمپلکس مس (II)

فرآیند تهیه کمپلکس $[C_2H_5COO(CH_2PPh_3Br)] [Cu_2Cl_6]$

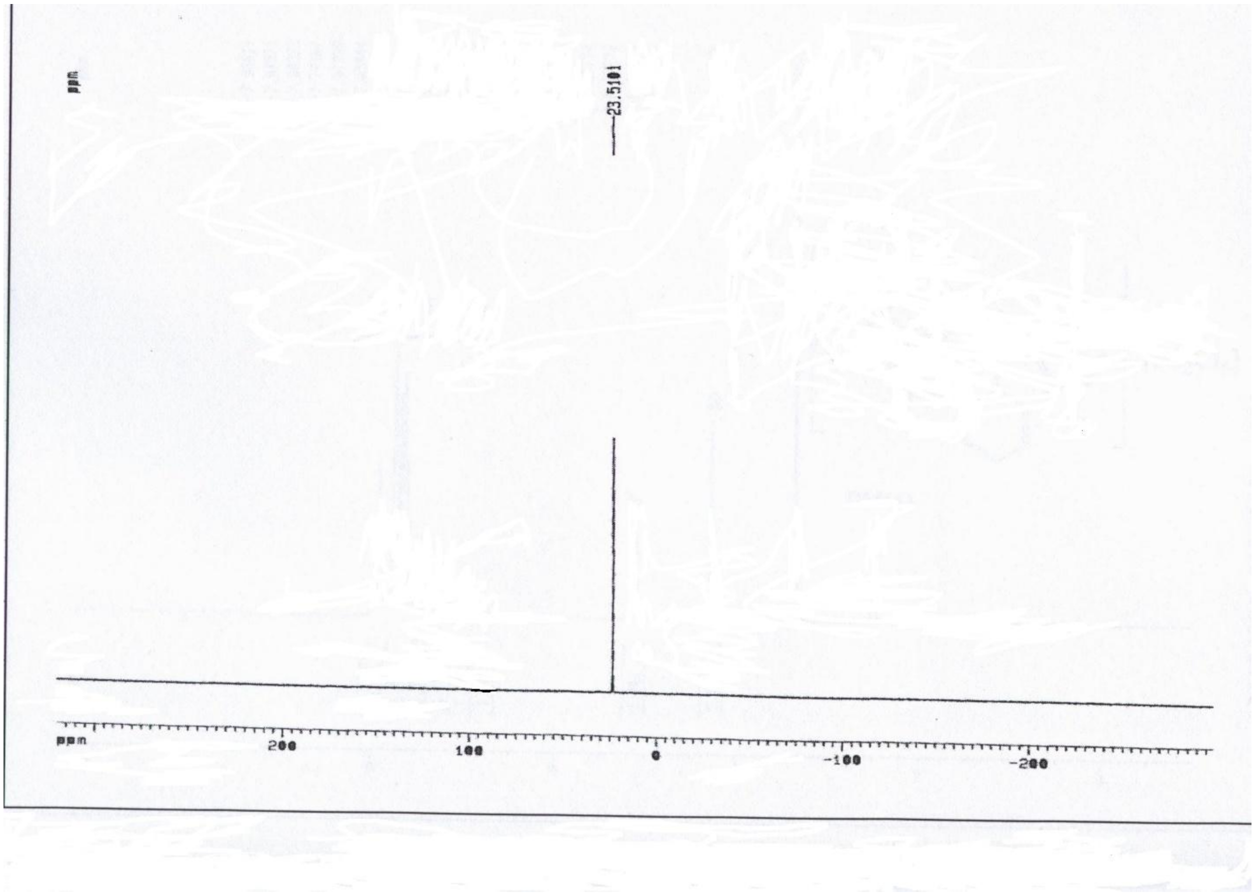
دراین مرحله 0/1 گرم $CuCl_2$ (0.74 m mol) و 0/17 گرم NaCl (2.9 m mol) در یک شیلنگ لوله ای ریخته شد. سپس 10 ml متانول به آن اضافه شد. و محلول در دمای 50 ^0c به مدت 5 ساعت هم زده شد .تا یک محلول شفاف سبز مایل به زرد مطابق طرح زیر به دست آمد. سپس مقدار 0/32 گرم ترکیب فسفونیوم (0/76 m mol) به آن افزوده شد.که سریعا شروع به تشکیل رسوب آبی فیروزه ای رنگی کرد . که وزن آن 0/15 گرم و بازدهی واکنش 25.86٪ بوده و در دمای 218 ^0c ذوب شد.

نتایج

به منظور تعیین ترکیب های بدست آمده طیف NMR شامل PNMR – CNMR – HNMR با استفاده از FT-NMR400 اندازه گیری شد. و طیف مادون قرمز با استفاده از دستگاه مدل FT-IR.Bommen و روغن نوژول وقرص KBr ارزیابی شد.ونتایج زیر بدست آمد.

طیف 1. طیف ^{31}PNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)] [Cu_2Cl_6]$ را نشان می دهد. دراین طیف , رزونانس فسفر در $\delta = 23.66$ PPm به شکل یک پیک یکتایی ظاهر می شود.شکل پیک در مقایسه با پیک فسفر دارای لیگاند آزاد در فنیل فسفین $\delta = 4.8$ PPm ظاهر می شود, نشان می دهد که اتم فسفر با اتم کربن یک پیوند جدید بوجود آورده است.که با کاهش چگالی الکترون در اتم فسفر, پیک فسفر به میدان های پایین تر تغییر مکان می دهد. همچنین این پیک برای ترکیب های مشابه در $\delta = 24.22$ PPm ظاهر می شود. [16]

این پیک نشان دهنده شکل گیری ترکیب مورد نظر می باشد . وپیک یکتایی فسفر در این طیف نشان دهنده ی خلوص بالای ترکیب است.



طیف 1 . ^{31}PNMR ترکیب [Cu_2Cl_6] [$C_2H_5COO(CH_2PPh_3Br)$]

طیف 2. طیف ^{1}HNMR ترکیب [$C_2H_5COO(CH_2PPh_3Br)$] [Cu_2Cl_6] را نشان می دهد.. در این طیف پیک یکتایی در 21281 مربوط به گروه متیل متصل به فسفر می باشد .پیک 5 تایی مربوط به هیدروژن های گروه اتیل متصل به اتم اکسیژن است که به دلیل افزایش چگالی الکترون ناشی از اتصال به اتم اکسیژن در میدان 24397 ظاهر می شود.و پیک های متعدد در 38456 تا 38456 مربوط به هیدروژن های آروماتیک ترکیب است. که خلاصه نتایج این طیف در جدول زیر آمده است.

شکل پیک	تعداد پروتون	δ (PPm)	نوع پروتون
پیک یکتایی	2	21281	CH_2 P
پیک 5 تایی	5	24397	C_2H_5 O
پیک های متعدد	15	14702	3 C_6H_5

سنتز و شناسایی کمپلکس های مس (II) با استفاده از نمک فسفونیوم حاصل از ترکیب تری فنیل فسفین با اتیل برمو استات, با استفاده از روش های استروسکوپی

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چکیده

نمک های فسفونیم دارای فرمول کلی $R_4\,P^+X^-$ بودهمانند $[P(CH_3)^+{}_4]^-$.بطور کلی فسفونیوم به یک مشتق آلی گفته می شود که از یون فرعی فسفونیوم چهارضلعی (PH^+) مشتق شده اند. ..مانند تترا متیل فسفونیوم کلرید و تترا متیل فسفونیوم یدید.

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واکنش آیلید با آلدهیدها یا کتون ها، که یکی از رایج ترین روشها برای تولید آلکن هایی در یک طیف خاص است، اولین باز توسط جورج ویتیگ معرفی شد. این واکنش مرحله اصلی تولید تعداد زیادی از فراورده های طبیعی و بیولوژیکی است. مزیت اصلی واکنش ویتیگ انتخاب فضایی آن است. انتخاب فضایی به چند عامل بستگی دارد. ساختار نمک فسفونیم وجود کاتیون های فلزی و شرایط آزمایشگاهی است [2].

واکنش ویتیگ علاوه بر تحقیقات کاربردی استفاده های گسترده ای در تولید مواد دارویی و صنعتی دارد. برای آغاز واکنش، ابتدا الکیل هالید با یک فسفین وارد واکنش می شود تا فسفین کاتیون چهار وجهی بدست آید. برای تولید یک ترکیب خنثی، که آیلید فسفونیم نامیده می شود، این کاتیون با یک باز قوی مانند بوتیل لیتیم پروتون زدایی می شود.

آیلید کربن را با بار منفی باردار می کند، به عنوان یک نوکلئوفیل عمل کرده و به گروه کربونیل آلدهید یا کتون حمله می کند. فلزهای حفاظتی و مهارکننده خوردگی نقش مهمی در صنعت ایفا می کنند. اغلب محافظت کننده ها و مهارکننده ها ترکیب های آلی هستند که دارای هترو اتم هایی مانند فسفر، نیتروژن، سولفور و اکسیژن هستند. این ترکیب ها و مشتقات آنها آهن و فولاد را در مقابل خوردگی بازداری می کنند. بسیاری از این مهارکننده های خوردگی و حفاظتی اثرات زیان باری بر محیط زیست دارند. بنابراین دستیابی به مهارکننده های آلی موثر و غیر سمی برای آهن و فولاد موضوعی حائز اهمیت است. مهارکننده مناسب برای محیط زیست می بایست دارای ویژگی های زیست تخریب پذیری بوده و برای محیط زیست مخرب نباشد. ترکیب های فسفونیم در محلول های اسیدی به عنوان محافظ برای اغلب فلزات استفاده می شوند [3].

ترکیب های چهار وجهی فسفونیم در بسیاری از سیستم ها به عنوان عوامل مهارکننده رشد باکتری شناخته شده اند، که به طور گسترده در محیط زیست استفاده می شود [4]. مزایای این ترکیب ها شامل این موارد است: سمیت بسیار پایین، فرسایش سریع در محیط زیست (از طریق هیدرولیز، اکسیداسیون، تجزیه نوری و تجزیه بیولوژیکی)، و اثرات غیر تخریبی بر محیط زیست [5].

برای مثال، تری فنیل فسفونیم برومید در محلول اسی سولفوریک ۰/۵ مول به عنوان یک بازدارنده خوردگی برای آهن و فولاد شناخته شده است و توسط ارزیابی های گالوانوستات و پوتنتیو استاتیک و با استفاده از اسپکتروسکوپی FT-IR و تصاویر حاصل از میکرویکوپ الکترونی و محاسبه کوانتوم تایید شده است [6]. همچنین برخی گزارشات در مورد تهیه پلیمرهای فعال بیولوژیکی با استفاده از گروههای آمونیوم و فسفونیم چهار وجهی، که دارای استفاده دارویی است، ارائه شده اند [7].

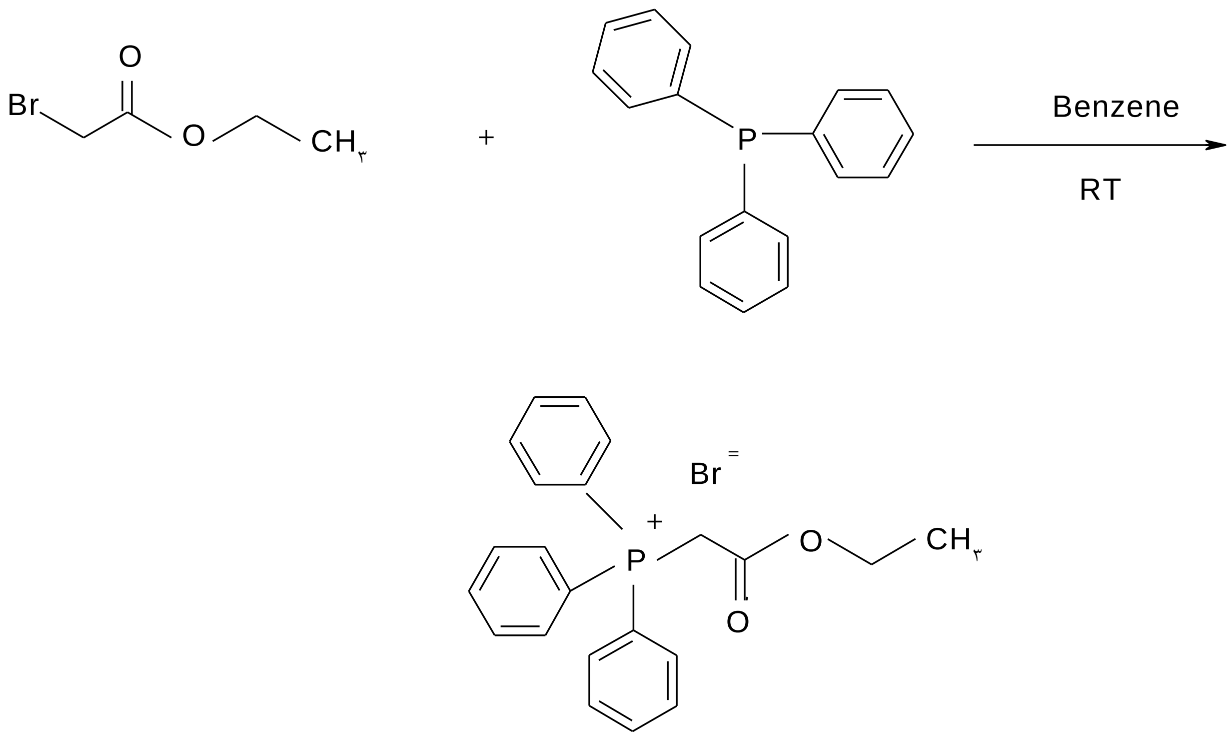
تولید مایعات یونی کاربرد دیگری از نمک های فسفونیم است که این مایعات نمک های آلی می باشند که در دماهای پایین (کمتر از ۱۰۰ درجه سناتیگراد) دارای حالت مایع بوده [8] و دارای مزیت هایی چون طیف دمایی گسترده خروجی مایع، پایداری حرارتی و شیمیایی بالا، حلال های قوی و فشار بخار بسیار پایین در ترکیب با ترکیب های آلی، کاتالیست های شیمیایی، روشهای مختلف جداسازی و نقش در الکترولیت های جدید در ساخت سلول های خورشیدی و سوختی هستند [9]. در سالهای اخیر مطالعات زیادی روی سیستم های فسفونیم چهار وجهی و ترکیب های جدید فسفونیم به نام مایعات یونی صورت گرفته است و استفاده از نمک های فسفونیم بیشتر از هر زمان دیگری است [10].

در سالهای اخیر حسگرهای رطوبتی پلیمر مهمی ساخته شده اند. انواع مختلفی از مونومرهای حساس به رطوبت در ساخت سنسورهای رطوبتی مورد استفاده قرار گرفته اند، از جمله نمک کاتیونی و آنیونی. نمک های فسفونیم به دلیل سادگی و تهیه آسان و پایداری بالا تحت شرایط مختلف در مقادیر بسیار زیاد برای ساخت سنسورهای پلیمری رطوبت مورد استفاده قرار می گیرند. اخیراً نمک های تری فنیل فسفونیم کلرید تهیه و در تولید سنسورهای رطوبتی ضدآب استفاده شده اند. می توان از تری بوتیل فسفونیم کلرید به عنوان یک مونومر در تولید این سنسورها استفاده نمود [11]. نمک های فسفونیم به طور موفقیت آمیزی به عنوان کاتالیست در انواع بسیاری از واکنش های آلی استفاده شده اند بطوریکه می توان گفت که این فعالیت کاتالیزوری نمک نمک ساده فسفونیم به عنوان واکنش بنزیل کلرید فسفونیم آلکوکسیسیل سیانو کتون ها و استفاده از نمک فسفونیم به عنوان کاتالیزور اسید لوئیس بدون فلز است که رشد در زمینه کاتالیزورهای آلی را سرعت بخشیده است [13].

روش آزمایش :

فرآیند تهیه ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$

در این مطالعه 10 m mol اتیل برمو استات (1.1 ml)و 10 m mol تری فنیل فسفین (2.62 gr) را بصورت جداگانه در 50 ml بنزن حل کرده و سپس به یک بالن 100 ml اضافه می کنیم. که پس از 2 الی 3 دقیقه شروع به رسوب می کند و تا 24 ساعت در دمای اتاق هم زده شد.سپس محلول را پس از شستشو با دی اتیل اتر . صاف کرده و سپس در دسیکاتور خشک گردید. وزن رسوب بدست آمده 2.98 gr و بازدهی واکنش 69٪ بود. که این رسوب در دمای $165\ ^0c$ ذوب شد.



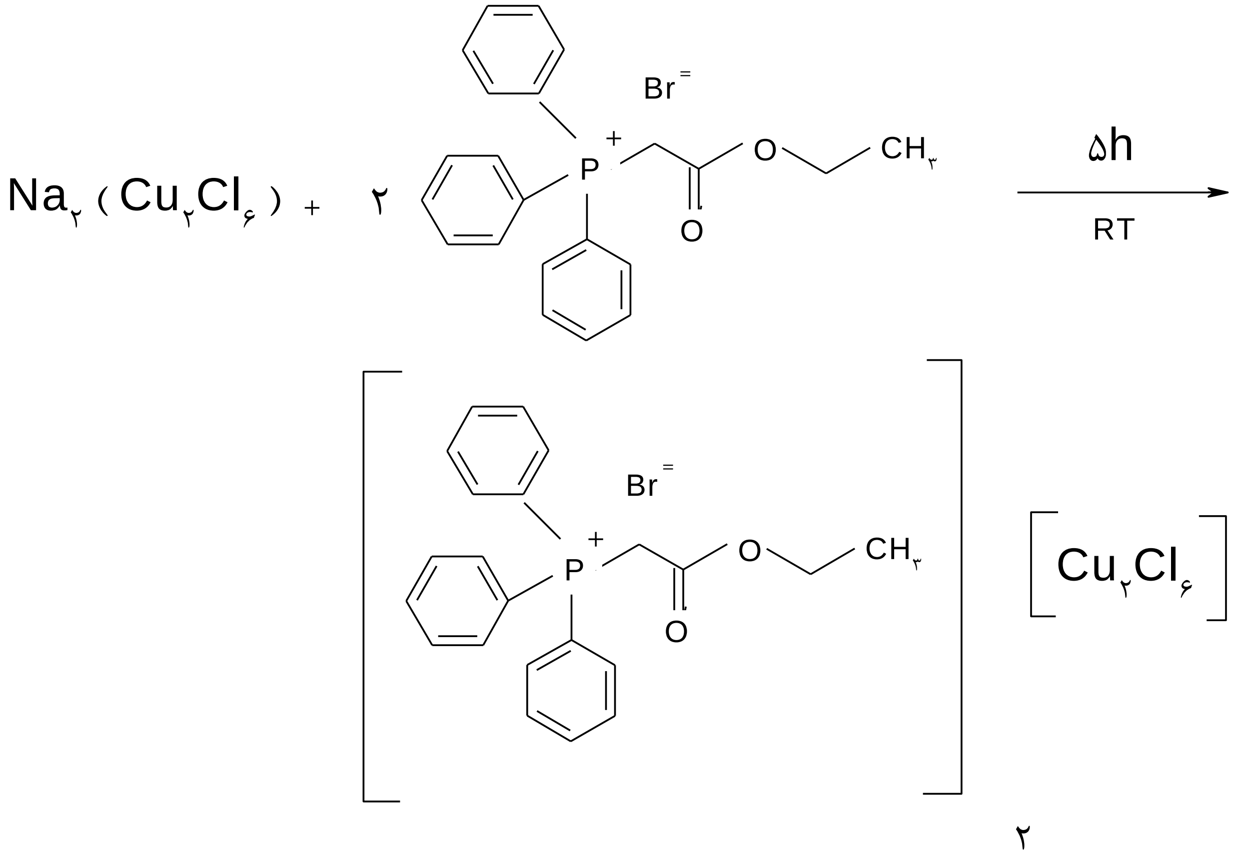
فرآیند تهیه $[C_2H_5COO(CH_2PPh_3Br)]$

تهیه کمپلکس مس (**II**)

فرآیند تهیه کمپلکس $[C_2H_5COO(CH_2PPh_3Br)]\ [Cu_2Cl_6]$

دراین مرحله 0/1 گرم ($CuCl_2$ (0.74 m mol) و 0/17 گرم (NaCl(2.9 m mol) در یک شیلنگ لوله ای ریخته شد. سپس 10 ml متانول به آن اضافه شد. و محلول در دمای 50 ^0c به مدت 5 ساعت هم زده شد تا یک محلول شفاف سبز مایل به زرد مطابق طرح زیر به دست آمد. سپس مقدار 0/32 گرم ترکیب فسفونیوم (0/76 m mol) به آن افزوده شد.که سریعا شروع به تشکیل رسوب آبی فیروزه ای رنگی کرد . که وزن آن 0/15 گرم و بازدهی واکنش 25.86٪ بوده و در دمای 218 ^0c ذوب شد.

