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Invited Lectures

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The chemistry of polyoxometalates based hybrids and polycarboxylic acid complexes in view of crystal engineering concepts

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At present, research into polyoxometalates (POMs) is a hot topic in many scientific fields, mainly because of their vast range of potential applications. Recently, the coordination ability of POMs has attracted the attention of the scientific community because it allows them to behave as unusual inorganic ligands. Currently, the design and assembly of hybrid inorganic–organic compounds has become an area of rapid growth due to their structural diversities as functional materials. POMs, as a unique class of inorganic metal oxide clusters, possess intriguing structures, unexpected reactivity and abundant potential applications. To date, a great deal of POMs-based hybrid compounds constructed from various metal ions and different kinds of POMs have been reported. A direct consequence of this ability is the assembly of high-dimensional architectures, which have been reported during the past decade. Thus, this presentation considers the latest achievements in the construction of hybrid inorganic-organic materials based on POMs, with a specific focus on their various coordination modes, particularly Keggin-type anions, which are widely available in our research group. [1-4] Herein, we describe the fascinating architectures of POMs-based hybrid compounds constructed using metal ions and different kinds of POMs. Complementing, the important role of POMs, the choice of adequate ligands is fundamental to modulate the properties of hybrids inorganic-organic as highlighted in this presentation. In addition to the important role of POMs, the choice of adequate ligands is important to modulate the properties of hybrid inorganic-organic materials. Moreover, flexible ligands with strong coordination capacity have been used for construction of POMs-based compounds with attractive topologies and different dimensionality. Thus, this presentation puts into perspective latest research on this topic focusing to the construction of hybrid inorganic-organic materials based on flexible ligands. Remarkably, they provide to POMs-based systems the flexibility and conformational freedom necessary to satisfy the coordination environment of the metal centers creating unprecedented topologies, such as entangled structures. In addition, this presentation also describes recent works devoted to analyze how the negative charge of POMs influences the supramolecular assembly of hybrid inorganic–organic materials. In second part of this talk, we report the syntheses and X-ray crystal structures of supramolecular frameworks based on polycarboxylic acid and amines prepared under ambient/solvothermal conditions using the proton-transfer mechanism in views of crystal engineering concepts. [5-7] The solid state architecture of the complexes has been analyzed and the energetics of the noncovalent interactions has been studied by means of high level DFT calculations. The evaluation of the binding energies associated with each noncovalent interaction is useful for rationalizing their mutual influence in the crystal packing.

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Coordination and Bioinorganic Chemistry of Metal-Drug Complexes

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The molecule resulting from the coordination of an organic drug (or an array of drugs) to a transition metalcenter is called a metal-drug complex. Metal-drug complexes are important both in coordination and bioinorganic chemistry and play a very important role in medicine, pharmacy, and diagnostics.

Recently, we have been interested in the design and synthesis of transition metal complexes based on oxicam ligands that can target DNA and BSA.Oxicams are one of seven chemical classes of non-steroidal anti-inflammatory drugs (NSAIDs) which suppress inflammation in a manner similar to steroids, but with fewer side effects. Coordination of oxicams to metal ionssuch as Ru(II), Pd(II), Zn(II), Co(II), Ni(II), and Cu(II) can provide an enhanced activity of the drug because of the synergism between the ligand and metal properties. In this regard, potential anticancercytostatic and cytotoxic effects of oxicam complexes have been investigated, revealing a synergistic activity when a transition metal ion is co-administered with anti-inflammatory drugs.An *in vitro* cytotoxicity investigation of the oxicam complexes on human cancer cell lines indicates that the oxicam complexes exhibit a considerable cell growth-inhibitory effect and most of the oxicam complexes show a remarkable increase in their cytotoxic activity in comparison to their free ligands and their metal salt precursors.In addition,we used molecular docking and ONIOM methodsformodeling the binding of the oxicam complexes to biomolecules.

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Zeolites, Properties and Applications

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Zeolites are hydrated aluminosilicate minerals made from interlinked tetrahedral of alumina (AlO_4) and silica (SiO_4). In simpler words, they're microprous solids with a relatively open, three-dimensional crystal structure built from the elements aluminum, oxygen and silicon, with alkali or alkaline-earth metals (such as sodium, potassium, and magnesium) plus water molecules trapped in the gaps between them.