$$۲\ NaCl + ۲\ CuCl_{۲} \xrightarrow[۵۰\ C]{Me\ oH} Na_{۲}(Cu_{۲}Cl_{۶})$$

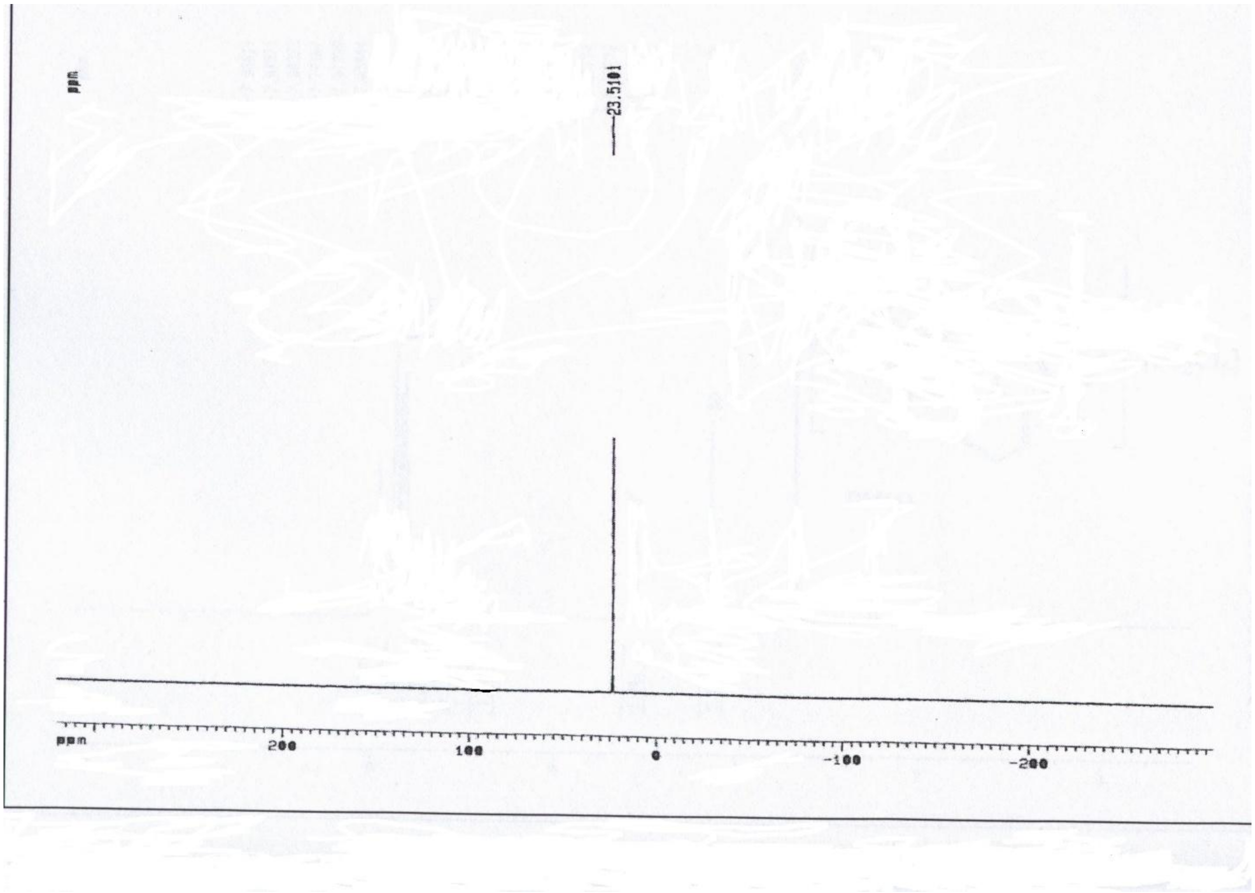


نتایج

به منظور تعیین ترکیب های بدست آمده طیف NMR شامل PNMR – CNMR – HNMR با استفاده از FT-NMR400 اندازه گیری شد. و طیف مادون قرمز با استفاده از دستگاه مدل FT-IR.Bommen و روغن نوژول وقرص KBr ارزیابی شد و نتایج زیر بدست آمد :

طیف ۱. طیف ^{31}PNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]\ [Cu_2Cl_6]$را نشان می دهد. دراین طیف ، رزونانس فسفر در $\delta = 23.66$ PPm به شکل یک پیک یکتایی ظاهر می شود. شکل پیک در مقایسه با پیک فسفر دارای لیگاند آزاد در فنیل فسفین $\delta = 4.8$ PPm ظاهر می شود، نشان می دهد که اتم فسفر با اتم کربن یک پیوند جدید به وجود آورده است که با کاهش چگالی الکترون در اتم فسفر، پیک فسفر به میدان های پایین تر تغییر مکان می دهد. همچنین این پیک برای ترکیب های مشابه در $\delta = 24.22$ PPm ظاهر می شود. [16]

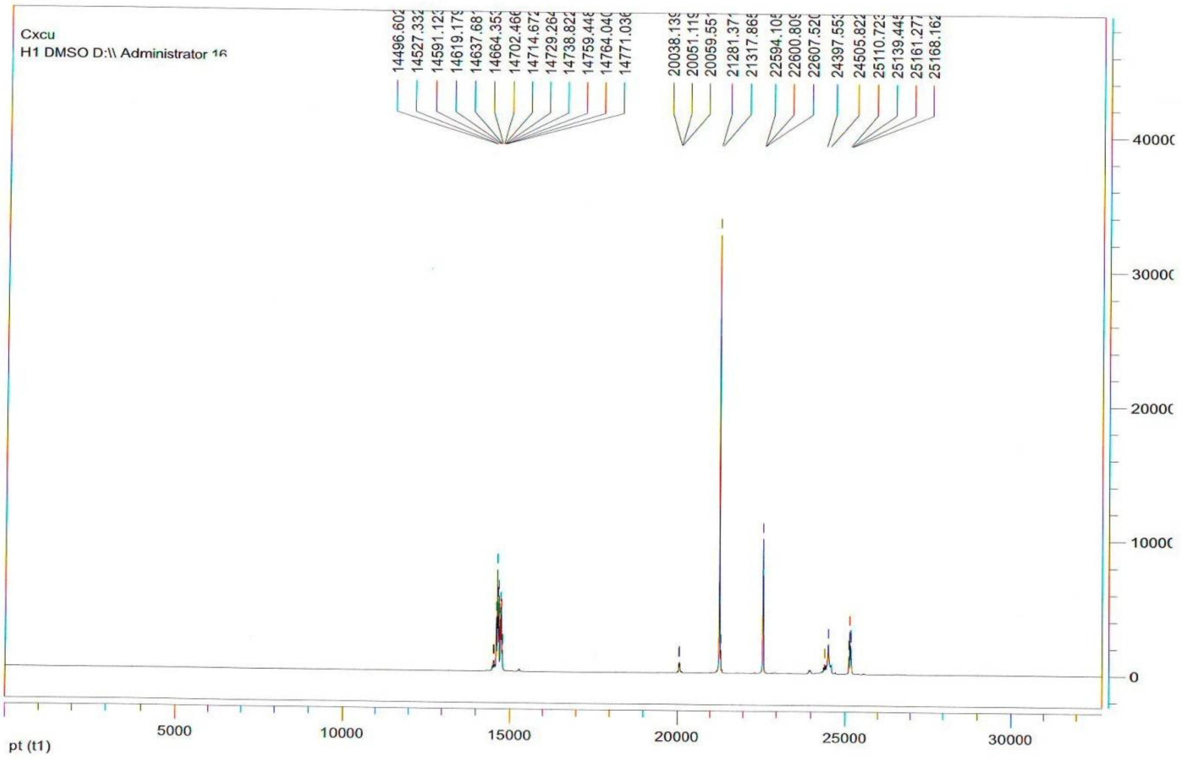
این پیک نشان دهنده شکل گیری ترکیب مورد نظر می باشد و پیک یکتایی فسفر در این طیف نشان دهنده ی خلوص بالای ترکیب است.



طیف ۱ . ^{31}PNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$ $[Cu_2Cl_6]$

طیف ۲. طیف ^{1}HNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$ $[Cu_2Cl_6]$ را نشان می دهد.. در این طیف پیک یکتایی در 21281 مربوط به گروه متیل متصل به فسفر می باشد .پیک ۵ تایی مربوط به هیدروژن های گروه اتیل متصل به اتم اکسیژن است که به دلیل افزایش چگالی الکترون ناشی از اتصال به اتم اکسیژن در میدان 24397 ظاهر می شود.و پیک های متعدد در 14496 تا 14771 مربوط به هیدروژن های آروماتیک ترکیب است که خلاصه نتایج این طیف در جدول زیر آمده است.

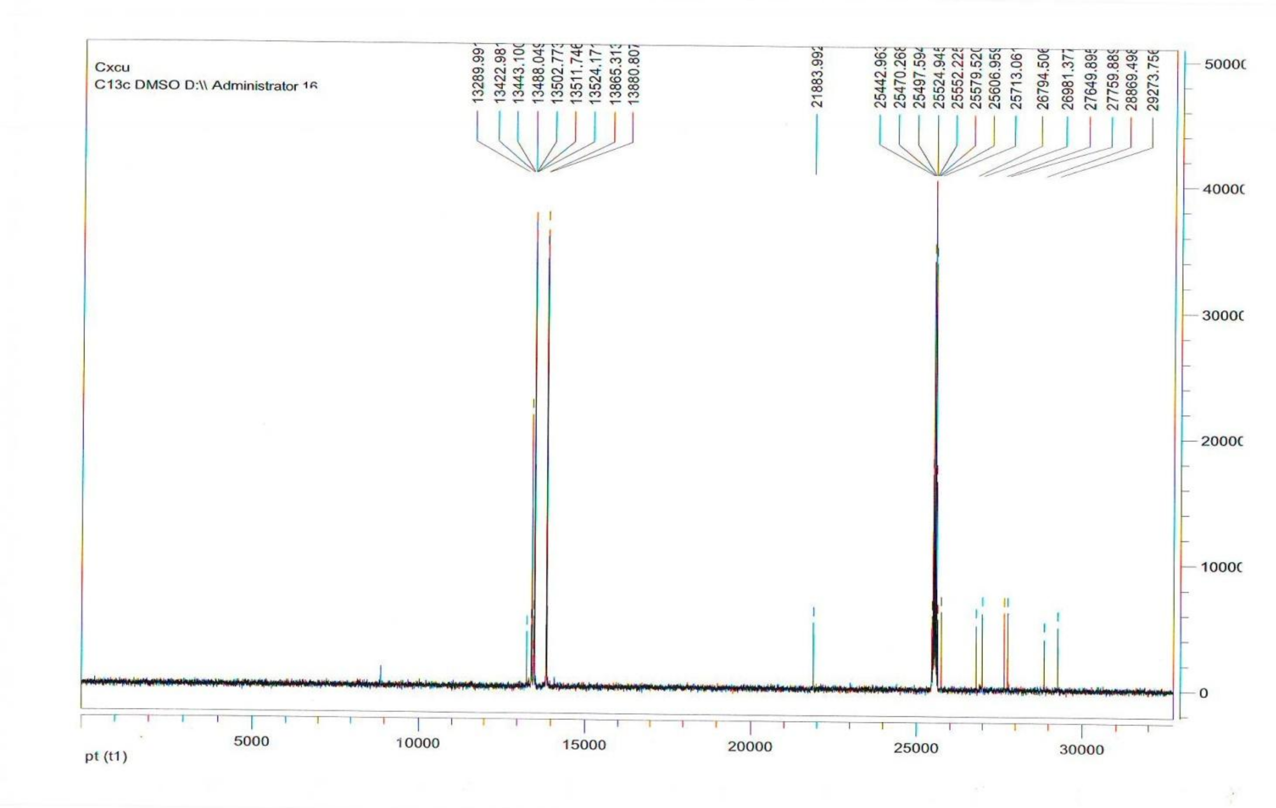
شکل پیک	تعداد پروتون	δ (PPm)	نوع پروتون
پیک یکتایی	2	21281	CH_2 P
پیک ۵ تایی	5	24397	C_2H_5 O
پیک های متعدد	15	14702	3 C_6H_5



طیف ۲. طیف ^{1}HNMR ترکیب $[Cu_2Cl_6]$ $[C_2H_5COO(CH_2PPh_3Br)]$

طیف ۳ . طیف CNMR ترکیب $[Cu_2Cl_6]$ $[C_2H_5COO(CH_2PPh_3)]$ را نشان می دهد . در این طیف ، پیک دوتایی در 26981 -26794 مربوط به کربن های گروه اتیل متصل به اتم اکسیژن است و پیک های موجود در 25713- 25442 مربوط به حلال DMSO می باشد . پیک های دوتایی موجود در 29273- 28869 مربوط به کربن متیل متصل به اتم فسفر و پیک های دوتایی موجود در 27759- 27649 مربوط به کربن های فنیل متصل به اتم فسفر و پیک یکتایی موجود در 21883 مربوط به کربن گروه کربونیل و پیک های چندتایی موجود در 13880- 13289 مربوط به کربن های آروماتیک حلقه های بنزن می باشد که خلاصه نتایج آن در جدول زیر آمده است .

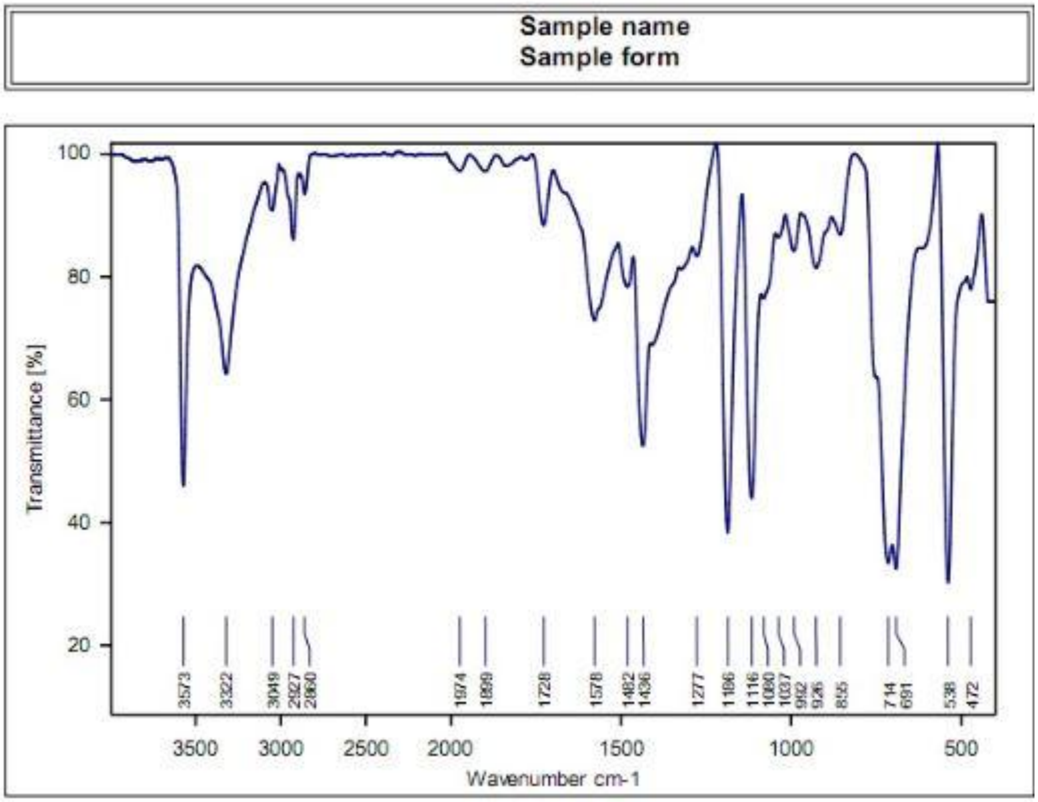
شکل پیک	δ (PPm)	نوع کربن
پیک دوتایی	26794 - 26981	C_2H_5O
پیک دوتایی	28869 - 29273	CH_2P
پیک یکتایی	21883	C - O
پیک چندتایی	13289 - 13880	آروماتیک
پیک دوتایی	27649 - 27759	P - C



طیف ۳ . طیف CNMR ترکیب $[Cu_2Cl_6]$ $[C_2H_5COO(CH_2PPh_3)]$

طیف ۴ . طیف IR ترکیب $[C_2H_5COO(CH_2PPh_3)]$ $[Cu_2Cl_6\ Br]$ را نشان می دهد. در این طیف، جذب قوی در ناحیه 538 مربوط به ارتعاشات کششی پیوند C - Br است . همچنین جذب قوی ناشی از ارتعاشات کششی C - O غیر استری در ناحیه 734 ظاهر می شود . جذب های مشاهده شده در 1116 و 1186 به ترتیب مربوط به ارتعاشات کششی پیوندهای C - C و C - O استری می باشد . جذب نوری در ناحیه 1436 مربوط به ارتعاشات کششی $P - CH_3$ و ارتعاشات پیوند فسفر - کربن در فنیل می شود و جذب در ناحیه 1728 مربوط به ارتعاشات کششی پیوند C = O می باشد .

در نهایت جذب های طیف در 2860 ،جذب متوسط در 3322 و جذب قوی در 3573 به ترتیب مربوط به ارتعاشات کششی متقارن CH_3 ، ارتعاشات کششی متقارن و نامتقارن CH_2 و همچنین ارتعاشات کششی C - H های حلقه متیل موجود در ترکیب می باشد .



طیف ۴ . طیف IR ترکیب $[C_2H_5COO(CH_2PPh_3)]$ $[Cu_2Cl_6\ Br]$

نتایج آنالیز عنصری این ترکیب با فرمول تجربی $C_{44}H_{44}Cl_6Cu_2BrO_4$ در جدول زیر آمده است :

%N	%H	%C	$C_{44}H_{44}Cl_6Cu_2BrO_4$
ــــ	3.92	45.15	آزمایشی
ــــ	3.87	46.49	نظری

نتیجه گیری

در این پژوهش ، سنتز کمپلکس مس (II) با استفاده از نمک فسفونیوم حاصل از ترکیب PPh_3 با اتیل برمو استات بررسی شد . این ترکیب کاربردهای متنوعی در صنایع شیمیایی دارد که از جمله آن ها می توان به کاتالیزور در واکنش Heck ، واکنش Suzuki و واکنش هیدروژنه کردن کربن ، ایزومره کردن الفین های ترمینال و تغییر گروه در وینیل اتر ها اشاره کرد .

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سنتز و شناسایی کمپلکس های مس (II) با استفاده از نمک فسفونیوم حاصل از ترکیب تری فنیل فسفین با اتیل برمو استات, با استفاده از روش های استروسکوپی

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چکیده

نمک های فسفونیم دارای فرمول کلی $R_4 P^{+} X^{-}$ بودهمانند $[P(CH_3)^{+}_{4}]^{-}$.بطور کلی فسفونیوم به یک مشتق آلی گفته می شود که از یون فرعی فسفونیوم چهارضلعی (PH^{+}) مشتق شده اند. ..مانند تترا متیل فسفونیوم کلرید و تترا متیل فسفونیوم یدید.

در این پروژه ترکیبات فسفونیوم $[C_2H_5COO\ (CH_2PPh_3Br)]$ و کمپلکس مس (II) آن $[C_2H_5COO\ (CH_2PPh_3Br)]$ $[Cu_2Cl_6]$ تهیه و مشخص گردیدند.نمک فسفونیوماز واکنش اتیل برمو استات با تری فنیل فسفین تهیه و مشخص گردیدند.آنگاه با استفاده از واکنش بین ترکیب فسفونیوم با $Na_2[Cu_2Cl_6]$ ترکیب های نهایی تهیه شدند. سپس با استفاده از روش های طیف سنجی تهیه ی این ترکیب ها مورد بررسی قرار گرفت.

واژگان کلیدی : *فسفونیوم , ترکیب های مس (II) , تری فنیل فسفین , اتیل برمو استات*

مقدمه :

نمک های آلکیل تری فنیل فسفوینم برای تهیه واکنشگر wittig در واکنش wittig به طور گسترده استفاده شد. این نمک ها به آسانی توسط واکنش تری فنیل فسفین با یک الکید آلدهید ساخته می شوند. اگر الکیل، متیل یا الکیل گروه اصلی بازداری فضایی نشده باشند، واکنش بخوبی انجام می شود. اما معمولاً واکنش با الکیل هالید ثانویه یک واکنش ضعیف است. گروههای الکیل سه گانه نمی توانند ایلید را تولید کنند. نمک فسفونیم ترکیب پایداری است که غالباً از اتانول و از طریق تبلور مجدد بدست می آید [1]. در سالهای اخیر، نمک های فسفونیم به دلیل ساختار، ویژگیها و واکنش پذیری خود بسیار مورد پسند قرار گرفته اند.

واکنش آیلید با آلدهیدها یا کتون ها، که یکی از رایج ترین روشها برای تولید آلکن هایی در یک طیف خاص است، اولین باز توسط جورج ویتیگ معرفی شد. این واکنش مرحله اصلی تولید تعداد زیادی از فراورده های طبیعی و بیولوژیکی است. مزیت اصلی واکنش ویتیگ انتخاب فضایی آن است. انتخاب فضایی به چند عامل بستگی دارد. ساختار نمک فسفونیم وجود کاتیون های فلزی و شرایط آزمایشگاهی است [2].

واکنش ویتیگ علاوه بر تحقیقات کاربردی استفاده های گسترده ای در تولید مواد دارویی و صنعتی دارد. برای آغاز واکنش، ابتدا الکیل هالید با یک فسفین وارد واکنش می شود تا فسفین کاتیون چهار وجهی بدست آید. برای تولید یک ترکیب خنثی، که آیلید فسفونیم نامیده می شود، این کاتیون با یک باز قوی مانند بوتیل لیتیم پروتون زدایی می شود.

آیلید کربن را با بار منفی باردار می کند، به عنوان یک نوکلئوفیل عمل کرده و به گروه کربونیل آلدهید یا کتون حمله می کند. فلزهای حفاظتی و مهارکننده خوردگی نقش مهمی در صنعت ایفا می کنند. اغلب محافظت کننده ها و مهارکننده ها ترکیب های آلی هستند که دارای هترو اتم هایی مانند فسفر، نیتروژن، سولفور و اکسیژن هستند. این ترکیب ها و مشتقات آنها آهن و فولاد را در مقابل خوردگی بازداری می کنند. بسیاری از این مهارکننده های خوردگی و حفاظتی اثرات زیان باری بر محیط زیست دارند. بنابراین دستیابی به مهارکننده های آلی موثر و غیر سمی برای آهن و فولاد موضوعی حائز اهمیت است. مهارکننده مناسب برای محیط زیست می بایست دارای ویژگی های زیست تخریب پذیری بوده و برای محیط زیست مخرب نباشد. ترکیب های فسفونیم در محلول های اسیدی به عنوان محافظ برای اغلب فلزات استفاده می شوند [3].

ترکیب های چهار وجهی فسفونیم در بسیاری از سیستم ها به عنوان عوامل مهارکننده رشد باکتری شناخته شده اند، که به طور گسترده در محیط زیست استفاده می شود [4]. مزایای این ترکیب ها شامل این موارد است: سمیت بسیار پایین، فرسایش سریع در محیط زیست (از طریق هیدرولیز، اکسیداسیون، تجزیه نوری و تجزیه بیولوژیکی)، و اثرات غیر تخریبی بر محیط زیست [5].

برای مثال، تری فنیل فسفونیم برومید در محلول اسی سولفوریک ۰/۵ مول به عنوان یک بازدارنده خوردگی برای آهن و فولاد شناخته شده است و توسط ارزیابی های گالوانوستات و پوتنتیو استاتیک و با استفاده از اسپکتروسکوپی FT-IR و تصاویر حاصل از میکرویکوپ الکترونی و محاسبه کوانتوم تایید شده است [6]. همچنین برخی گزارشات در مورد تهیه پلیمرهای فعال بیولوژیکی با استفاده از گروههای آمونیوم و فسفونیم چهار وجهی، که دارای استفاده دارویی است، ارائه شده اند [7].