Several transition metals have been substituted into crystalline silica or aluminophosphate frameworks to yield the corresponding metallosilicates or metalloaluminophosphate molecular sieves. Under controlled synthesis conditions, the metal can enter into the framework with the same coordination geometryas the parent element, which is tetrahedral. Some of transition metals which are believed to be incorporated into crystalline silica frameworks are V, Fe, Mn, Co, Cr, etc., although the exact nature and coordination of these metals are still in debate tetrahedral coordination in thesesystems.

There are about 40 naturally occurring zeolites and the artificial synthetic zeolites (around 800) have been designed for specific purposes, the best known of which are zeolite A (commonly used as a laundry detergent), zeolites X and Y (two different types of faujasites, used for catalytic cracking), and the petroleum catalyst ZSM-5 (a branded name for pentasil-zeolite).

Zeolites are widely used as ion-exchanger, molecular sieve, solid acid, catalyst or catalyst support, adsorbent of water or other molecules and etc.

In our recent researches, it can be distinguished that one of the conventional methods for enhancing the activity of a semiconductor as a photocatalyst is to use an efficient support material such as metalosilicate, which can increase its effective surface area and also provides an effective and homogenous dispersion of semiconductor particles on the external surface or within the pores of its structure. Moreover, the metalosilicate structure with electron-accepting and donating properties can play an important role in the control of charge transfer process. Thus using metalosilicates leads to an improvement the photocatalytic activity of the prepared semiconductor nanoparticles.

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Key role of heteropoly acids as nano catalyst
My research group and Me

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The application of catalysis to reduced toxicity systems, benign and renewable energy systems, and efficiency makes it a central focus area for green chemistry research in the 21th century. It is possible to prepare heterogeneous analogous of the most commonly used soluble and homogeneous catalysts by immobilization of them on various insoluble supports. The use of heterogeneous catalysts in chemical processes would simplify catalyst removal and minimizing the amount of waste formed. However, although heterogeneous catalysts can be recovered by filtration or precipitation through adding precipitating agents to the reaction media, these methods are time- and energy-consuming. Moreover, a substantial decrease in activity and selectivity of the immobilized catalysts is frequently observed due to the heterogeneous nature of the support materials in reaction media, steric and diffusion factors. A great proportion of active species are deep inside the supporting matrix and thus reactants have limited access to the catalytic sites. Therefore, to maintain economic viability, a suitable heterogeneous system must not only minimize the production of waste, but should also exhibit activities and selectivities comparable or superior to the existing homogeneous route. The advances in nano science and nano technology have led to a new research interest in employing nano-sized particles to construct a recyclable nano catalyst system in the heterogeneous catalysis.

Keeping in mind above statements, among heterogeneous solid acids, supported heteropoly acids (HPAs) with Keggin structures have received the most attention due to their unique structure and strong acidity.Flexibility in their acid strength, low toxicity and fairy high thermal stability make them as excellent and versatile catalysts for a wide variety of acid catalyzed reactions in homogeneous and heterogeneous media.[1-4] Thus heterogenization of HPAs produce nano catalysts and combine both advantages of nano support and HPAs, undoubtedly opened a new horizon for scientists and made them take a different and more precise look at heterogeneous nano catalysts.

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Affinity, hole-size fitting, preorganization and solvent role in host-guest complexation

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In traditional supramolecular chemistry the selectivity is mainly characterized by the hole-size fitting concept. However, nowadays, we know that the selectivity depends on several factors like ‘‘hole-size fitting’’ but also on ‘‘affinity’’, ‘‘strain energy’’, ‘‘solvent role’’ etc. [1] Following our interest in predicting the formation constants of metal complexes of macrocyclic and macroacyclic ligands[2–4] we studied the origin of the selectivity of some 3D hosts for alkaline cations or halide anions.[5–8] Two types of host-guest systems were studied: (i) protonated azacryptands with halide anions; (ii) calix[4] tubes with alkali metal cations (see Fig. 1). In all cases, our calculations showed that the solvent molecules play an important role in the formation of these complexes. Indeed, always there is a solvent hindrance against the desolvation of host and guest ions that occurs during the formation of host-guest complex in solution. However, whenever the process of desolvation of isolated host and guest ions is not very endothermic and solvation of new host-guest complex is exothermic enough, then the solvent hindrance against the host-guest complexation decreases and formation constant of corresponding complex increases. Thus, in order to design a good host for a special guest, in addition to all important parameters such as a good host-guest interaction, hole size fitting and a good degree of preorganization, we must also think about its structure/charge and strength of its interaction with solvent molecules.

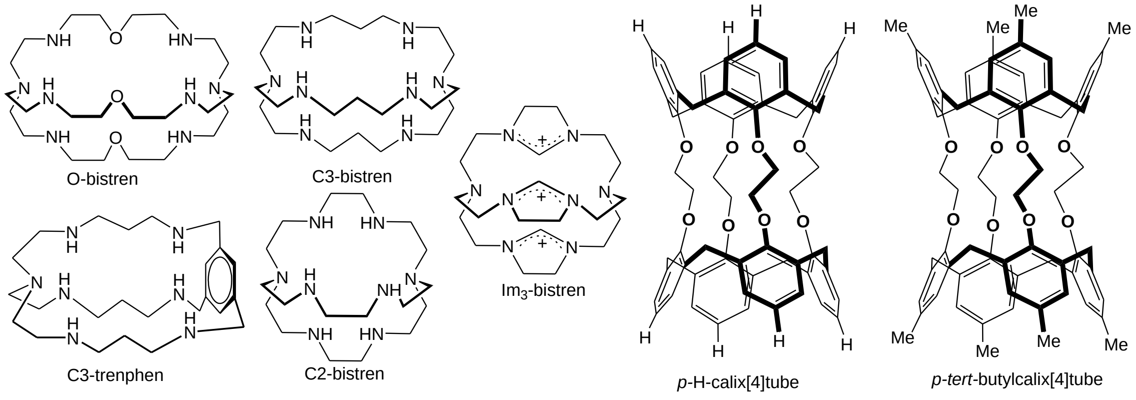

Fig. 1. Molecular structures of host species studied in our group during recent years.

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Manganese Compounds for Water Oxidation Catalysis – From Biological to Artificial Leaves

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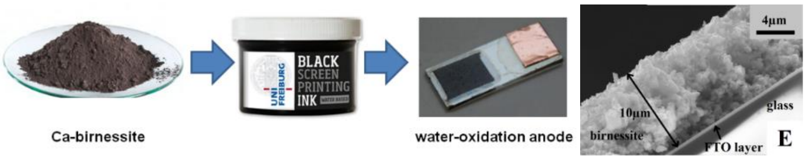
The efficient catalysis of the four-electron oxidation process of water to molecular oxygen (eq.1) is a central challenge for the development of devices for the use of renewableenergy to produce chemical fuels. This is equally true for artificial leaf-type structures and electrolyser systems.

$$2\ H_2O \rightarrow O_2 + 4\ H^+ + 4\ e^- \quad (1)$$

Inspired by the composition of the oxygen evolving complex (OEC) of Photosystem II, the very efficient biological catalyst for reaction (1), we have developed synthetic routes for calcium manganese oxides and successfully used these materials as heterogeneous catalysts for water oxidation. In screenings where Ce^{4+} was used as chemical oxidant, calcium-containing, layered manganese oxides from the birnessite mineral family clearly emerged as most active oxide phase. These oxides have rather complex elemental compositions (e.g. a typical stoichiometry is $K_{0.20}Ca_{0.21}MnO_{2.21}\cdot 1.4H_2O$) and structurally contain layers of edge-sharing $[MnO_6]$-octahedra with manganese in average oxidation states of +3.5 to +3.9. [1] The synthetic parameters during their preparation proved to be of great importance for catalytic rates and we found that especially the Ca/Mn ratio and the temperature used during the post-synthetic treatment in air have to be optimized to enhance catalytic performances. [2]



As a next step towards the use of suchMnO_x catalysts in combination with light-absorbing semiconductors (“artificial leaves”), we searched for a method to coat conductive surfaces like FTO or nickel with Ca-birnessite layers (see Figure). After several optimization steps, we developed a screen-printing method yielding electrodes covered by ~10µm-thick layers of Ca-birnessite. These anodes can be operated for hours at water-oxidation current densities of $>1 mA\cdot cm^{-2}$ in an aqueous electrolyte at pH 7 without a significant loss in activity.[3]

The presentation will start from a description of the “static” properties of both the as-prepared birnessite materials and the screen-printed electrodes. Next, it will be described how some of these properties are significantly altered when manganese oxides are used as (electro)catalysts for water oxidation, which can be detected by using analytical tools like IR, XRD, XAS or XPS. Because birnessites are highly-disordered, porous materials of variable composition and Mn redox state, such *in operando* investigations are very complex. On the other hand, the detected features of chemical and structural flexibility might be central to explain the observed good electrocatalytic performance of birnessite anodes and thus a deeper understanding of these dynamic properties is needed to improve the performance of MnO_x-based anodes in water oxidation.