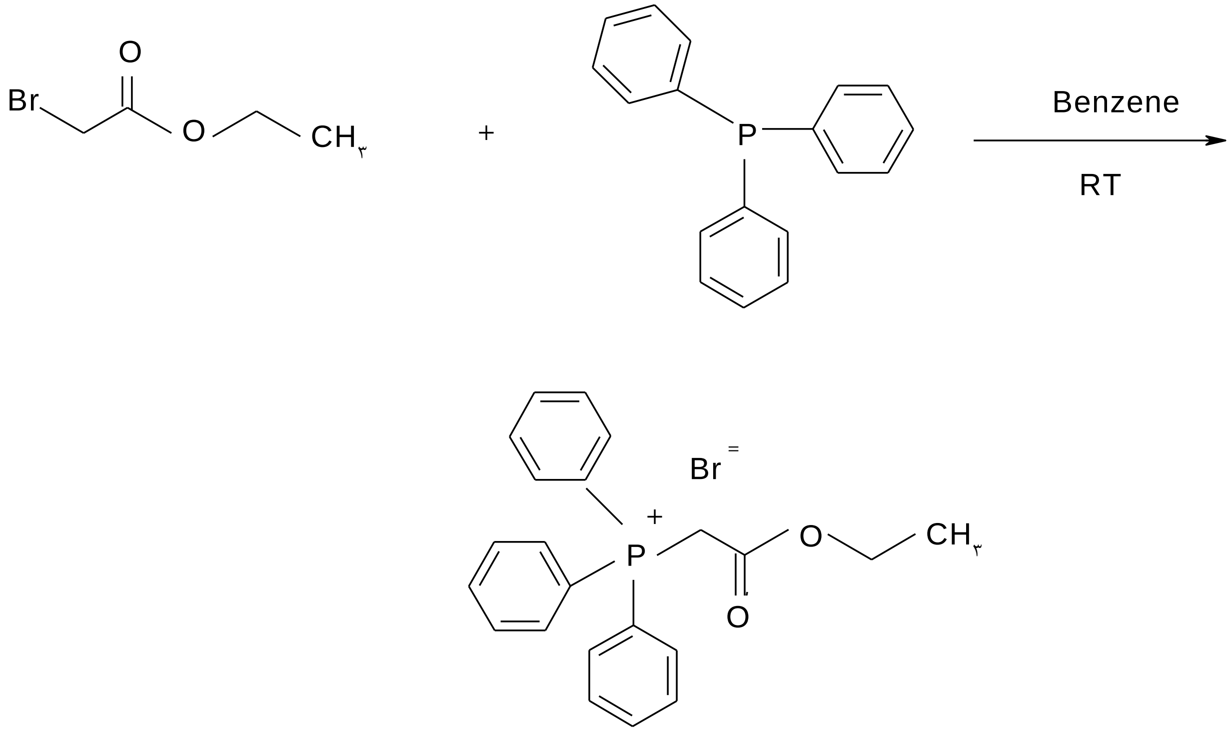
تولید مایعات یونی کاربرد دیگری از نمک های فسفونیم است که این مایعات نمک های آلی می باشند که در دماهای پایین (کمتر از ۱۰۰ درجه سناتیگراد) دارای حالت مایع بوده [8] و دارای مزیت هایی چون طیف دمایی گسترده خروجی مایع، پایداری حرارتی و شیمیایی بالا، حلال های قوی و فشار بخار بسیار پایین در ترکیب با ترکیب های آلی، کاتالیست های شیمیایی، روشهای مختلف جداسازی و نقش در الکترولیت های جدید در ساخت سلول های خورشیدی و سوختی هستند [9]. در سالهای اخیر مطالعات زیادی روی سیستم های فسفونیم چهار وجهی و ترکیب های جدید فسفونیم به نام مایعات یونی صورت گرفته است و استفاده از نمک های فسفونیم بیشتر از هر زمان دیگری است [10].

در سالهای اخیر حسگرهای رطوبتی پلیمر مهمی ساخته شده اند. انواع مختلفی از مونومرهای حساس به رطوبت در ساخت سنسورهای رطوبتی مورد استفاده قرار گرفته اند، از جمله نمک کاتیونی و آنیونی. نمک های فسفونیم به دلیل سادگی و تهیه آسان و پایداری بالا تحت شرایط مختلف در مقادیر بسیار زیاد برای ساخت سنسورهای پلیمری رطوبت مورد استفاده قرار می گیرند. اخیراً نمک های تری فنیل فسفونیم کلرید تهیه و در تولید سنسورهای رطوبتی ضدآب استفاده شده اند. می توان از تری بوتیل فسفونیم کلرید به عنوان یک مونومر در تولید این سنسورها استفاده نمود [11]. نمک های فسفونیم به طور موفقیت آمیزی به عنوان کاتالیست در انواع بسیاری از واکنش های آلی استفاده شده اند بطوریکه می توان گفت که این فعالیت کاتالیزوری نمک نمک ساده فسفونیم به عنوان واکنش بنزیل کلرید فسفونیم آلکوکسیسیل سیانو کتون ها و استفاده از نمک فسفونیم به عنوان کاتالیزور اسید لوئیس بدون فلز است که رشد در زمینه کاتالیزورهای آلی را سرعت بخشیده است [13].

روش آزمایش :

فرآیند تهیه ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$

در این مطالعه 10 m mol اتیل برمو استات (1.1 ml)و 10 m mol تری فنیل فسفین (2.62 gr) را بصورت جداگانه در 50 ml بنزن حل کرده و سپس به یک بالن 100 ml اضافه می کنیم. که پس از 2 الی 3 دقیقه شروع به رسوب می کند و تا 24 ساعت در دمای اتاق هم زده شد.سپس محلول را پس از شستشو با دی اتیل اتر . صاف کرده و سپس در دسیکاتور خشک گردید. وزن رسوب بدست آمده 2.98 gr و بازدهی واکنش 69٪ بود. که این رسوب در دمای $165\ ^0c$ ذوب شد.



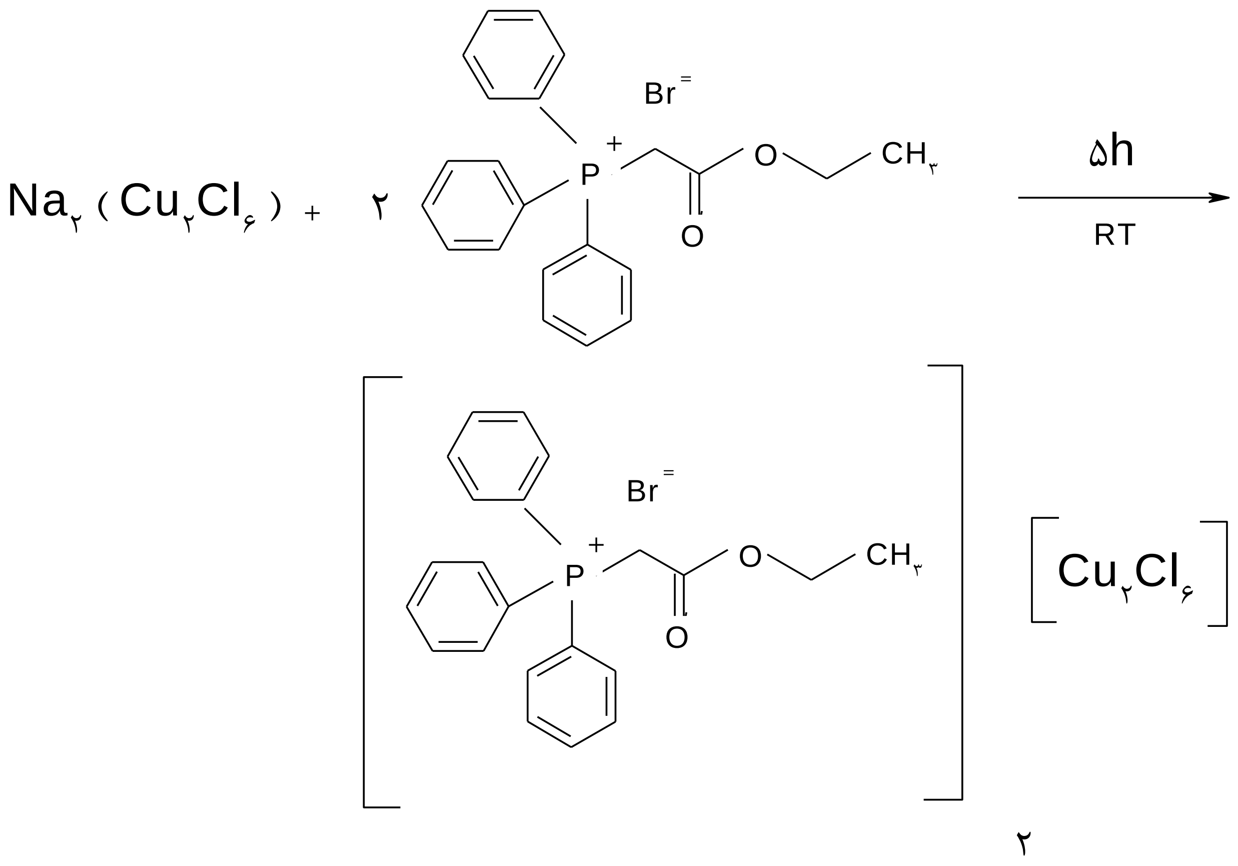
فرآیند تهیه $[C_2H_5COO(CH_2PPh_3Br)]$

تهیه کمپلکس مس (II)

فرآیند تهیه کمپلکس $[C_2H_5COO(CH_2PPh_3Br)]\ [Cu_2Cl_6]$

دراین مرحله 0/1 گرم $CuCl_2$ (0.74 m mol) و 0/17 گرم NaCl(2.9 m mol) در یک شیلنگ لوله ای ریخته شد. سپس 10 ml متانول به آن اضافه شد. و محلول در دمای $50\ ^0c$ به مدت 5 ساعت هم زده شد تا یک محلول شفاف سبز مایل به زرد مطابق طرح زیر به دست آمد. سپس مقدار 0/32 گرم ترکیب فسفونیوم (0/76 m mol) به آن افزوده شد.که سریعا شروع به تشکیل رسوب آبی فیروزه ای رنگی کرد . که وزن آن 0/15 گرم و بازدهی واکنش 25.86٪ بوده و در دمای $218\ ^0c$ ذوب شد.

$$۲\,NaCl + ۲\,CuCl_۲ \xrightarrow[۵۰\ C]{Me\,oH} Na_۲(Cu_۲Cl_۶)$$

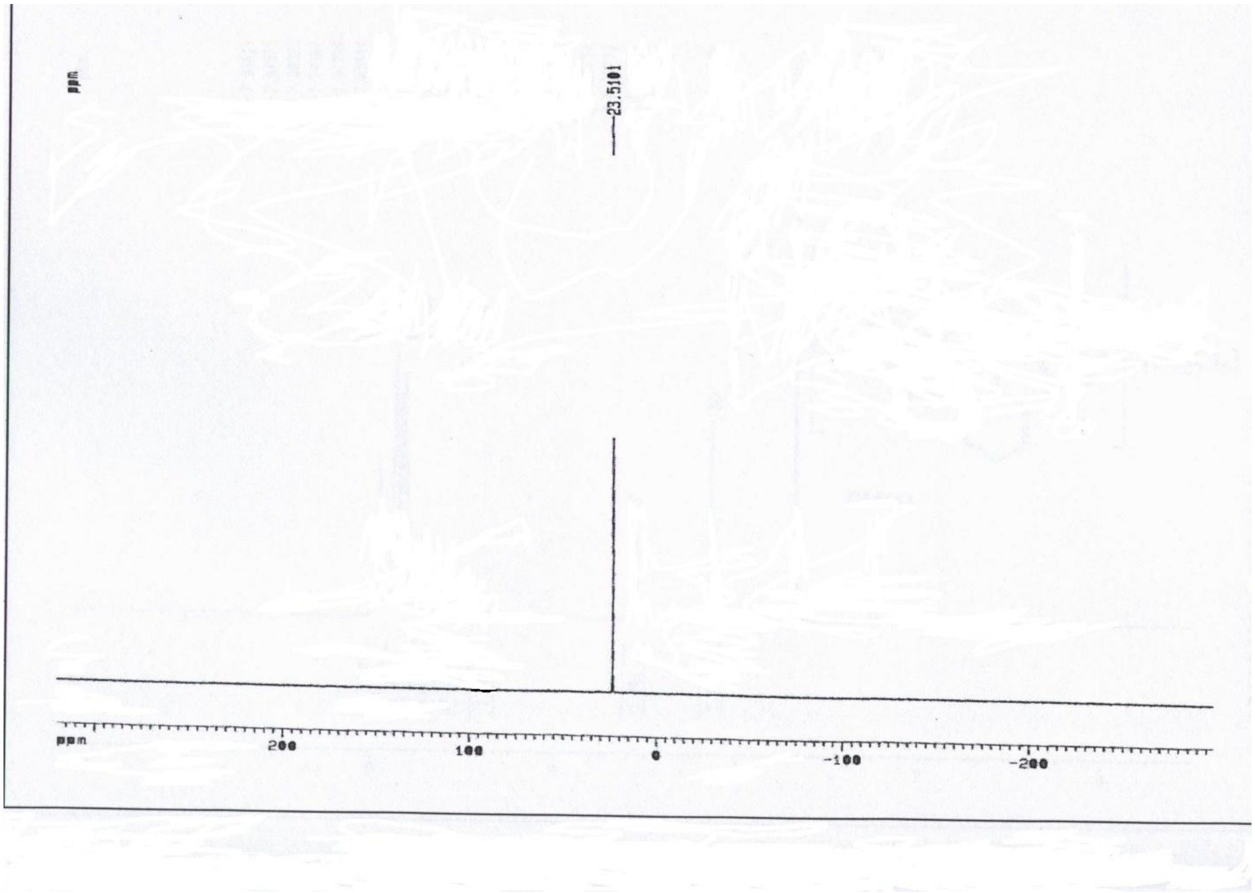


نتایج

به منظور تعیین ترکیب های بدست آمده طیف NMR شامل PNMR – CNMR – HNMR با استفاده از FT-NMR400 اندازه گیری شد. و طیف مادون قرمز با استفاده از دستگاه مدل FT-IR.Bommen و روغن نوژول وقرص KBr ارزیابی شد و نتایج زیر بدست آمد :

طیف ۱. طیف ^{31}PNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]\ [Cu_2Cl_6]$را نشان می دهد. دراین طیف ، رزونانس فسفر در $\delta = 23.66$ PPm به شکل یک پیک یکتایی ظاهر می شود. شکل پیک در مقایسه با پیک فسفر دارای لیگاند آزاد در فنیل فسفین $\delta = 4.8$ PPm ظاهر می شود، نشان می دهد که اتم فسفر با اتم کربن یک پیوند جدید به وجود آورده است که با کاهش چگالی الکترون در اتم فسفر، پیک فسفر به میدان های پایین تر تغییر مکان می دهد. همچنین این پیک برای ترکیب های مشابه در $\delta = 24.22$ PPm ظاهر می شود.

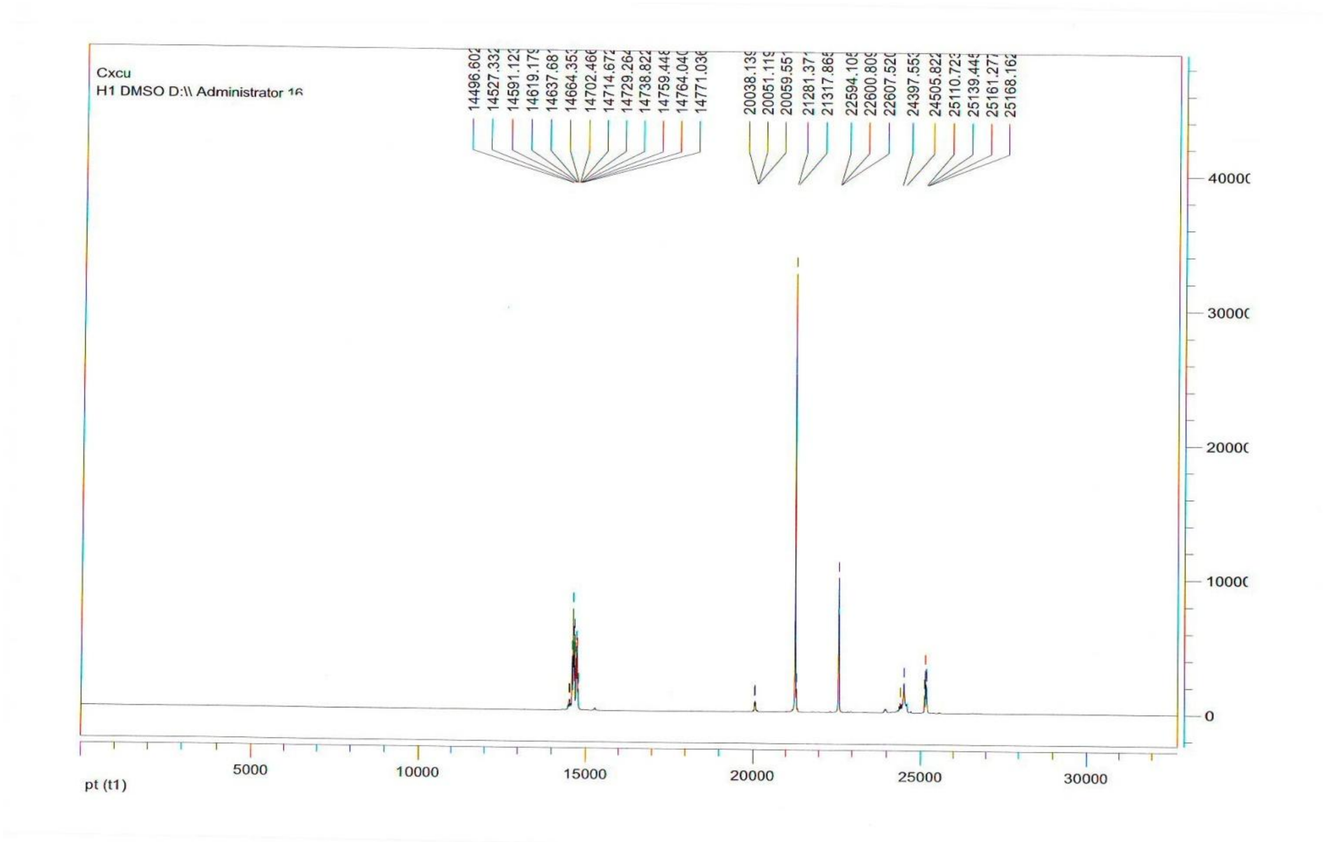
این پیک نشان دهنده شکل گیری ترکیب مورد نظر می باشد و پیک یکتایی فسفر در این طیف نشان دهنده ی خلوص بالای ترکیب است.



طیف ۱ . ^{31}PNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$ $[Cu_2Cl_6]$

طیف ۲. طیف ^{1}HNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$ $[Cu_2Cl_6]$ را نشان می دهد.. در این طیف پیک یکتایی در 21281 مربوط به گروه متیل متصل به فسفر می باشد .پیک ۵ تایی مربوط به هیدروژن های گروه اتیل متصل به اتم اکسیژن است که به دلیل افزایش چگالی الکترون ناشی از اتصال به اتم اکسیژن در میدان 24397 ظاهر می شود.و پیک های متعدد در 14496 تا 14771 مربوط به هیدروژن های آروماتیک ترکیب است که خلاصه نتایج این طیف در جدول زیر آمده است.

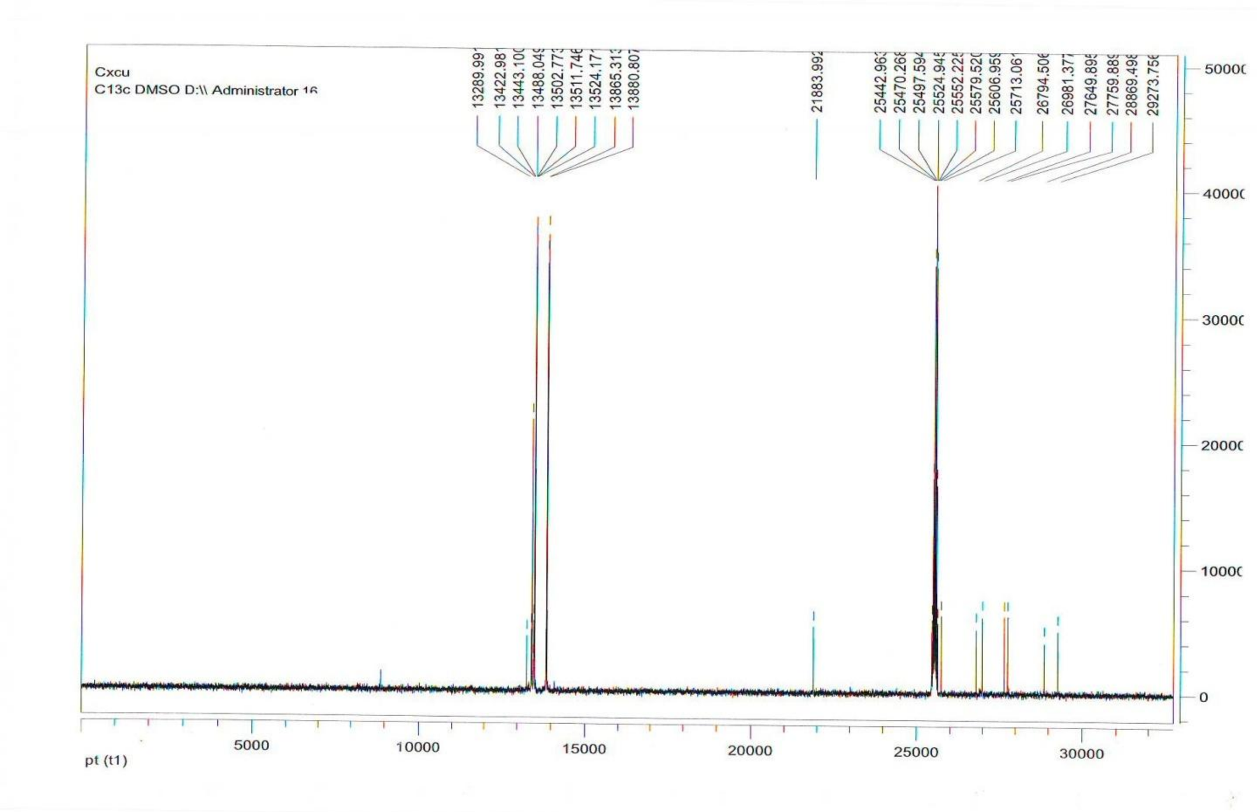
شکل پیک	تعداد پروتون	δ (PPm)	نوع پروتون
پیک یکتایی	2	21281	CH_2 P
پیک ۵ تایی	5	24397	C_2H_5 O
پیک های متعدد	15	14702	3 C_6H_5



طیف ۲. طیف ^{1}HNMR ترکیب $[C_2H_5COO(CH_2PPh_3Br)]$ $[Cu_2Cl_6]$

طیف ۳ . طیف CNMR ترکیب $[C_2H_5COO(CH_2PPh_3)]$ $[Cu_2Cl_6]$ را نشان می دهد . در این طیف ، پیک دوتایی در 26981 -26794 مربوط به کربن های گروه اتیل متصل به اتم اکسیژن است و پیک های موجود در 25713 -25442 مربوط به حلال DMSO می باشد . پیک های دوتایی موجود در 29273 -28869 مربوط به کربن متیل متصل به اتم فسفر و پیک های دوتایی موجود در 27759 -27649 مربوط به کربن های فنیل متصل به اتم فسفر و پیک یکتایی موجود در 21883 مربوط به کربن گروه کربونیل و پیک های چندتایی موجود در 13880 -13289 مربوط به کربن های آروماتیک حلقه های بنزن می باشد که خلاصه نتایج آن در جدول زیر آمده است .