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Precise and accurate crystal structure determination: Tuff crystal structures with disorder and twinning

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A real perfect periodic crystal is a solid object in which a special pattern is repeated over and over in three- dimension. The crystal structure determined from the diffraction data is the spatial averageover the whole crystal which doesn’t give real image of the changes in the solid state by the conventional routine structure determination method. An ideal crystal isconsideredto be constructed byregular arrangement of unit cells, eachhaving an identical composition of atoms or molecules. Therefore, for the spatially averaged data a correct modelling should be done to describe the crystal structure precisely. There are two major kinds of irregularityin crystal structure determination *viz.* disorder and twinning. In this talk we will review different case of occurring disorder and twinning in crystal structure to get a better view for modelling and description of such structures.

Boron-rich borides – Synthesis, crystal structures, physical properties and bonding

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The crystal structures of elemental boron are unique. The explanation is its behaviour as a non-metal, which fulfils not the 8-N rule. As a consequence boron shows a unique variety of bonding modes with the formation of B_{12}-icosahedra as the most prominent feature. [1] This is continued in boron-rich borides, which can serve a model structures.

One class of compounds can directly be derived from the structure of β-rhombohedral boron. In $LiB_{\sim 10}$, $BeB_{\sim 20}$ and $MgB_{\sim 20}$ the interstitial B-atoms of β-rhombohedral boron are substituted by metal cations. [2]

A second class relates to the simple structure of α-rhombohedral boron, which is characterised by a *ccp* arrangement of B_{12} icosahedra and 2e-2c bonds. In binary compounds $B_{12}P_2$, $B_{12}As_2$ and $B_{12}S_{2-x}B_2$ the 2e-3c bonds are substituted by diatomic units. Deviations from the stoichiometric composition, i.e. $B_{12}P_{2-x}$, are seen from the colour and manifest in the EPR spectra. A similar situation is observed in ternary representatives of boron carbide $B_{13}C_2/B_4C$. The uptake of Li and Be changes the colour. In the case of Al and Si there is additionally a substitution within the CBC-unit.

Boron-rich borides show a strong tendency to form electron-precise compounds. In $MgB_7$the B_{12} –icosahedra and interstitial B_2-units constitute a covalent framework with Mg^{2+}cations in its voids. In other representatives belonging to this structure the B_2-unit is substituted by C_2, PC or CBC-units, while charge and number of the cationsare changed according to the electronic requirements. [3] Another way to achieve a stable structure is to fit the connectivity of the B_{12}-icosahedra and the interstitial units. Examples are compounds of the system Mg/B/C ($MgB_{12}C_2$, $Mg_3B_{50}C_8$, $Mg_2B_{24}C$). [4]

We have used the Electron Localizability Indicator (ELI-D) [5] to describe different bonding properties in elemental structures of boron aind in a number of boron-rich borides. This method enables a distinction between exohedral B–B bonds and endohedral bonds within a polyhedron, independent from distance and valence electron density.

The elemental analysis of boron-rich borides is a special problem. Careful examination of high-quality single crystal data and electron micro probe analyses (EMPA, EDX) of single crystals will well-defined surfaces allow a simultaneous determination of all elements.

Boron carbide is known as one of the hardest materials ever. Therefore, we have measured the micro-hardness of our new compounds and confirmed hardness values between those for Al_2O_3 and boron carbide. In combination to the high chemical and thermal stability this makesboron-r ich borides to an interesting class of materials for high-temperature materials.