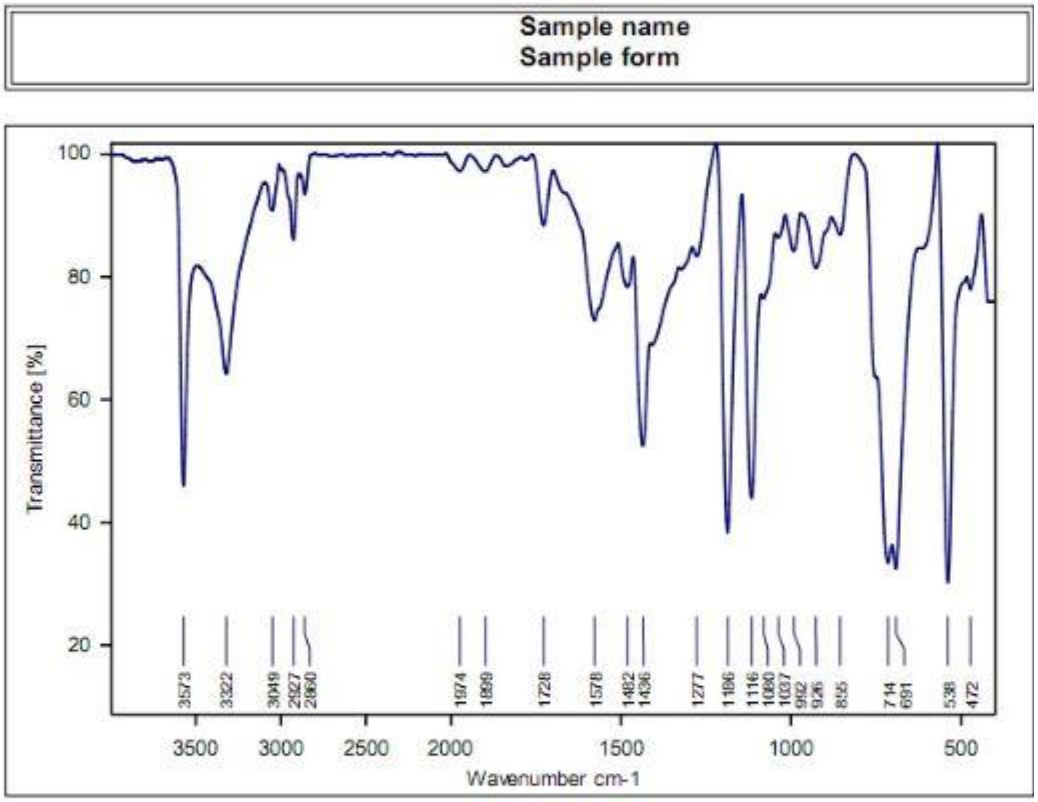
شکل پیک	δ (PPm)	نوع کربن
پیک دوتایی	26794 - 26981	C_2H_5O
پیک دوتایی	28869 - 29273	CH_2P
پیک یکتایی	21883	C - O
پیک چندتایی	13289 - 13880	آروماتیک
پیک دوتایی	27649 - 27759	P - C



طیف ۳. طیف CNMR ترکیب $[C_2H_5COO(CH_2PPh_3)]\ [Cu_2Cl_6]$

طیف ۴ . طیف IR ترکیب $[C_2H_5COO(CH_2PPh_3)]$ $[Cu_2Cl_6\ Br]$ را نشان می دهد. در این طیف، جذب قوی در ناحیه 538 مربوط به ارتعاشات کششی پیوند C - Br است . همچنین جذب قوی ناشی از ارتعاشات کششی C - O غیر استری در ناحیه 734 ظاهر می شود . جذب های مشاهده شده در 1116 و 1186 به ترتیب مربوط به ارتعاشات کششی پیوندهای C - C و C - O استری می باشد . جذب نوری در ناحیه 1436 مربوط به ارتعاشات کششی $P - CH_3$ و ارتعاشات پیوند فسفر - کربن در فنیل می شود و جذب در ناحیه 1728 مربوط به ارتعاشات کششی پیوند C = O می باشد .

در نهایت جذب های طیف در 2860 ،جذب متوسط در 3322 و جذب قوی در 3573 به ترتیب مربوط به ارتعاشات کششی متقارن CH_3 ، ارتعاشات کششی متقارن و نامتقارن CH_2 و همچنین ارتعاشات کششی C - H های حلقه متیل موجود در ترکیب می باشد .



طیف ۴ . طیف IR ترکیب $[C_2H_5COO(CH_2PPh_3)]$ $[Cu_2Cl_6\ Br]$

نتایج آنالیز عنصری این ترکیب با فرمول تجربی $C_{44}H_{44}Cl_{6}Cu_{2}BrO_{4}$ در جدول زیر آمده است :

%N	%H	%C	$C_{44}H_{44}Cl_{6}Cu_{2}BrO_{4}$
___	3.92	45.15	آزمایشی
___	3.87	46.49	نظری

نتیجه گیری

در این پژوهش ، سنتز کمپلکس مس (II) با استفاده از نمک فسفونیوم حاصل از ترکیب PPh_3 با اتیل برمو استات بررسی شد . این ترکیب کاربردهای متنوعی در صنایع شیمیایی دارد که از جمله آن ها می توان به کاتالیزور در واکنش Heck ، واکنش Suzuki و واکنش هیدروژنه کردن کربن ، ایزومره کردن الفین های ترمینال و تغییر گروه در وینیل اتر ها اشاره کرد .

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19th Iranian Inorganic Chemistry Conference
Chemistry & Chemical Engineering Research Center of Iran
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5-7 September 2017
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Synthesis and identification of copper II complexes using phosphonium salt From the combination of trinylphosphine with ethyl bromoacetate, using stereoscopic methods

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Phosphonium salts have the general formula $R_4 P^+ X^-$ such as $[P(CH_3)^{+}{}_{4}]^{-}$. Phosphonium is generally referred to as an organic derivative derived from the quaternary Phosphonium ion PH such as tetramethylphosphonium chloride and tetramethylphosphonium iodide .

In this paper , Phosphonium compounds $[C_2H_5COO\ (CH_2PPh_3Br)]$ and its copper II complex $[C_2H_5COO\ (CH_2PPh_3Br)]\ [Cu_2Cl_6]$ were prepared and identified. Phosphonium content was prepared from the reaction of ethyl bromoacetate with terphenylphosphine . Then, with The reaction was prepared by the combination of phosphonium with $Na_2[Cu_2Cl_6]$ final compounds. Then, using these spectroscopic methods, preparation of these compounds was investigated .

Keywords : Phosphonium , Copper (II) , Triphosphine , Ethylbromoacetate

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Partial interaction studies of a synthesised Platinum (II) antitumor complex with BSA and DNA.

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Anti-cancer properties of cisplatin have been discovered by B.Rosenberg in 1960. Its commercially successful analogues, carboplatin, oxaliplatin, nedaplatin…..etc are second generation drugs. These properties are mostly due to their interaction with cell DNA.

Present research work includes synthesis of a platinum (II) complex of formula [Pt (en) (2-py)] Cl (Where en = ethylenediamine and 2-py = 2-pyridinecarboxylate) and characterized by elemental analysis (C, H, N), conductivity measurement, and by UV-Visible, IR, and ^{1}H NMR spectroscopic techniques[1].

The interaction of the complex with calf thymus DNA (CT-DNA) and bovine serum albumin (BSA) were carried out using UV-Visible spectroscopy in 30 mmol/L Tris-HCl buffer of pH =7.0 at two temperatures of 300 and 310K. In these studies, K_{app}, the apparent equilibrium constant are 2.3×10^{4} M^{-1} and 2.5×10^{4} at 300K and 1.7×10^{4} M^{-1} and 1.4×10^{4} M^{-1} at 310K for BSA and DNA respectively. The above compound can interact with BSA as well as DNA and the concentration of the complex in the midpoint of transition, $[L]_{1/2}$, is increased by increasing the temperatures from 0.028 mmol/L to 0.033 mmol/L for BSA and from 0.029 mmol/L to 0.035 mmol/L for DNA at 300K and 310K respectively. This complex can inhibit the growth of K562[2] cancer cells and has Cc_{50} value (50% cytotoxic concentration) of 40 µM.

Keywords: antitumor activity, Pt (II) complex, BSA/DNA-binding

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Reduction and Dechlorination of Chlorinated ethylenes by nano Particles of Iron doped on Graphen Oxide Sheets

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Abstract

In this paper, a new criterion for reducing chlorinated ethylenes is proposed. The proposed method is based on converting graphene oxide into magnetic sheets by nano zero valent iron particles. A laboratory study conducted to investigate to remove chlorinated ethylenes from aqueous solution. Dechlorination reaction of two important pollutants in the environment, 1,1,2-tri-chloroethene(TCE) and tetra-chloroetene(PCE) studied. The results showed that both pollutants converted almost completely in presence of magnetic graphene oxide surfaces.

Keywords: Magnetic graphene oxide surfaces, Graphene magnetic nanoparticles of iron, Removal of chlorinated contaminants

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Introduction

The most chlorinated pollutant that in the groundwater resources are found as chlorinated ethenes. Remediation of groundwater contaminated with chlorinated ethenes has been a major environmental challenge because of their wide occurrence and limitations associated with conventional pump-and-treat approach [8].

Nanotechnology can been an effective method for removing organic pollutants such as chlorinated organic dyes, inorganic compounds and heavy metal ions [2-4]. In this regard, the use of zero-valent metals to degrade contaminants represents are an active research area environmental field.

One of popular techniques in removing pollutants is adsorption especially as eco-friendly. In addition, in the fields of environment, this method can be provide the decontamination efficiency from organic pollutants [5]. It has been shown that many of nano-based environmental technologies (e.g., sensors, sorbents) have been expected to improve or replace various conventional environmental technologies in the near future [5].

There are different methods for providing stability nZVI particles, one of the method is using of carbon materials. It was found that the carbon-based nano-materials such as carbon black (CB), carbon nanotubes (CNTs), graphene, functionalized graphene and carbon nanofibers (CNF) have been extensively investigated to use as sensors or support in various fields. Among the different carbon-based nano-materials, Graphene oxide (GO) has involved great attention on its unique electronic properties arising from the presence of both sp^2 and sp^3 carbons. In addition, Graphene oxide consists of a two-dimensional (2D) sheet of covalently decorated C atoms bearing various oxygen functional groups (e.g., hydroxyl, epoxy, and carboxyl) either on the basal plane or at the edges. In addition, layered nanostructures GO allow to regard it as support for preparation of nano composites with high thermal and chemical stabilities [6].

Since the incorporation of magnetite part into Graphene can be considered as a rapid and effective technique for removing pollutants and so it is possible to separate nanoparticles from aqueous solutions [7].

In reductive dechlorination reaction, like oxidation, it is need that the contaminant molecular structure modified such that the contaminant structure can be transformed to a more benign substance and then removes chlorine atoms from hydrogen-carbon molecules. In this regard, electron donating or reductive properties of nZVI have been considered[8]. In addition, it was notable that iron with its relative low standard potential (E_0, 0.41V) is an effective and environmentally friendly electron donor [9-11].

In this paper, our research experiment results is showed that magnetic surface of GO can be provide a high efficiency in properties enhancement of nano-zero valent iron catalytic activation for dechlorination of chlorinated ethenes, also it is interesting to note that GO-iron oxide hybrid materials have high adsorption capabilities for organic pollutants. In addition, the large surface area and stability of GO as a stable support to motivate us to employed magnetite-GO hybrids for organic pollutant removal.

Experimental Section

Synthesis of GO-iron nanocomposites: All of reagents and solvents employed for synthesis were purchased from Sigma-Aldrich or Merck and used as received. GO was synthesized using modified Hummers method [1] from natural flake graphite (48 μm, 99.95 % purity). Briefly, 1.0 g of graphite, 1.0 g of $NaNO_3$, and 40 mL of H_2SO_4 were mixed and stirred in a three-neck flask in a cool bath, and then 6.0 g of $KMnO_4$ was slowly added and stirred for about 1 h. Then 80 mL Milli-Q water added and the solution stirred for 30 min at temperature 90 ± 1 ^{o}C. Finally, 150 mL Milli-Q water added again, and 6 mL H_2O_2 (30%) slowly added, turning the color of the solution from dark brown to yellow. The warm solution filtered and rinsed with 100 mL of Milli-Q water. The filter cake dried under vacuum and a dark brown GO powder obtained.

Fe-GO: 0.15 g GO ultrasonicated in 200 mL Milli-Q water to form a homogeneous suspension. So that, the solution transferred to a three-neck flask and purged with N_2. An aqueous solution of $FeCl_2.6H_2O$ (0.33 g) and $FeSO_4$-$7H_2O$ (0.38 g) in Milli-Q water (5 mL) was injected to the GO suspension. The mixture heated to 80 ^oC and stirred constantly under N_2. Following, 10 mL 30% ammonia solution added to adjust pH to 10 and, the mixture stirred and kept at 80 ^{o} C for 30 min. At last, 1.0 g tri-sodium citrate added to the solution while the temperature raised to 95 ^{o} C. The product (black suspension) separated with a permanent magnet, rinsed with Milli-Q water for several times, and dried at 60 ^oC. The GO-iron oxide composite obtained.

The GO-iron composite characterized by FT-IR spectra and using of a Perkin-Elmer RXI spectrometer. The chemical structure of nano-composite examined using of X-ray photoelectron spectroscopy (XPS). XPS measurements performed by Bestec spectrometer. The surface areas were determined by nitrogen adsorption-desorption isotherms (Belsorp mini). Brunauer-Emmett-Teller (BET) specific surface area and pore volume measured by nitrogen sorption using a micromeritics model PHS 1020.

The total amount of un-reacted PCE or TCE, both in aqueous solution and sorbet by nZV-related surfaces measured using a modified extraction method and injection to GC(HP5890) for performing of analysis.

The TCE or PCE concentration in the organic phase measured by GC(pentane (1.6 mL) added into the reactors, and then the reactors shaken), the concentration of TCE and byproducts in pentane solution was measured using GC.

Catalytic Experiment: Degradation PCE and TCE performed in the presence of GO-Fe nanocomposites and different concentrations of the regents at 25 °C. Stock n-hexane solutions of Fe-GO (2-10 mg), TCE or PCE (34 μL), and neat dodecane (2 μL) as an internal standard put into a 5-mL round-bottomed flask containing n-hexane (2 mL) and H_2O (0.25 mL) was added to initiate the reaction. The reaction solution stirred for the required time, and then aliquots (2 μL) removed from the reaction solution and injected into the GC column (before the sample injected, filtered through 0.2 mm Milipore syringe filters and so immediately injection into the GC column). The temperature program for the analysis was 1 min at 70 °C, and the rate program was set at 10 $°Cmin^{-1}$ up to 200 °C and 5 min at 200 °C. Data were obtained in triplicate to ensure precision, and the repeatability of the data was within ±5%. The concentration of the acetone and vinyl chloride determined by comparing of its peak area with internal standard.

3. Results and Discussion

Zero-valent iron has been shown to be very effective in the dechlorination of chlorinated olefins. The objective of this research study based on use of Graphene oxide (GO) decorated with nanoparticles Fe^0 for removing chlorinated organic compounds such as 1,1,2-tri-chloroethene (TCE) and tetra-chloroetene (PCE) that are usually found in groundwater systems. In fact, our goal is investigation the reductive dechlorination of trichloroethylene (TCE) and tetrachloroethylene (PCE), by nano-zero valent iron (Fe^0) supported on GO sheets in water-limiting conditions for removing chlorinated organics contaminants from aqueous solution. These results suggest that catalytic properties nano particle Fe-zero valent decorated on graphene sheets can have an important role in transferring electron to halogenated ethylenes.

According to Table 1, it was found that the reductive elimination occurred by atoms the iron supported on surface GO in which electron transfer of nano particles iron leads to dechlorination of

TCE and PCE. The advantage of major use of nano zero-valent iron as reductive displayed that nano zero valent iron decorated on graphene sheets more stable and effective than nano particle zero valent iron alone. In the other hand, GO-sheet acted as a supporter for nano particles Fe^0. The results of reductive dechlorination TCE and PCE showed that graphene oxide could be provide a large specific surface for iron nanoparticls by their supported on graphene sheets and lead to enhanced future foster reactivity for the conversion of recalcitrant environmental pollutants.

We developed a new method for reducing halogenated ethylenes by graphene oxide decorated by Fe^0 nano-particle structures using some process that involves transfer electrons and reduction halogenated samples to dechlorination regents. Our recent work has shown that dechlorination of chlorinated solvents by zero-valent iron are proportional to the specific iron surface area. In addition, it was found that for dechlorination of TCE and PCE, water is a critical reactant (proton donor) and may function as an electrolyte medium (electron transfer) for the reduction of TCE or PCE to occur, see Table 1.

According to GC data on PCE and in the presence of GO-Fe^0, losing of PCE and TCE measured. Thus, reaction TCE or PCE by zero-valent iron surfaces indicate that reducing of chloroethylenes comparable energetically to hydrogenolysis at neutrally pH. Although dehydrohalogention does occur for haloethylenes, it requires extreme conditions in homogeneous solution.

In this research, the groundwater contaminated to different ratio of TCE and PCE (5, 10, 25, 50 ppm) were exposed in the presence of the two value of nZV Fe-GO (2 and 5 mg) in batch reactor. Experimental data showed that more than 95 percent of TCE and PCE were removed from solution within 24 hours, Table 1.

Our results showed that degradation of chlorinated hydrocarbons using of nano-valent iron supported on GO sheets is very effective and iron nano particles doped on GO-sheets actually provided a valuable opportunity to demonstrate its positive effect on environmental quality.

In general, our proposed mechanism represented TCE or PCE as RCl in the presence of nanocompsite (Fe-GO) that transferred electrons to RCl and then converted them to the corresponding hydrocarbon RH:

$RCl + H^+ + Fe^\circ \rightarrow RH + Fe^{2+} + Cl^-$

In this research studies we concerned on the reducing power of nano-zero valent iron supported on GO toward degradation PCE and TCE. Our finding showed that Fe-dopped on GO-sheets could readily do dechlorinated reaction in aqouse media. Because zero-valent iron (Fe^0) recognized as an excellent electron donor, regardless of its particle size when it dopped on GO, the resultant composite exhibits a strong tendency to release electrons in aquatic environments. In fact, the synthesis nanocomposite also readily reacts with a wide variety of redox-amenable contaminants.

Characterization

Brunauer Emmett Teller (BET): The nitrogen sorption measurement was performed to investigate the textural characteristic of resulting nano-composites. The pore size distribution is in the range of 3 to 13 nm. It was appeared that nano particle Fe^0 dispersed on GO sheets and intercalated between the GO sheets. In addition, the nitrogen isotherm shows that the mean pore size distributions of GO- Fe nanocomposites are in range of 13 nm, Fig.1. The specific surface area ($a_{s,\ BET}$ 122.42 $m^2\ g^{-1)}$ and pore volume (0.4003 $cm^3 g^{-1}$) of the prepared nanocomposite suggest that the GO-Fe have got a mesoporouse structure.

In this work, the process of reaction followed by GC and GC-Mass instrument for determination of products. According to our result obtained by the GC-Mass, PCE and TCE converted mainly to acetone and vinyl chloride. The prepared nanocomposite analyzed using XPS to verify the phase of NP, interaction between Fe and GO. As seen in Fig. 2, the XPS spectra of nanocomposite exhibited photoelectron lines at binding energies of 317, 446, 611 eV which are ascribed to C 1s, O 1s and Fe 2p, respectively.

CONCLUSIONS

Our results display that the catalytic activity nanocomposite can be attributed to the presence of nano-particles zero valent Fe on the GO sheets. Nanoscale zero valent iron (nZVI) is becoming an increasingly popular method for treatment of hazardous and toxic wastes and for remediation of contaminated soil and groundwater.

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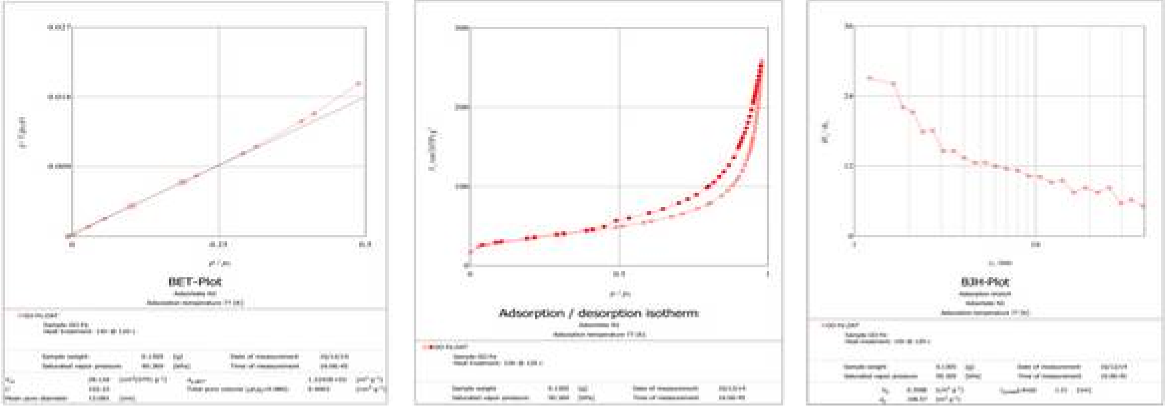

Figure 1. Nitrogen adsorption-desorption isotherms, S $_{BET}$ and pore volume of GO-Fe nanocomposite.

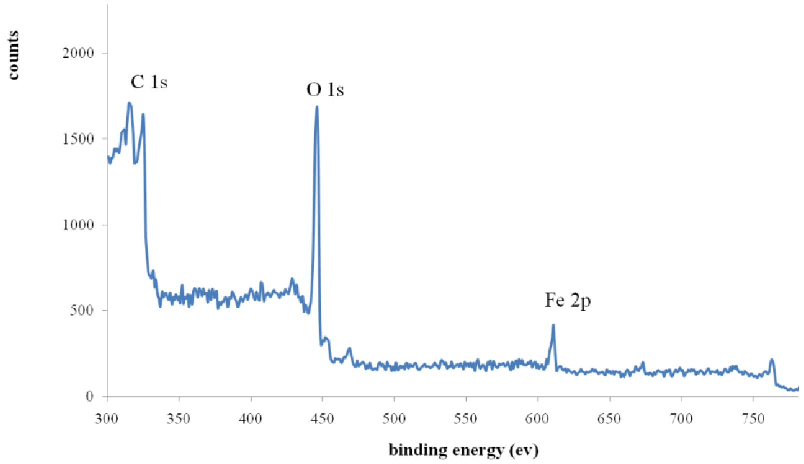

Figure. 2. XPS spectra of nano-zero valent iron-GO nanocomposite.

Table 1. Dechlorination results of TCE and PCE in presence of nZV-Fe^0

Entry	**RCl**	**Time(h)**	**Yield (**acetone and vinyl chloride **(%)**
1*	PCE	1	23(5)**
		5	67(13)**
		24	92(24)**
2*	TCE	1	26(7)**
		5	69(16)**
		24	96(31)**
3	PCE	24(1 mg)	51
		(10 mg)	97
4	TCE	24(1 mg)	47
		(10 mg)	94

*The reactions were run by 5 mg of Fe-GO composite. The all of reactions were carried out in n-hexane (1 mL)/ H_2O (0.25 mL), at 22±2 °C. All of the reactions were run at least in triplicate, and the data represent an average of these reactions with ±5–8%. The dechlorination yields (%) were measured relative to the starting reagents. Peak heights and peak areas were used to measure the concentration of various species; averaging of the two methods usually gave the most consistent results.

**The reactions were carried out in absence of H_2O.

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

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During the past decade, a great deal of attention has been paid to developing greener chemical processes and synthetic methods [1]. Catalysts bound to inorganic solids are widely used for organic transformations due to environmental and economical considerations [2]. Nanoparticles supported on a metal oxide as an inorganic solid, in particular magnetic nanoparticles (MNPs), have been extensively studied in the field of chemical catalysis, environmental protection, sensors, magnetic storage media, and clinical diagnosis treatments [3]. MNPs have great potential in view of the their recovery, since the magnetic separation of MNPs from the reaction mixture with an external magnet is simpler and more efficient than conventional separation with filtration or centrifugation. On the other hand, MNPs are accessible from inexpensive materials and can be easily supported by organic and inorganic materials [4]. Recently, MNP-supported-copper ions have been used extensively in organic transformations.[5].

In this work, a new magnetically recoverable nanocatalyst was developed by covalent binding of a ligand, 2-amino banzhydrazide and 2-hydroxy naphtaldehyde on the surface of silica coated magnetite nanoparticles (SCMNPs) and followed complexation with $CuCl_2.4H_2O$. Characterization of the prepared nanocatalyst was performed with different physicochemical methods such as FT-IR, TCP-AES, VSM, SEM EDS and TGA analyses. Finally, catalytic activity of the prepared nanocatalyst was examined in the preparation of 2-amino-4*H*-benzo[*h*]chromene derivetives through a one-pot, three component reactions of 1-naphthol, various aldehydes and malononitrile.

Keywords: Heterogeneous catalysts, Magnetic nanoparticles, Three component reactions

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www.IICC19.ccerci.ac.ir
5-7 September 2017

Dioxo-molybdenum Schiff base complex immobilized on surface modified magnetite as a nanocatalyst for the oxidation of organic compound

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Nanoscale materials have been a subject of particular interest due to properties, which differ from their bulk counterparts [1]. They have been used extensively in chemistry [2], physics [3], biology and catalysis [4]. Recently, magnetic core–shell nano-structures have attracted more attention due to their unique magnetic properties. In contrast to the difficulty observed in recovering and reusing most solid catalysts, core–shell nanostructure magnetic catalysts can be easily retrieved under the influence of a magnetic field and used in subsequent reactions. Due to this property, using magnetic core–shell structure composites as catalysts has been recommended in literature. Schiff base transition metal complexes have been extensively studied because of their potential use as catalysts in a wide range of reactions. These complexes have been extensively used for hydrogenation of organic substrates, epoxidation of olefins, conversion of epoxides into halohydrines, asymmetric ring opening of terminal epoxides and oxidation reactions [5].

In this work, a new magnetically recoverable nanocatalyst was developed by covalent binding of a ligand, 2-amino banzhydrazide and 2-hydroxy naphtaldehyde on the surface of silica coated magnetite nanoparticles (SCMNPs) and followed complexation with $MoO_2(acac)_2$. Characterization of the prepared nanocatalyst was performed with different physicochemical methods such as FT-IR,TCP-AES, VSM, SEM, EDS and TGA analyses. Finally, catalytic activity of the prepared complexes was examined in the oxidation of sulfids and epoxidation of olefins.

Keywords: Nanoscale ,materials Schiff base , nanocatalyst.

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Synthesis of phosphoramidate and it's graphene oxide composite, anticholinesterase activity and study fluorescence spectra

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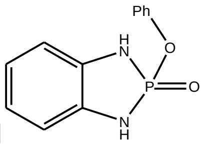
Phosphoramidates are best known for their highly toxic effect as agricultural chemicals. Phosphoramidates with the general structure of X–(NH)2P(O) skeleton are important class of compounds that exhibit the insecticide properties to inhibit the acetylcholinesterase (AChE) enzymes [1, 2]. little attention has been given on the interaction mechanism of the ChE enzymes and Phosphoramidate. Spectrophotometric studies of the interaction of Acetylcholinesterase and phosphoramide ligands have shown that it can binds to Acetylcholinesterase .If two partial composites of this compounds by GO synthesized, this compounds have highly exceed AChE properties than Phosphoramide. That this matter recognized by Fluorescence spectrum. this analyze shown times that Phosphoramide(PA) without synthesize GO/PA composite has approximately 1/1000 AChE properties into GO/PA composite and this matter very important due to very little pollutant materials enter the nature. The chart and table of this analysis IC50 for GO, PA and GO/PA composite exhibit in the following.[3]

L1 ligand



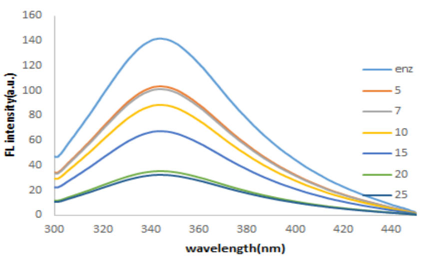


Figure 1: Fluorescence spectrum of AChE in presence GO in 5,7,10,15,20,25 µl

$((0.01)_{grGO}/(6)_{mL\ Ethanol})$

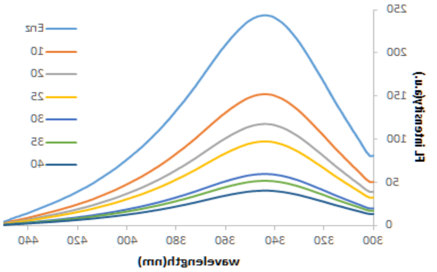


Figure 2: : Fluorescence spectrum of AChE in presence L1 in 10,20,25,30,35,40 µl

(4Mm)

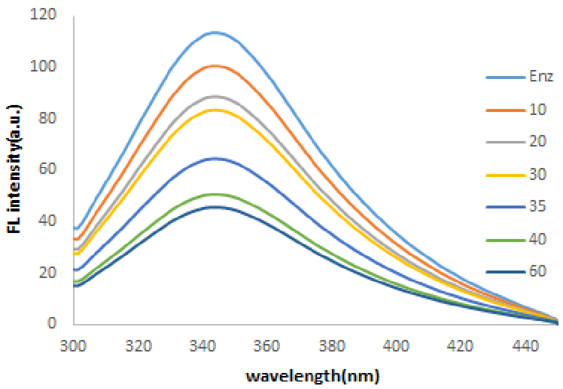


Figure 3: Fluorescence spectrum of AChE in presence GO/L1 composite in 10,20 ,30,35,40,60 µl

3µM L1 in 0.01$_{gr}$ GO/5cc$_{solvent}$

sample	L1 ligand	GO	GO/L1 composite
IC50	84mM	0.027gr/lit	0.013mM

Keywords: AChE, Fluorescence, Phosphoramidates , GO composite

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Synthesis of New Sodium Lanthanide Tungstate $NaM(WO_4)_2$ [M=Dy and Ho] Via Solid-State Method And Investigation Of Their Optical, Magnetic And Electrical Properties

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Recently, tungstate with a scheelite-type structure has been attracting attention. Because of their good photoluminescence (PL) properties, optical fibers and scintillators [1].They are used as solid-state laser materials [2].And they can provide properties such as negative thermal expansion (NTE),high anisotropic transport[3]. Moreover some of them are receiving attention as laser host materials and stimulated-Raman-scattering active media .These materials exhibit high potential for a wide range of applications, such as in phosphorescent materials , solar cells and luminescent diodes [4].

In this paper, we were synthesized new $NaRE(WO_4)_2$ (RE=Dy and Ho) at 800 ºc for 10 h by solid state method. The products characterized by X-Ray powder diffraction analyses that shown as a single phase and IR spectroscopy that demonstrated all bands were as we expected .The SEM and EDS analysis emphasized that compounds have almost the same morphology and also the size of nanoparticles was measured .Also the electrical conductivity was determined. The magnetization curve under the external magnetic field was measured and VSM curve shown that each of them is paramagnetism. Furthermore their spectroscopic properties i.e. absorption emission, excitation and luminescence was investigated at room temperature.

Keywords: Tungstate, Lanthanide, laser, optical properties , scheelite-type structure

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Synthesis of New Sodium Lanthanide Tungstate NaM(WO$_4$)$_2$ [M=Dy and Ho] Via Solid-State Method And Investigation Of Their Optical, Magnetic And Electrical Properties

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In this paper, we were synthesized new NaRE(WO$_4$)$_2$ (RE=Dy and Ho) at 800 ºc for 10 h by solid state method. The products characterized by X-Ray powder diffraction analyses that shown as a single phase and IR spectroscopy that demonstrated all bands were as we expected .The SEM and EDS analysis emphasized that compounds have almost the same morphology and also the size of nanoparticles was measured .Also the electrical conductivity was determined. The magnetization curve under the external magnetic field was measured and VSM curve shown that each of them is paramagnetism. Furthermore their spectroscopic properties i.e. absorption emission, excitation and luminescence was investigated at room temperature.

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Properties and application of Dimethyl carbonate

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Dimethyl carbonate (DMC) is an established solvent and a green reagent which continues to attract attention. DMC is classified in the greenest “recommended” bracket according to the solvent selection guide, and can be a potential replacement for methyl ethyl ketone, ethyl acetate, methyl isobutyl ketone, and most other ketones. Currently, the most prevalent commercial pathway for the production of DMC is through oxidative carbonylation of methanol using O_2; in addition, new alternative processes for DMC from CO_2 are being developed. DMC has found several applications such as the electrolyte in lithium rechargeable batteries and as a solvent in several reactions including pharmaceutically relevant synthesis and in biocatalysis. This report provides a brief overview of physical- thermodynamic-, toxicological- and ecotoxicological properties, production methods, reactivity, and applications of DMC as an environmentally benign chemical in chemical processes.

Keywords: Dimethyl carbonate, green solvent , production, electrolyte

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Synthesis, Characterization, Density Functional Theory Calculation and Antibacterial Activities of Five-Coordinate Complexes of iron (II) and cobalt (II) Transition Metals Containing a Benzoyl Thiourea Derivative

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In recent years, much research has been focused on the development of efficient antimicrobial agents to inhibit the growths of various drug-resistant strains [1]. Using Elemental Analysis, Fourier Transform Infrared (FTIR) and UV-visible spectroscopies, as well as conductivity measurements, synthesis of 2 first-row transition metal complexes, including $[M(L')(H_2O)_2]$ (M = Fe (C1) and Co (C2)) relevant to a benzoyl thiourea ligand, which was derived by condensing 2-chlorobenzoyl-isothiocyanate with 2,6-diaminopyridine, to produce 1,1'-(pyridine-2,6-diyl)bis(3-(2-chlorobenzoyl) thiourea) (L) was conducted. The structures proposed for the 2 complexes were confirmed through the application of conformational analysis and geometry optimization by utilization of Gaussian 09 suite of programs and Beck's 3-parameter hybrid method at the B3LYP level with the 6-31G(d,p) basis set as a supplementary tool due to inaccessibility to suitable crystals from pure solid thiourea compounds for X-ray measurements. These compounds were studied in vitro in terms of antibacterial properties against Staphylococcus aureus and Enterococcus faecalis and Escherichia coli and Pseudomonas aeruginosa as 2 standard gram-positive and 2 standard gram-negative bacterial strains, respectively, through minimum Inhibitory Concentration by using the broth macrodilution procedure and inhibition zone via the disk diffusion method [2] and their superior antibacterial activities compared to those of the new thiourea derivative were proven through the experiments.

Keywords: Density Functional Theory; Antibacterial Activity; Benzoyl Thiourea; 2,6-Diaminopyridine

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Preparation of magnetic nickel nanoparticles from their coordination compounds in amorphous silica

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ABSTRACT

Nickel nanoparticles have received a lot of attention because of their unique magnetic properties [1-3]. Magnetic materials are used in a broad range of applications, including the production of magnetic fluids, stealth technology, refrigeration, optoelectronic, catalysis and biological applications. These materials have also been used as catalysts for hydrogenation of organic synthesis [4]. In this work, nickel nanocrystallites have been prepared by reduction of nickel complexes. In a mechanochemical method, nickel complexes were reacted with hydrazinium sulfate as a reducing agent. Nickel nanoparticles were formed due to the silica substrate and the reduction potential of Ni^{II} complexes. These nanoparticles were characterized by X-ray diffractometer (XRD), scanning electron microscopy (SEM), vibrating sample magnetometer (VSM), EDX analysis and IR spectroscopy.

Keywords: Amorphous silica, Chemical reduction, Nickel complexes, Nanoparticles, Magnetic particles size.

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Co-Precipitation method for synthesis of Fe-Ni oxide Nanoparticles supported by Nano Alumina and Investigation of the Calcination conditions on their Structures

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In this study, Nano particles Fe-Ni oxide was synthesized with Co-precipitation method. The nanoparticles synthesis in various time and different temperatures of calcination conditions. The synthesized particles were characterized by X-ray Diffraction (XRD), Field Emission Scanning Electron Spectroscopy (FESEM), Energy-dispersive X-ray Spectroscopy (EDS). According to the XRD pattern, products were crystallized and structure was cubic. The crystal size ranged from 10-30 nm. Because of the obtained Fe_3O_4, NiO and $NiFe_2O_4$ compounds and the smaller particles the best time and temperature of calcination was 6 hours and $550C^0$.

Keywords: Co-precipitation; Calcination; Alumina; Fe-Ni Nanoparticles

A new Methodology in Drug Delivery

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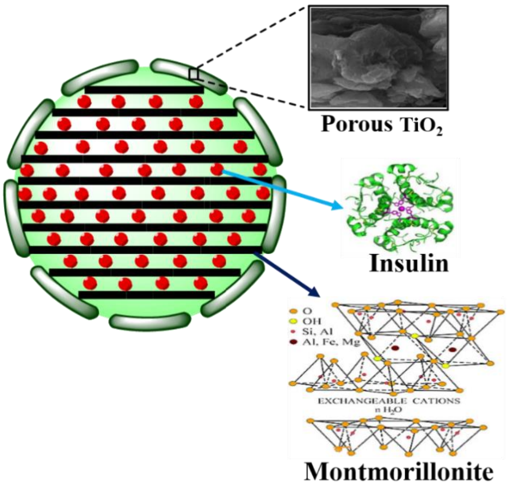
Our main goal in presenting this methodology was to modify the conventional systemic delivery of drugs because such procedures may cause toxicity; for example, polymeric coatings may present some disadvantages such as limited chemical stability, local inflammatory reactions and so on. As a result, we thought that it could be interesting to embed bioactive compounds and biomolecules within inorganic coating such as TiO_2, ZrO_2, and SiO_2. This type of coating increases drug passage time through its small and long pores forward intended fluid (whether *in vitro* or *in vivo*) and eliminates different stimuli such as (temperature, pH, ultrasonic irradiation,...) to remove the coating on the surface of drug carrier system. This could be very effective economically and time spent. Moreover, if such inorganic coatings have nanostructure properties, they improve cellular adhesion, enhances osteoblast proliferation, and increase biomineralization. In this talk, emphasis is placed on presenting the technique, and would like to explore it as a new methodology in drug delivery.



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Metallodrugs in Medicinal Inorganic Chemistry

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Metal ions play important roles in biological processes, and the field of knowledge concerned with the application of inorganic chemistry to therapy or diagnosis of disease is medicinal inorganic chemistry. Among the natural sciences, medicinal inorganic chemistry is still considered a rather young discipline by many, but this is contrary to the historically proven use of metals in pharmaceutical potions, which traces back to the ancient civilizations of Mesopotamia, Egypt, India, and China.

Twelve metals are essential for the human body that has developed a sophisticated and sensitive system of pathways for their transport as different and diverse as the essential metals; consequently, this diversity amounts to a core challenge for the systematic development of metallodrugs. In addition, other nonessential metals can be used for therapy as well.

To exploit fully the potential of metallodrugs, it is absolutely essential to understand what happens to the coordination complex and its components, the metal and the ligand(s), once the metal−ligand complex enters the body. To what extent can the active metabolite be defined for drugs that are essentially delivery vehicles for metal ions to undergo dissociation and ligand exchange once administered? What role does the design of the ligand itself play in this? Are the pharmacological and toxicological properties of novel metallodrugs predictable based on an improved understanding of metal ion speciation in vivo? In what way does the oxidation state of the metal influence this? How important are the thermodynamic versus kinetic considerations for metallodrugs in the body? What is there still to learn from the biochemistry of essential metals and metal ion distribution in the human body? These are questions that were raised years ago,and the answers are slow in coming.

If the scientific community succeeds to communicate the benefit of metallodrugs to the public, in addition to answering the questions raised above and gaining an increased understanding of the metal homeostasis in the body, the chances that the public and thereby as well “Big Pharma” will become more receptive to medicinal inorganic chemistry approaches will improve. The revenue from such successful metallodrugs as imaging agents, anticancer drugs, and metal supplements ought to be a persuasive argument to invest in this interdisciplinary area of medicinal chemistry. Particularly, metal coordination compounds in therapy open an array of possibilities, which traditional organic or biological molecules cannot fulfill any longer due to growing drug resistance. Metallodrugs hold still tremendous potential to help mankind overcome drug resistance and to find new cures in medicine.

Cooperativity of chemical bonds; where, how and how much?

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Unlike covalent interaction which leads to the formation of a classical molecule, non-covalent interaction leads to the formation of molecular clusters. When a pair of non-covalent interactions strengthen each other, it is called cooperative while when they weaken each other they are defined as operating in an anticooperative manner. Cooperativity implies that the sum of at least two interactions is larger than the simple addition of the individual interactions [1, 2]. A quantitative measure of the cooperative effect is made by decomposing the many-body interaction energy (MBIE) of a system of n bodies. But in above method total interaction energy cannot be calculated using a series of defined interactions and we need the many-body term which is not corresponded to any defined type of interaction. In ABC triad system, the appearance of three-body term in any proposed equation for calculation of total interaction energy of a triad means “there is one or more types of interactions but we don't know what they are”. A new equation having four defined interactions that for the first time gives the total interaction energy in a non-cyclic ABC triad without using three-body term is reported [3]. A new method is also proposed for calculating the changes in values of A···B and B···C interactions when a non-cyclic triad forms from the corresponding dyads.

Figure 1. Formation of a triad from the corresponding dyads and total interaction energies.

Keywords: Non-covalent interactions, Cooperativity, MBIE, Interaction energy, Non-cyclic triad

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A new sensor for selective detection of Pb^{2+} based on dithiazolopyridine derivative

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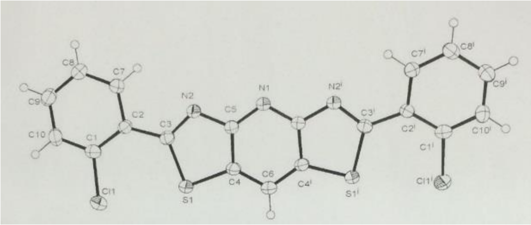
With the high speed development of industry, the discharge of waste water containing various excessive ions is becoming more and more serious, which can cause irreversibly destroy for natural environment especially waste water containing Pb^{2+} ions.

Herein, 2,6-di-(ortho-hydroxyphenyl)di[1,3]thiazolo[4,5-b:4',5'-e]pyridine was synthesized by Willgerodt-Kindler reaction for the first time. The molecule was characterized by NMR and as well as x-ray crystallographic analysis (scheme 1). Its absorption and emission spectra was also measured leading to obtain photophysical data.

Furthermore, its cation and anion recognition was studied. From the obtained results utilizing of UV-Visible and fluorescence spectroscopy it was manifested that ligand has more sensivity and selectivity to Pb^{2+}toward other metal ions.



Scheme 1: X-ray structure of ligand

Keywords: Methals ion, Intraction of ligand, UV-Visible and fluorescence

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Opportunities and challenges in catalytic applications of Keplerate polyoxometalates

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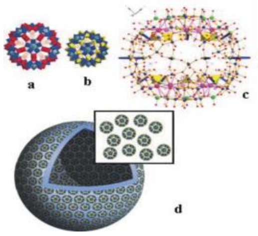
Keplerate-type polyoxometalates as a significant class of inorganic nanocapsules have attracted more and more attention of scientists in the areas of chemistry, physics, biology, and materials. They have overwhelming variety of fascinating and unusual properties, which make the supramolecular clusters become good candidates to construct functional materials in the fields of magnetics, optics, electrochemistry, and materials science.[1] However, their catalytic activity in organic transformation has been underestimated.[2]

Following our discovery on catalytic efficiency of $\{Mo_{132}\text{-}OAc\}$ nanoball in aerobic olefin epoxidation, [3], a few works on catalytic activity of Keplerates has been done.[4] However, self-assembly of Keplerates in different conditions as well as degradation at neutral and basic environments and particularly under redox conditions are major concerns for their catalytic applications. The use of different linkers joining $\{(Mo)Mo_5\}$ unites provides new opportunities for development of novel catalyst with appropriate efficiency and stability. Attractive reactivities of amorphous and crystalline forms of Keplerates in chemical and photochemical reactions were observed. Organic-inorganic hybrids of title clusters form a honeycomb nanostructure enabling their uses in organic solvents and enlarge their scope of catalytic activity. Their potential for using in photo-controlled and reaction-controlled phase-transfer catalysis [4] are another important advantages of Keplerates.



Keywords: Keplerate polyoxometalates; Catalytic activity; Inorganic Nanocapsules

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نوزدهمین کنفرانس شیمی معدنی ایران
19th Iranian Inorganic Chemistry Conference
Chemistry & Chemical Engineering Research Center of Iran
www.IICC19.ccerci.ac.ir
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Homogeneous and Heterogeneous Catalysis

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In recent two decades, the use of oxazoline, oxazine, Schiff base, porphyrin and carbene type ligands has been developed by our research group for a broad range of catalytic reactions based on a variety of metals such as manganese, iron, vanadium, copper, molybdenum, tungsten, and palladium [1-3]. Many complexes with these ligands show excellent catalytic activity in various homogeneous and heterogeneous catalytic processes including oxidation, reduction and carbon-carbon coupling reactions. Homogeneous catalysts usually exhibit remarkable catalytic activities and selectivity. A major drawback of homogeneous catalysts is difficult recovery from the reaction medium. One of the important approaches to overcome this limitation is heterogenizing homogeneous catalysts via immobilization of the catalytically active species onto/into the surface of supports. A part of our attempts have been focused on the development of new ligand-loaded supports such as MOF, SBA-15, silica-coated and polymeric-anchored magnetic nanoparticles, supported ionic liquid phase (SILP), and zeolite for the attachment of metals and the design of new approaches to improve their oxidative stability, selectivity and the catalytic performance because of the support environment and other advantages with respect to recovery and reuse.

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Biomimetic catalysis: Targeted synthesis of coordination complexes

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Chemical catalysis that mimics certain key features of enzymatic systems is generally referred to biomimetic catalysis [1]. In this regard, different heme and non-heme catalysts were employed to mimic the active site of cytochrome P450 enzymes, heme and non-heme peroxidases and catalases, catechol dioxygenase, superoxide dismutase, oxygen evolving complex of photosystem II, copper enzymes and molybdenum enzymes [2]. Biomimetic catalysis of the oxidation reactions of organic compounds has been the subject of many studies over the past decades [1-5]. While the active site of most enzymes contains simple heterocylic porphyrinic, porphyrinoid or non-heme ligands, more complicated ligands and metal complexes are needed to mimic the active site of these biological catalysts. The aim of this lecture is to review different aspects of targeted synthesis of transition metal complexes for application in the field of biomimetic catalysis. Furthermore, biomimetic oxidations will be discussed from an industrial point of view.

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Green synthesis of Inorganic nanomaterials

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In general, green production refers to realizing reasonable utilization of resources and reducing harm to the environment and humans, which includes the main ways of comprehensive utilization of resources and waste, green production process, and the improvement and development of green technology. Recently, green processes for nanotechnology have been receiving more and more attention, which has favored environmental protection and sustainable economic development. Various green processes for nanotechnology have been reported such as hydrothermal/solvothermal, sol–gel, microwave-assisted method, ultrasound agitation and mechanochemical method. The synthetic method only is a part of the green processes. Besides green synthetic route, the other green processes such as green solvents, green resources, green materials, green design, and green production also should be considered. Here in, the green preparation of some inorganic nanomaterials will be presented. The nanostructures of these compounds were nanoparticles, plate, cauliflower, rod, flower and … Also the properties of these compounds were investigated.

Keywords: Green synthesis, Inorganic nanomaterials, Environment.

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Metal oxide/Zeolite composites as the active catalysts for dehydrogenation of ethylbenzene to styrene process

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Zeolites are crystalline aluminosilicates with regular and uniform porous structures. In these materials, Si/Al molar ratio can be varied from 1 to ∞; so highly hydrophobic aluminum-free synthetic zeolites can also be attainable .Thanks to the development of the synthetic techniques, there are grated many synthetic zeolites with different compositional elements and frameworks. Other elements, especially transition metals, can incorporate into the zeolite framework such as Fe,Cr,Mn&etc. In this speech, synthesis and characterization of Nano Fe_2O_3/Zeolite composites are presented. Styrene (ST) is one of the most essential materials in the petrochemical industry for production of synthetic polymers and plastics. The most conventional process for the commercial production of styrene is ethylbenzene (EB) dehydrogenation by the K−Fe-based catalysts with high iron loading in the presence of a large amount of superheated steam at a high temperature of 600−650 °C. However, this traditional process has many disadvantages such as high energy consumption and thermodynamic equilibrium limitations. Hence, a worldwide investigation of the alternative process is being considered. Recently, as a substitute for steam, CO_2 gas has received great attention as a co-feed gas for dehydrogenation of ethylbenzene. The presence of CO_2 in the ethylbenzene dehydrogenation reaction suppresses coke formation and also helps remove the carbonaceous deposits.

This investigation introduces novel composites of Fe_2O_3/ K-metalosilicate with high performance in oxidative dehydrogenation (ODH) of ethylbenzene to produce styrene with CO_2. Regarding K-metalosilicate as catalyst support, various amounts of iron oxide nanoparticles (γ-Fe_2O_3) were introduced into porous support by different methods such as solid-stated dispersion (SSD),hydrothermal,sol gel and… in order to enhance catalytic activity. The prepared samples were characterized by

X-ray diffraction (XRD), scanning electron microscopy (SEM) coupled with the energy dispersive analysis–EDX, and N_2 physical adsorption analysis.The high performance of catalytic activity of the composites in ethylebenzene dehydrogenation process can be attributed to the synergistic effect of transition metal oxide ,K^+ and Fe^{3+} ions in the structure of catalysts.

When EXAFS helps Crystallography

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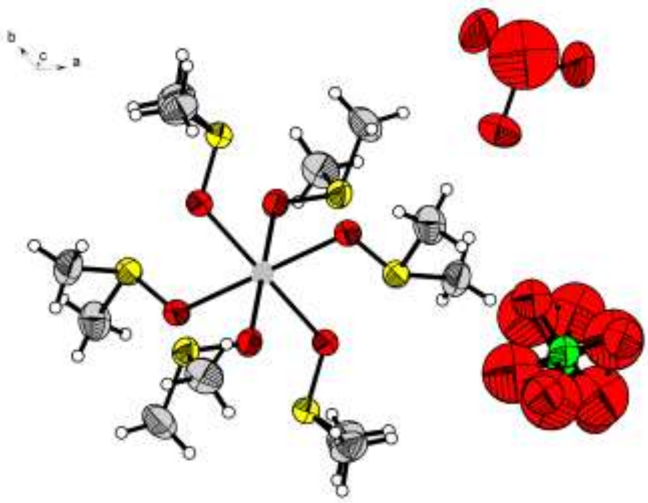
The structure of dimethyl sulfoxide solvate of thallium(III) perchlorate have been studied in the solid state. Space groups R3 (No. 146) and R-3 (No. 148) were suggested from systematic absences. Low value of $|E^2 -1| \approx 0.62$ indicates the acentric space group or possible twinning. However, the structure could be solved and described in both space groups. In the acentric (R3) the absolute structure could not be determined, and the structure had to be refined as a racemic twin. In the centrosymmetric (R-3) the description of the complex improved significantly with fewer parameters but one of the perchlorate must be modeled as disordered.

Low temperature (150 K) data set did not help and this issue could not be resolved. From our crystallographic data, we were not able to distinguish between a twinning and a statistical disorder. An EXAFS study shows the Tl-O and Tl…S distances of 2.221(4) and 3.282(6) Å, respectively, consistent with a Tl-O-S bond angle of 120(1)°. The low Debye-Waller factors approve a regular coordination without the disorder of the dimethyl sulfoxide ligands, confirming the alternative choice of space group R-3.



Keywords: Crystallography, EXAFS, Space group, Thallium, DMSO

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Short report on organoboron compounds

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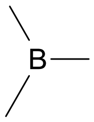
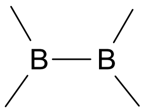
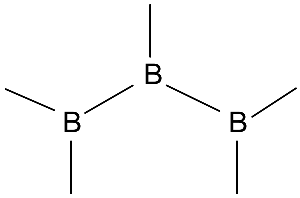
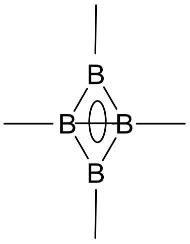
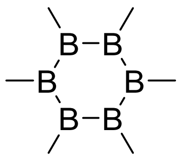
The electron deficiency on boron atom causes the Lewis character of boron compounds and also enables the formation of three-center-two-electron(3c2e) bonds between the boron atoms. In the lecture will be reported on the synthesis of linear or cyclic boron compounds of types: borane, diborane(4), triborane(5), aromatic bicyclotetraborane(4), cyclohexaborane and synthesis of organoboron compounds such as boracyclopropene, diboracyclopentane, diborylethene, borinc ester and derivatives of ferrocenylborane. The spectroscopic characterization of boron compounds and X-ray structure analyses will also be discussed.

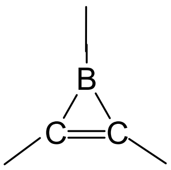


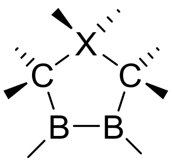


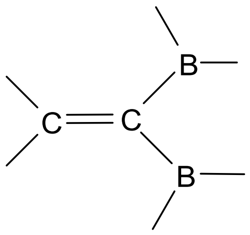


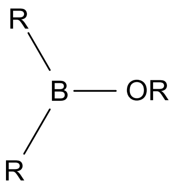


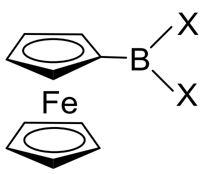












Synthesis and Identification of Copper (II) Complexes using phosphonium salt resulting from the combination of trinylphosphine and ethyl bromoacetate, using stereoscopic methods

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Abstract

Phosphonium salts have the general formula $R_4P^+X^-$ and are derived from the sub-ion phosphonium tetrahedral(pH_4^+), such as phosphonium iodide $[p(CH_3)_4^+]^-$. Generally, phosphonium is attributed to an organic derivative, such as tetra-phenyl phosphonium chloride and tetra tetra-methyl phosphonium iodide. .

In this project, the phosphonium compounds [C2H5COO (CH2PPh3Br)] and its copper (II) complex [C2H5COO (CH2PP3Br)] [Cu2Cl6] were prepared and identified. Phosphonium species were prepared from the reaction of ethyl bromoacetate with terphenylphosphine. Then the final compounds were prepared using the reaction between the phosphonium compound with Na2 [Cu2Cl6]. Then, using spectroscopic methods, preparation of these compounds was investigated.

Key words: phosphonium, copper (II) compound, triphenylphosphine, ethyl bromoacetate

Introduction

Alkyl tri- phenyl Phosphonium salts are used to prepare Wittig reagents in Wittig reaction, widely. Such salts are made easily by using tri-phenyl phosphine reaction with an Alkyl halide. If the alkyl, methyl or primary group alkyl have not space prevention , the reaction well done. But usually react with **secondary** alkyl halides is a weak reaction. Tertiary alkyl groups can't form Aylyd. Phosphonium salt is a stable compound which often is achieved from ethanol, by recrystallization [1]. In recent years, Phosphonium salts are of great interest due to their structure, properties and reactivity.

Aylyd reaction with aldehydes or ketones, which is one of the most common methods for the formation of region specific alkenes, was first reported in 1953 by George Wittig. This reaction is a key step to produce a large number of natural and biological products. The Main reagent in the Wittig process is prepared through the deprotonated

Phosphonium salt, which has been achieved through four coordination of phosphine with a combination of Hollow. The main advantage of Wittig reaction is it’s stereo selectivity. Stereochemistry depends on several factors. Phosphonium salt structure is The presence of metal cations and laboratory conditions [2].

Wittig reaction in addition to done applied research, has broad applications to produce pharmaceutical and industrial materials. Wittig, to start the reaction, react an alkyl halide with a phosphine to obtain four coordinate kation phosphine. To produce a neutral compound, Which is called P aylyd, this cation is then deprotonated by a strong base such as butyl lithium.

Aylyd negatively charged carbon, acts as nucleophile and attacks to carbonyl Aldehyde group or ketone. Protective and corrosion inhibitor metals play an important role in industry. Most of protectors and inhibitors are organic compounds which have hetero atoms such as phosphorus, nitrogen, sulfur and oxygen. These compounds and their derivatives are corrosion inhibitors for iron and steel. Many of these corrosion inhibitors and protective have hazardous effects on the environment. So achieving effective and non-toxic organic inhibitors for iron and steel is a crucial point. Suitable inhibitors for the environment should have biodegradability properties and should not be destructive for environment. Phosphonium compounds in Acidic solutions are used as protective for most metals [3].

Four coordinated Phosphonium compounds have been identified in many systems as factors inhibiting the growth of bacteria, which are highly adapted to the environment [4]. The benefits of these compounds including very low toxicity, rapid degradation in the environment (via hydrolysis, oxidation, light degradation and biodegradation), and destructive or non-destructive effects on the environment [5].

For example, tri phenyl phosphonium bromide in 0/5 M sulfuric acid solution is known as a corrosion inhibitor for iron and steel, and has been proven by Galvanostatic and Potentiostatic measurements and using FT-IR spectroscopy and images from electron microscopy and quantum computing [6]. Also some reports provided about the preparation of biologically active polymers using ammonium groups and Four coordinated Phosphonium, which have medical use [7].

Production of ionic liquids is another application of phosphonium salts, which the liquids are organic salts which are in liquid state at low temperatures (less than 100 ° C) [8] and has advantages such as wide temperature range of liquid output, high thermal and chemical stability, strong solvents and very low vapor pressure in the synthesis of organic compounds, chemical catalysts, different separation methods and the role of new electrolytes in the manufacture of solar and fuel cells [9]. In recent years, many studies have been done on Four coordinated Phosphonium systems and the new composition of the phosphonium known as ionic liquids and the use of phosphonium salts is more than ever [10].

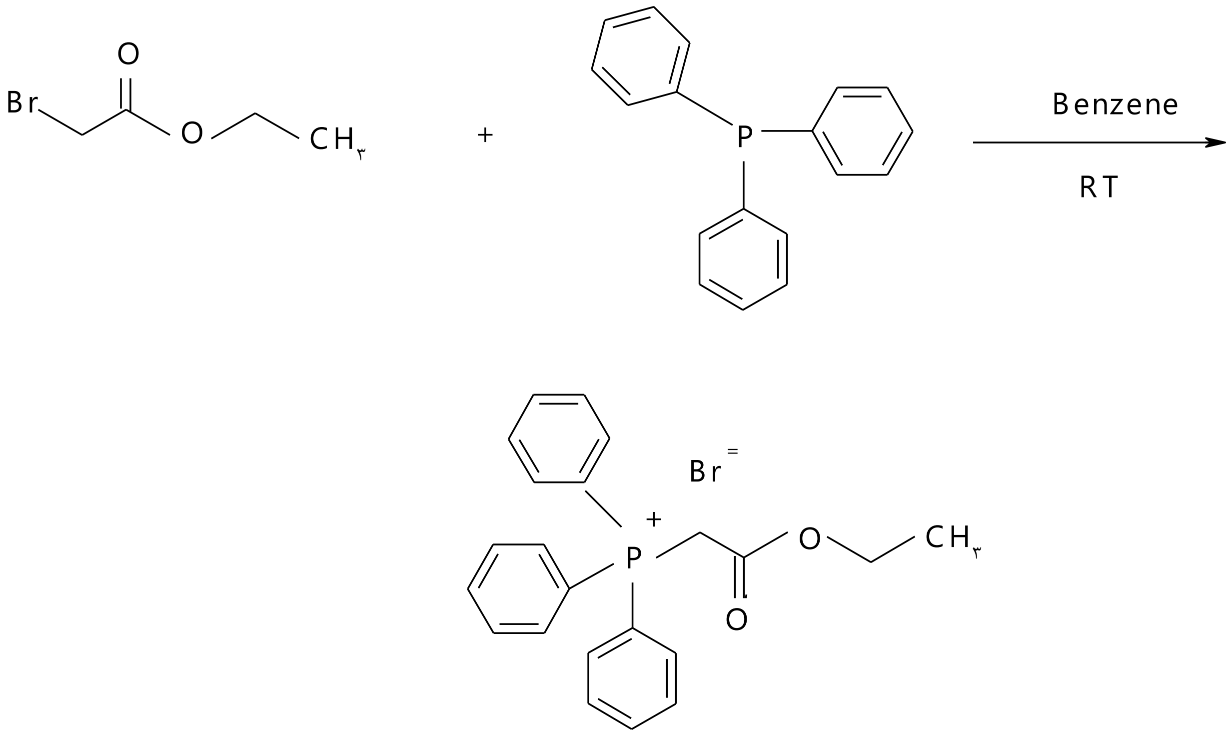
In recent years, important polymer humidity sensors are built. Different types of monomers sensitive to moisture have been used to build the humidity sensors, including cationic or anionic salt. Phosphonium salts due to the simplicity and easy preparation and high stability under different conditions are used, in a very large extent, for the manufacture of polymer humidity sensors. Most recently, tri-phenyl phosphonium chloride salts have been prepared and used for the production waterproof humidity sensors. You can also use tri-butyl phosphonium chloride, as monomer, to prepare the sensors [11]. Phosphonium salts successfully have been used as a catalyst for many types of organic reactions Such that it can be noted is simple phosphonium salt catalytic activity as benzyl chloride phosphonium Alkoxysilyl cyano reaction of the ketones [12] and the use of phosphonium salt as the catalyst Lewis acid without metal, which has been rapid growth in the field of organic catalysts [13].

Recent studies have been carried out on quasirone phosphonic systems and new compounds of phosphonium are known as ionic liquids. And has resulted in the use of more phosphonium salts. [14]. Phosphonium salts are used as phase transfer catalysts in organic synthesis. [15]. Phosphonium salts are also used to synthesize Macrocycle peptides in solution. [16]

Test Method

The process of preparing the compound [C2H5COO (CH2PPh3Br)]

In this study, 10 m mol Bromine ethyl acetate (1.1 ml) and 10 m mol tri phenyl phosphine (2.62 gr) was solved separately in 50 ml of benzene and then was added to a 100 ml balloon, which starts to precipitate after 2 to 3 minutes, and was stirred at room temperature for 24 hours. Then the solution was refined after washing with ethyl ether and then was dried in the desiccator. The resulting sediment weight was 2.98 gr and efficiency of reaction was 69%. The precipitate was melted at 165 ° C.

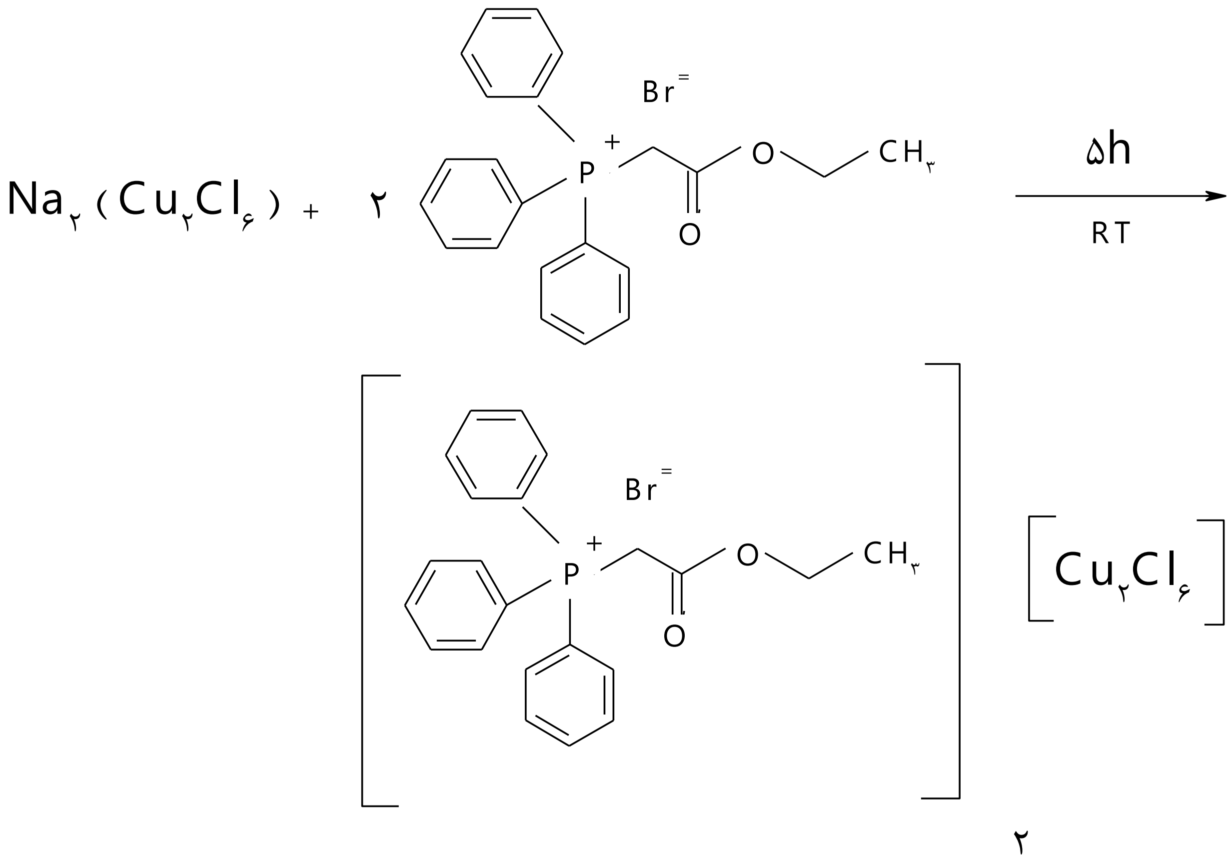


Preparation Process of [C2H5COO (CH2PPh3Br)]

Preparation of Copper Complex (II)

The process of preparing the complex [C2H5COO (CH2PPh3Br)] [Cu2Cl6]

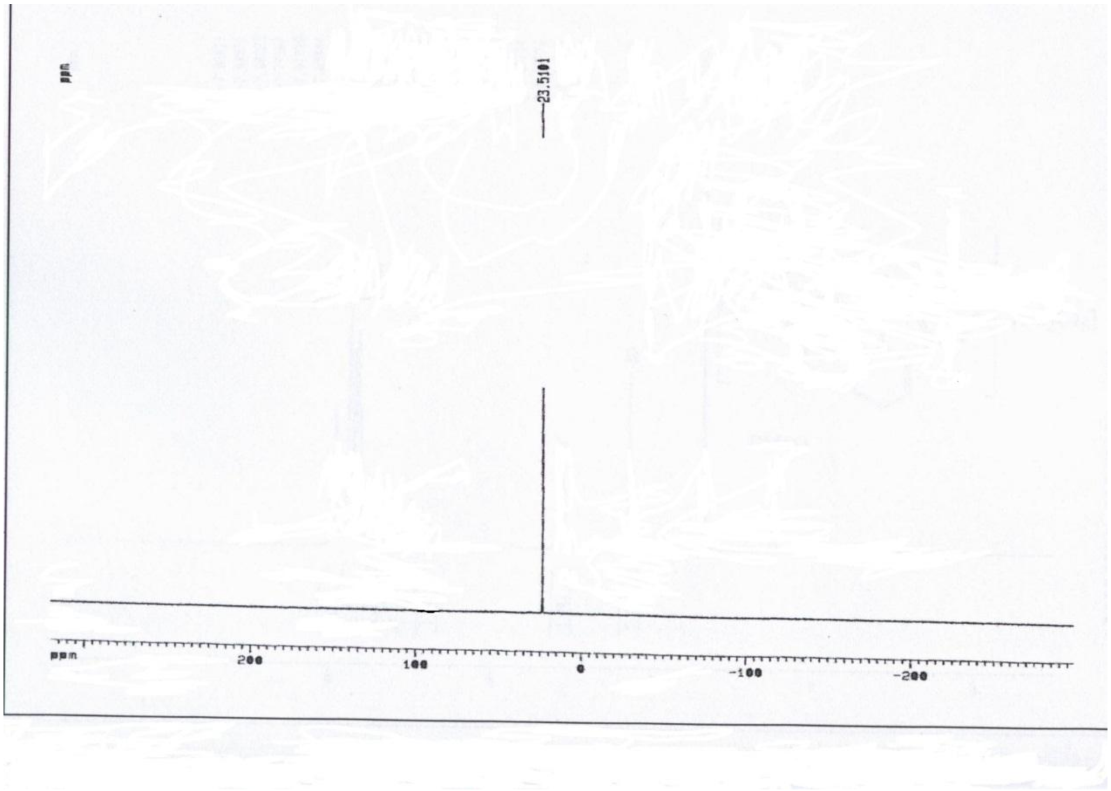
At this stage, 0.1 g CuCl2 (0.74 m mol) and 0.15 g NaCl (2.9 m mol) were poured into a tube hose. Then 10 ml of methanol was added to it. And the solution was stirred at 50 ° C for 5 hours until a clear greenish yellow solution was obtained according to the following scheme. Then, 0.32 g of phosphonium (76.8 m mol) was added to it, which quickly began to form turquoise blue sediment. Its weight was 15.0 g and the reaction efficiency was 25.86% and melted at 218 ° C.



Results

In order to determine the obtained combinations the NMR spectrum including PNMR-CNMR-HNMR was measured using FT-NMR400. The infrared spectrum was evaluated using the FT-IR.Bommen model and Nojol oil and KBr tablet, the following results was obtained:

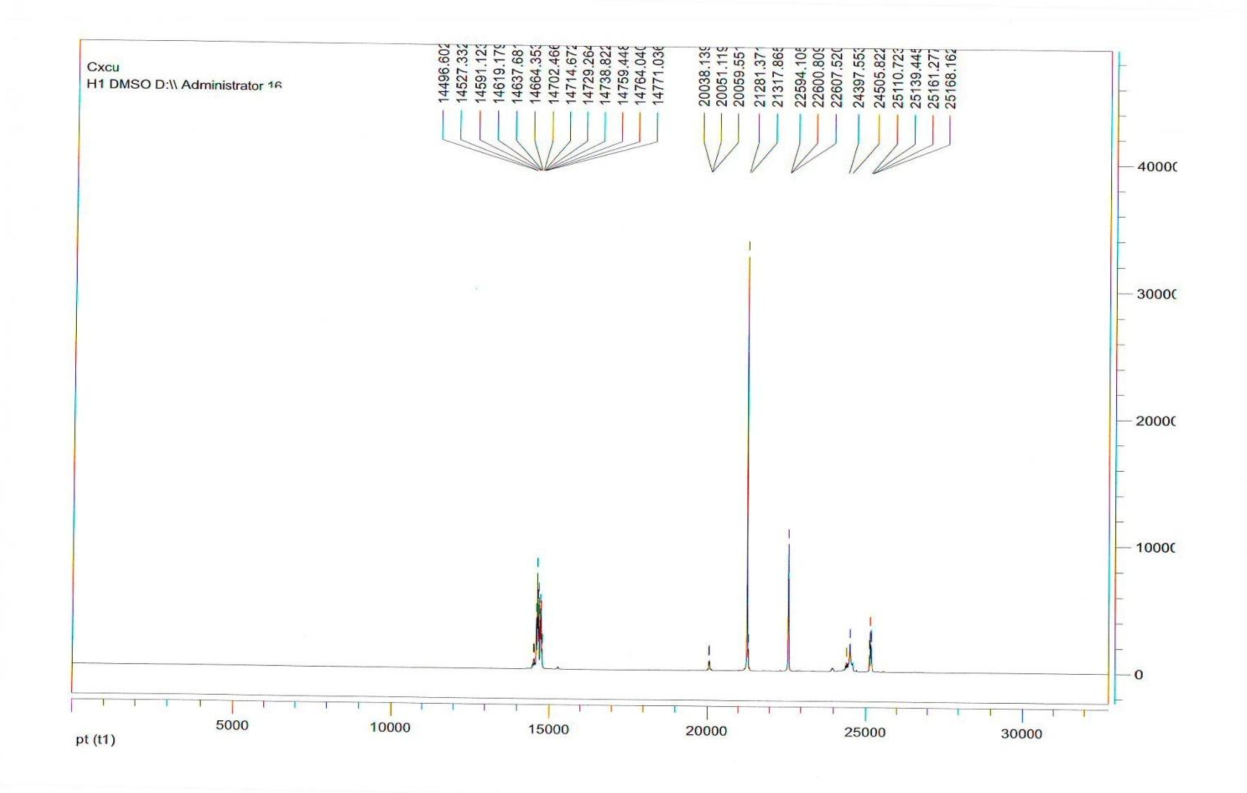
The spectrum 1 shows the 31PNMR spectrum of [C2H5COO (CH2PPh3Br)] [Cu2Cl6] composition. In this spectrum, the phosphor resonance in δ = 23.66 PPm appears in the form of a unique peak. δ = 4.8 PPm indicating that the atom of phosphorus has created a new bond with a carbon atom that, by decreasing the density of electrons in the phosphorus atom, the peak of phosphorus moves to the lower fields. For same compounds the peak appears in δ = 24.22 PPm. This peak represents the formation of the desired composition, and the unique P-peak in this spectrum represents the high purity of the composition.



Spectrum 1 .^{31} PNMR [C2H5COO (CH2PPh3Br)] [Cu2Cl6] Compound

Spectrum2. The 1HNMR spectrum shows [C2H5COO (CH2PP3Br)] [Cu2Cl6] composition. In this spectrum, the unique peak in 21281 corresponds to the methyl group attached to phosphorus. Quintuple peak is related to the hydrogen of the ethyl group, which appears in the field 24397 due to an increase in the electron density resulting from the connection to the oxygen atom. And multiple peaks in 14496 to 14771 are related to aromatic hydrocarbons. The summary of the results of this spectrum is presented in the table below.

The peak shape	The number of protons	δ (PPm)	Proton type
A unique peak	2	21281	CH_2 P
A quintuple peak	5	24397	C_2H_5 O
Multiple peaks	15	14702	3 C_6H_5



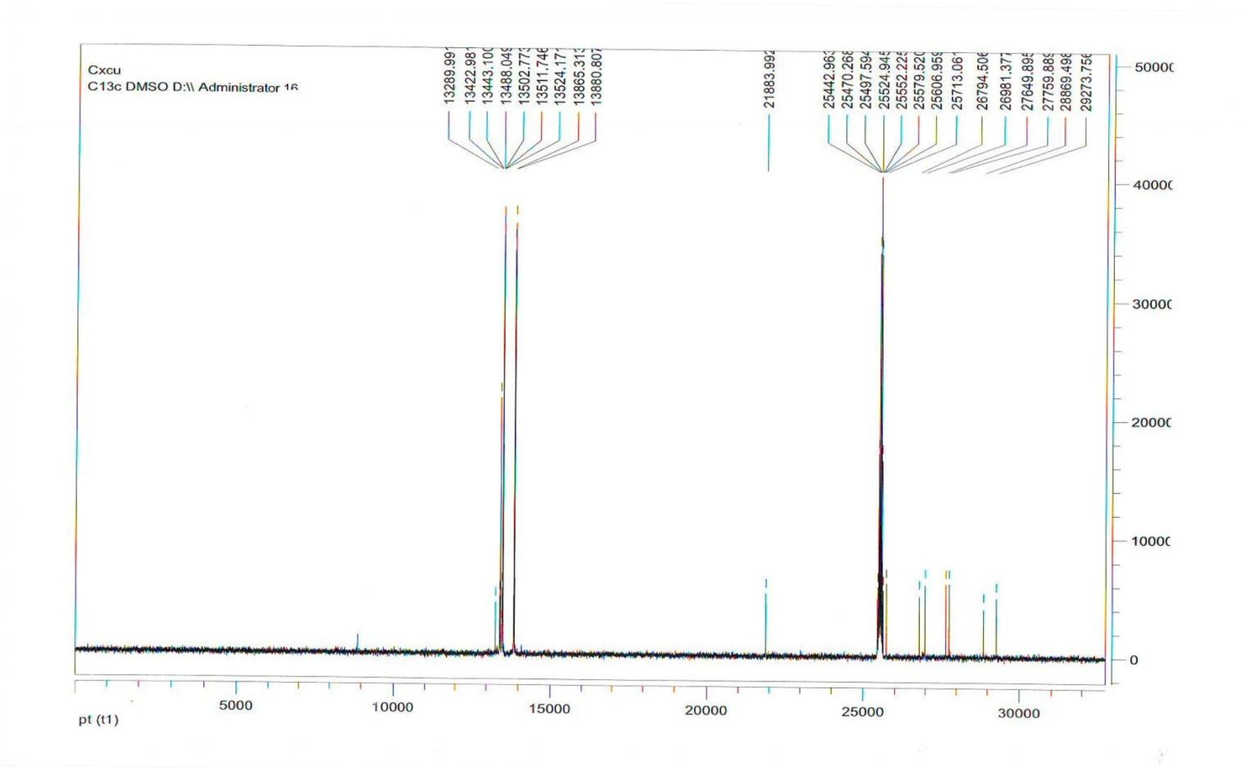
Spectrum2. The 1HNMR spectrum of the composition [C2H5COO (CH2PPh3Br)] [Cu2Cl6]

Spectrum3. The CNMR spectrum shows the composition of [C2H5COO (CH2PPh3)] [Cu2Cl6]. In this spectrum, the double peak at 26981-2694 corresponds to the carbon atoms of the ethyl group attached to the oxygen atom, and the peaks in the 25713-25442 correspond to the DMSO solvent. The double peaks in 29863-28869 are related to the carbon in methyl coupled to the phosphorus atom and double peaks in 27759- 27649 are correspond to carbon in phenyl attached to phosphorus atom, and unique peak in 21883 is correspond to the carbon of the carbonyl group and the existing multiple peaks In 13880-13289 are correspond to the aromatic carbons of benzene rings.

A summary of the results is presented in the table below.

Peak shape	δ (PPm)	Carbon type

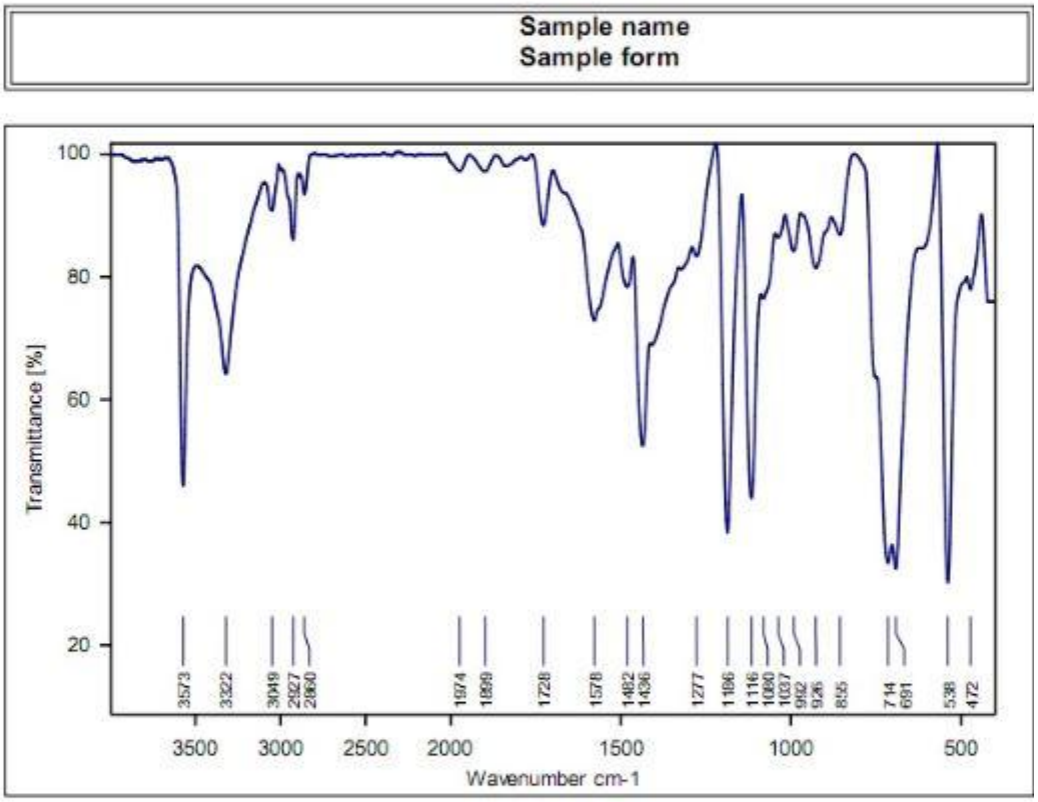
A double peak	26794 - 26981	C_2H_5O
A double peak	28869 - 29273	CH_2P
A unique peak	21883	C - O
Multiple peaks	13289 - 13880	aromatic
A double peak	27649 - 27759	P - C



Spectrum3. The CNMR spectrum of [C2H5COO (CH2PPh3)] [Cu2Cl6]

Spectrum4. The IR spectrum shows the composition of [C2H5COO (CH2PPh3)] [Cu2Cl6 Br]. In this spectrum, the strong absorption in region 538 is related to the tensile vibrations of the C-Br bond. Also, strong absorption due to non-steric C-O stretching vibrations appears in area 734. The adsorption observed in 1116 and 1186 are respectively correspond to the tensile vibrations of C-C and C-O-ester bonds. The optical absorption in region 1436 correspond to the tensile vibrations of P-CH3 and the vibration of the P-carbon bond in the phenyl, and absorption in the region 1728 is correspond to the tensile vibrations of the C = O bond.

Finally, spectral adsorption in 2860, an average absorption in 3322 and strong absorption in 3573 are correspond to symmetric tensile vibrations CH3, tensile symmetrical and asymmetric vibrations of CH2, as well as the tensile vibrations of the C-H of the methyl ring in the composition, respectively.



Spectrum4. The IR spectrum of the compound [C2H5COO (CH2PPh3)] [Cu2Cl6 Br]

The results of the elemental analysis of this composition with the experimental formula C44 H 44 Cl 6 Cu 2 BrO4 are given in the following table.

$C_{44}H_{44}Cl_6Cu_2BrO_4$	%C	%H	%N
Experimental	45.15	3.92	___
Theoretical	46.49	3.87	___

Discussion and conclusion

In this research, the synthesis of copper (II) complexes was investigated by using phosphonium salt produced by PPh3 with ethyl bromoacetate. And the composition [C2H5COO (CH2PPh3)] [Cu2Cl6 Br] was obtained by spectroscopic methods. Copper phosphonium complexes (II) can be excellent catalysts for different chemical reactions. It has a variety of applications in the chemical industry, including catalysts in the Heck reaction, Suzuki reaction and carbon hydrogenation reaction, terminal isomyramination of terminal olefins, and variation of the group in vinyl ethers. Therefore, more attention can be paid to the use of these compounds in different branches. The ability of phosphonium compounds to catalyze a wide variety of chemical reactions makes it very convenient to choose these compounds to work with.

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Synthesis and Identification of Copper (II) Complexes using phosphonium salt resulting from the combination of trinylphosphine and ethyl bromoacetate, using stereoscopic methods

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Abstract

Phosphonium salts have the general formula $R_4P^+X^-$ and are derived from the sub-ion phosphonium tetrahedral(pH_4^+), such as phosphonium iodide $[p(CH_3)_4^+]^-$. Generally, phosphonium is attributed to an organic derivative, such as tetra-phenyl phosphonium chloride and tetra tetra-methyl phosphonium iodide. .

In this project, the phosphonium compounds [C2H5COO (CH2PPh3Br)] and its copper (II) complex [C2H5COO (CH2PP3Br)] [Cu2Cl6] were prepared and identified. Phosphonium species were prepared from the reaction of ethyl bromoacetate with terphenylphosphine. Then the final compounds were prepared using the reaction between the phosphonium compound with Na2 [Cu2Cl6]. Then, using spectroscopic methods, preparation of these compounds was investigated.

Key words: phosphonium, copper (II) compound, triphenylphosphine, ethyl bromoacetate

Introduction

Alkyl tri- phenyl Phosphonium salts are used to prepare Wittig reagents in Wittig reaction, widely. Such salts are made easily by using tri-phenyl phosphine reaction with an Alkyl halide. If the alkyl, methyl or primary group alkyl have not space prevention , the reaction well done. But usually react with **secondary** alkyl halides is a weak reaction. Tertiary alkyl groups can't form Aylyd. Phosphonium salt is a stable compound which often is achieved from ethanol, by recrystallization [1]. In recent years, Phosphonium salts are of great interest due to their structure, properties and reactivity.

Aylyd reaction with aldehydes or ketones, which is one of the most common methods for the formation of region specific alkenes, was first reported in 1953 by George Wittig. This reaction is a key step to produce a large number of natural and biological products. The Main reagent in the Wittig process is prepared through the deprotonated

Phosphonium salt, which has been achieved through four coordination of phosphine with a combination of Hollow. The main advantage of Wittig reaction is it’s stereo selectivity. Stereochemistry depends on several factors. Phosphonium salt structure is The presence of metal cations and laboratory conditions [2].

Wittig reaction in addition to done applied research, has broad applications to produce pharmaceutical and industrial materials. Wittig, to start the reaction, react an alkyl halide with a phosphine to obtain four coordinate kation phosphine. To produce a neutral compound, Which is called P aylyd, this cation is then deprotonated by a strong base such as butyl lithium.

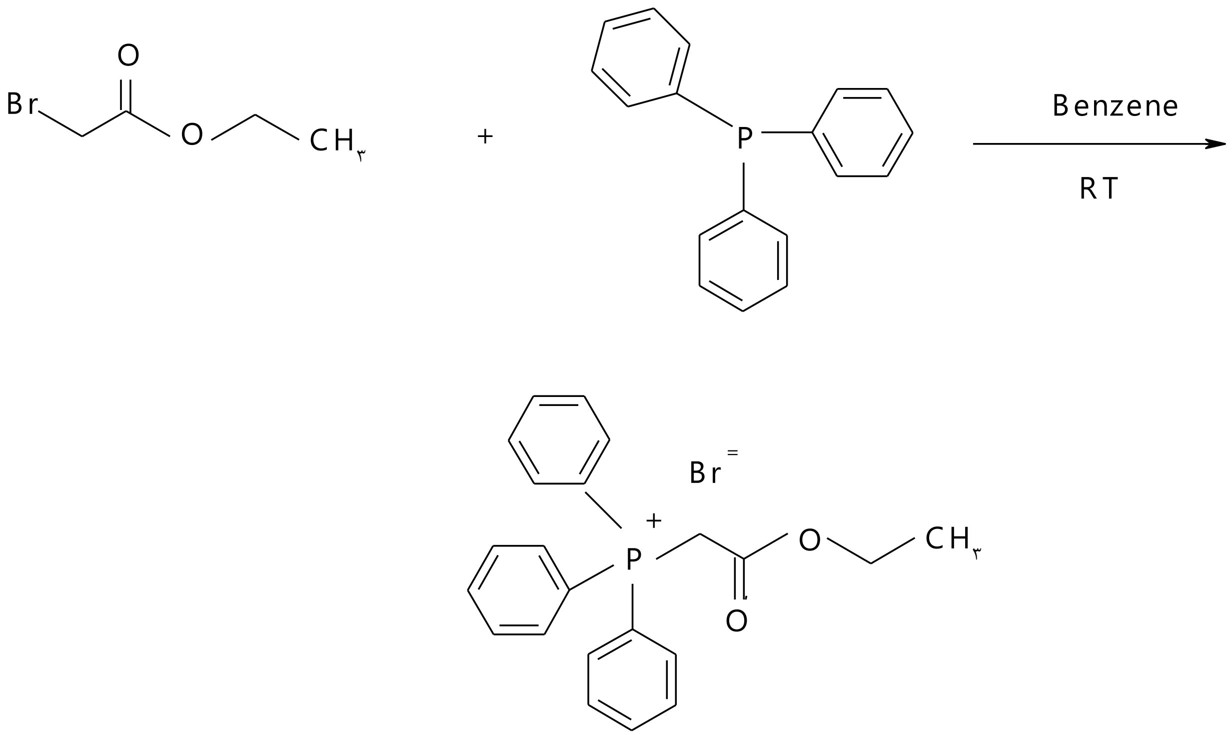
Aylyd negatively charged carbon, acts as nucleophile and attacks to carbonyl Aldehyde group or ketone. Protective and corrosion inhibitor metals play an important role in industry. Most of protectors and inhibitors are organic compounds which have hetero atoms such as phosphorus, nitrogen, sulfur and oxygen. These compounds and their derivatives are corrosion inhibitors for iron and steel. Many of these corrosion inhibitors and protective have hazardous effects on the environment. So achieving effective and non-toxic organic inhibitors for iron and steel is a crucial point. Suitable inhibitors for the environment should have biodegradability properties and should not be destructive for environment. Phosphonium compounds in Acidic solutions are used as protective for most metals [3].

Four coordinated Phosphonium compounds have been identified in many systems as factors inhibiting the growth of bacteria, which are highly adapted to the environment [4]. The benefits of these compounds including very low toxicity, rapid degradation in the environment (via hydrolysis, oxidation, light degradation and biodegradation), and destructive or non-destructive effects on the environment [5].

Test Method

The process of preparing the compound [C2H5COO (CH2PPh3Br)]

In this study, 10 m mol Bromine ethyl acetate (1.1 ml) and 10 m mol tri phenyl phosphine (2.62 gr) was solved separately in 50 ml of benzene and then was added to a 100 ml balloon, which starts to precipitate after 2 to 3 minutes, and was stirred at room temperature for 24 hours. Then the solution was refined after washing with ethyl ether and then was dried in the desiccator. The resulting sediment weight was 2.98 gr and efficiency of reaction was 69%. The precipitate was melted at 165 ° C.

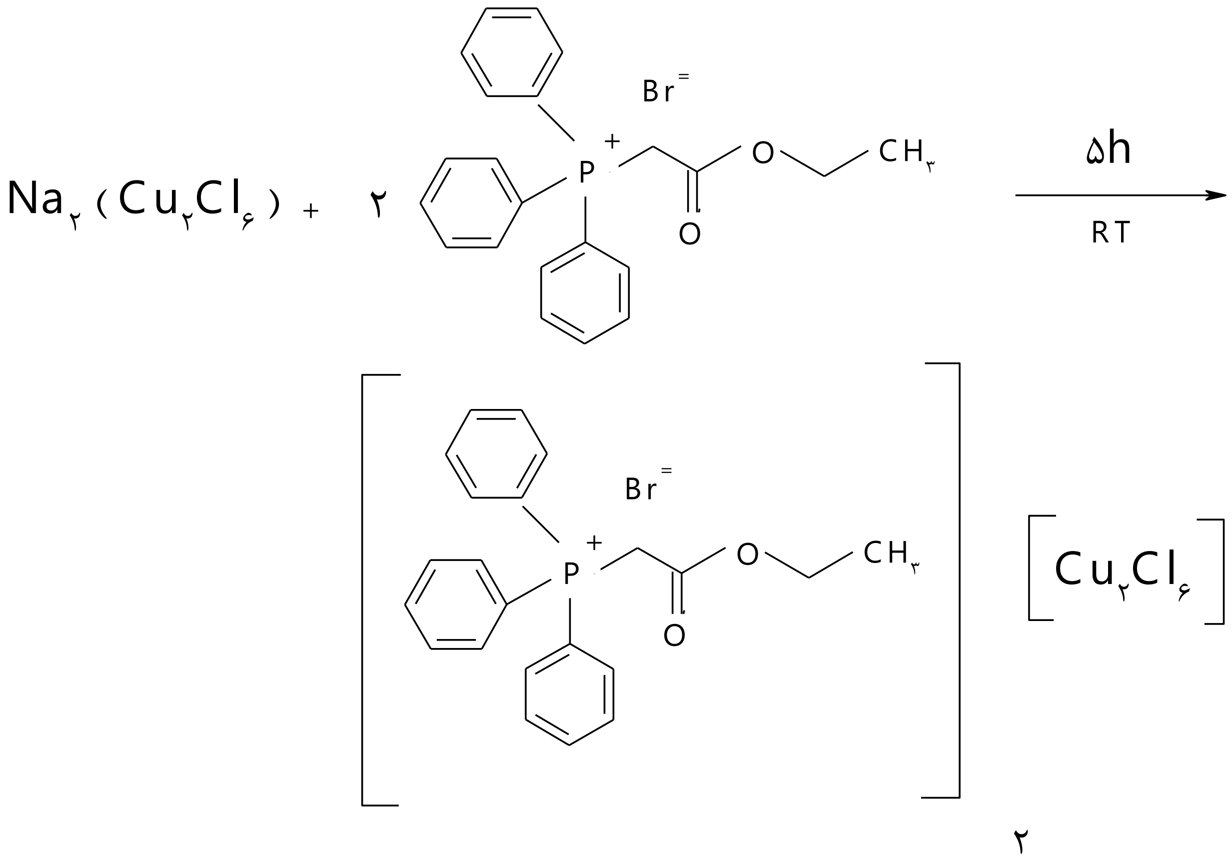


Preparation Process of [C2H5COO (CH2PPh3Br)]

Preparation of Copper Complex (II)

The process of preparing the complex [C2H5COO (CH2PPh3Br)] [Cu2Cl6]

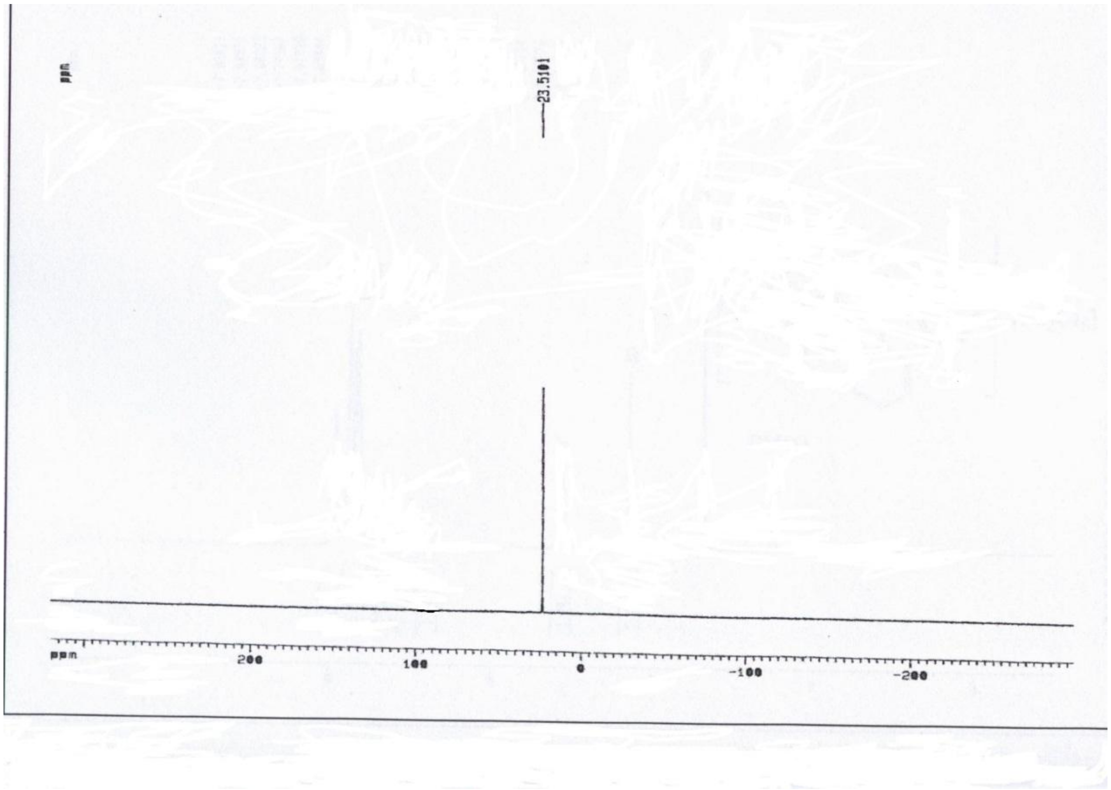
At this stage, 0.1 g $CuCl_2$ (0.74 m mol) and 0.15 g NaCl (2.9 m mol) were poured into a tube hose. Then 10 ml of methanol was added to it. And the solution was stirred at 50 ° C for 5 hours until a clear greenish yellow solution was obtained according to the following scheme. Then, 0.32 g of phosphonium (76.8 m mol) was added to it, which quickly began to form turquoise blue sediment. Its weight was 15.0 g and the reaction efficiency was 25.86% and melted at 218 ° C.



Results

In order to determine the obtained combinations the NMR spectrum including PNMR-CNMR-HNMR was measured using FT-NMR400. The infrared spectrum was evaluated using the FT-IR.Bommen model and Nojol oil and KBr tablet, the following results was obtained:

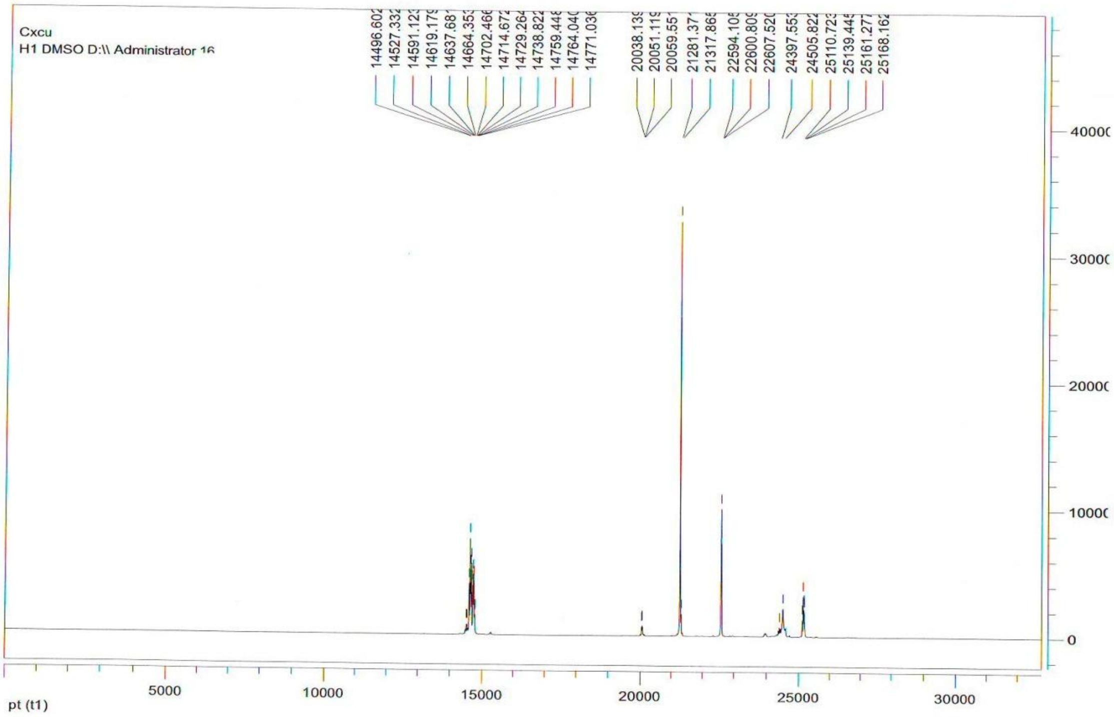
The spectrum 1 shows the 31PNMR spectrum of [C2H5COO (CH2PPh3Br)] [Cu2Cl6] composition. In this spectrum, the phosphor resonance in δ = 23.66 PPm appears in the form of a unique peak. δ = 4.8 PPm indicating that the atom of phosphorus has created a new bond with a carbon atom that, by decreasing the density of electrons in the phosphorus atom, the peak of phosphorus moves to the lower fields. For same compounds the peak appears in δ = 24.22 PPm. This peak represents the formation of the desired composition, and the unique P-peak in this spectrum represents the high purity of the composition.



Spectrum 1 .^{31} PNMR [C2H5COO (CH2PPh3Br)] [Cu2Cl6] Compound

Spectrum2. The 1HNMR spectrum shows [C2H5COO (CH2PP3Br)] [Cu2Cl6] composition. In this spectrum, the unique peak in 21281 corresponds to the methyl group attached to phosphorus. Quintuple peak is related to the hydrogen of the ethyl group, which appears in the field 24397 due to an increase in the electron density resulting from the connection to the oxygen atom. And multiple peaks in 14496 to 14771 are related to aromatic hydrocarbons. The summary of the results of this spectrum is presented in the table below.

The peak shape	The number of protons	δ (PPm)	Proton type
A unique peak	2	21281	CH_2 P
A quintuple peak	5	24397	C_2H_5 O
Multiple peaks	15	14702	3 C_6H_5



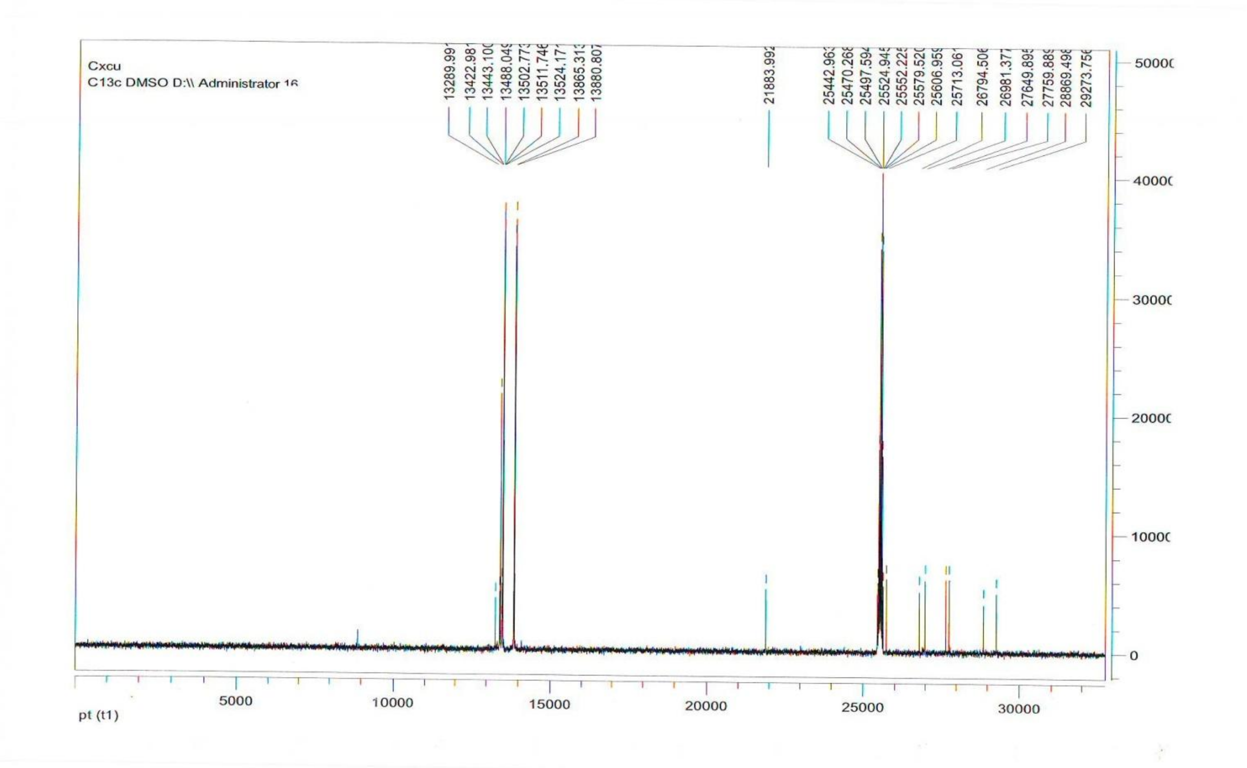
Spectrum2. The 1HNMR spectrum of the composition [C2H5COO (CH2PPh3Br)] [Cu2Cl6]

Spectrum3. The CNMR spectrum shows the composition of [C2H5COO (CH2PPh3)] [Cu2Cl6]. In this spectrum, the double peak at 26981-2694 corresponds to the carbon atoms of the ethyl group attached to the oxygen atom, and the peaks in the 25713-25442 correspond to the DMSO solvent. The double peaks in 29863-28869 are related to the carbon in methyl coupled to the phosphorus atom and double peaks in 27759- 27649 are correspond to carbon in phenyl attached to phosphorus atom, and unique peak in 21883 is correspond to the carbon of the carbonyl group and the existing multiple peaks In 13880-13289 are correspond to the aromatic carbons of benzene rings.

A summary of the results is presented in the table below.

Peak shape	δ (PPm)	Carbon type
A double peak	26794 - 26981	C_2H_5O
A double peak	28869 - 29273	CH_2P
A unique peak	21883	C - O

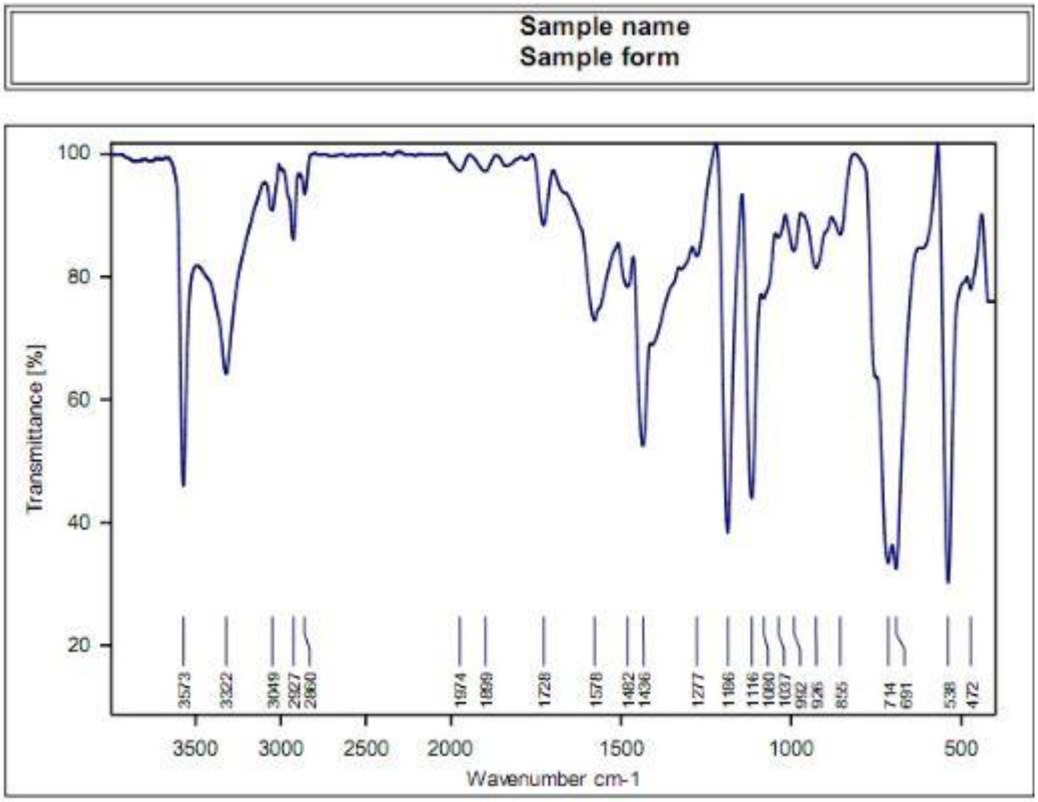
Multiple peaks	13289 - 13880	aromatic
A double peak	27649 - 27759	P - C



Spectrum3. The CNMR spectrum of [C2H5COO (CH2PPh3)] [Cu2Cl6]

Spectrum4. The IR spectrum shows the composition of [C2H5COO (CH2PPh3)] [Cu2Cl6 Br]. In this spectrum, the strong absorption in region 538 is related to the tensile vibrations of the C-Br bond. Also, strong absorption due to non-steric C-O stretching vibrations appears in area 734. The adsorption observed in 1116 and 1186 are respectively correspond to the tensile vibrations of C-C and C-O-ester bonds. The optical absorption in region 1436 correspond to the tensile vibrations of P-CH3 and the vibration of the P-carbon bond in the phenyl, and absorption in the region 1728 is correspond to the tensile vibrations of the C = O bond.

Finally, spectral adsorption in 2860, an average absorption in 3322 and strong absorption in 3573 are correspond to symmetric tensile vibrations CH3, tensile symmetrical and asymmetric vibrations of CH2, as well as the tensile vibrations of the C-H of the methyl ring in the composition, respectively.



Spectrum4. The IR spectrum of the compound [C2H5COO (CH2PPh3)] [Cu2Cl6 Br]

The results of the elemental analysis of this composition with the experimental formula C44 H 44 Cl 6 Cu 2 BrO4 are given in the following table.

$C_{44} H_{44} Cl_6 Cu_2 BrO_4$	%C	%H	%N
Experimental	45.15	3.92	___
Theoretical	46.49	3.87	___

Discussion and conclusion

In this research, the synthesis of copper (II) complexes was investigated by using phosphonium salt produced by PPh3 with ethyl bromoacetate. And the composition [C2H5COO (CH2PPh3)] [Cu2Cl6 Br] was obtained by spectroscopic methods. Copper phosphonium complexes (II) can be excellent catalysts for different chemical reactions. It has a variety of applications in the chemical industry, including catalysts in the Heck reaction, Suzuki reaction and carbon hydrogenation reaction, terminal isomyramination of terminal olefins, and variation of the group in vinyl ethers. Therefore, more attention can be paid to the use of these compounds in different branches. The ability of phosphonium compounds to catalyze a wide variety of chemical reactions makes it very convenient to choose these compounds to work with.

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