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Oral Presentations

Levofloxacin-intercalated layered zinc hydroxide as a bacteria inhibitor

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Layered double hydroxides (LDHs) and layered hydroxide salt (LHS) well known as anionic clays or hydrotalcite-like consist of positively charged layers and exchangeable anions, along with water molecules in the interlayer space.[1,2] Layered Zinc hydroxide (LZH) is an LHS with a general composition of $M^{2+}(OH)_{2-x}(A^{n-})_{x/n}.mH_2O$ where M^{2+} is a metallic cation and A^{n-} represents a counter ion with (n-) charge. LZH has also been used as a drug delivery system for compounds like ellagic acid [3], ciprofloxacin [4], and hippuric acid.[5] New organic-inorganic nanohybrid based on layered zinc hydroxide intercalated with an antibacterial agent was synthesized through direct reaction of levofloxacin at various concentrations with layered zinc hydroxide. The basal spacing of the pure phase nanohybrid was 16.57 Å, with the levofloxacin anions arranged in a monolayer form and an angle of 37 degrees between the layered zinc hydroxide interlayers. A Fourier transform infrared study confirmed the formation of the nanohybrid, while thermogravimetry and differential thermogravimetry analyses showed that the thermal stability of the nanohybrid was markedly enhanced. Antibacterial activity of the nanohybrid was also studied by an in-vitro test, such as the minimal inhibitory concentration (MIC) by agar dilution method. The antimicrobial activity of the nanohybrid against various Gram-positive bacteria (Staphylococcus aureus, Bacillus subtilis) and Gram-negative bacteria (Escherichia coli) was evaluated and found that the antibacterial activity of nanohybrid was greater than that of parent drug Levofloxacin.

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Structure Determination and DFT Studies of Some New Phosphite-based Cyclo platinated(II) Complexes Containing Biphosphine Ligands

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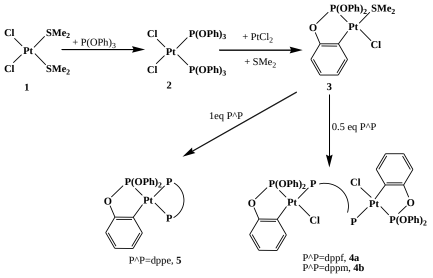
Phosphines and phosphites have widely been used in the structure of inorganic and organometallic complexes as good σ-donor π-acceptor ligands. These ligands present various steric and electronic effects when coordinated to transition metals. Chemical behaviors of phosphines and phosphites are tuned by changing the substituents at the phosphorus atom.[1]

Formation of a stable five-membered C^P cyclometal is one of the out-standing properties of the arylphosphite family. They can perform intramolecular C-H activation on ortho positions of their phenyl rings in appropriate conditions. Orthometallatedarylphosphite derivatives of palladium and platinum are known and show catalytic properties in organic solvents.[2-5]

In the present study, The starting complex $[Pt(C^\wedge P)Cl(SMe_2)]$, **3**,was made by a new method using the reaction of $[PtCl_2(P(OPh)_3)_2]$ with $PtCl_2$ and then SMe_2 under reflux condition. The new cyclometalatedphosphite complex, $[Pt(C^\wedge P)Cl(SMe_2)]$, is to be treated with some bidentate phosphine ligands to explore their mode of coordination.The schematic view of the syntheses is shown in Scheme 1. The complexes were fully characterized using multinuclear (^1H and ^{31}P) NMR spectroscopy and elemental analysis. The structure of typical complex **4a** was also determined by X-ray crystallography. The optimized structures of the complexes in their dichloromethane solutions were obtained from DFT calculations. These optimized structures were used to determine the frontier molecular orbitals of the complexes and also the nature of their electronic transitions.

In addition experiment the Suzuki biaryl coupling reaction has been performed with these synthesisedcyclometalatedphosphite complexes as catalyst.



Scheme 1

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Preparation of new nano composite of ZnO nanoplates- Poly aniline and application as new sorbent in solid phase microextraction

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Application of polymers were developed in research and industry field such as sorbent in adsorption of pollution in water, membrane, insulator, conductive polymers and etc at 70 decade. Recently composite of nanostructures and polymers could change properties such as surface area and thermal and chemical stability. [1,2] By developing 3-D nano structures such as nano-rods and nano-plates of metal oxides, a higher surface area can be achieved. Here we report on the investigations on ZnO nano-plates- poly aniline composite grown on fused silica, as a new sorbent for solid phase microextraction (SPME).

The results of the innovative study on a new stationary phase with high efficiency based on nano composite of ZnO-polyaniline nano plates coating on fused silica are reported in this paper. These composite of nanoplates with a thickness in the range of 30–60 nm and the length of about 100 nm, have been grown on fused silica fibers using a hydrothermal process. The extraction properties of the fiber were investigated using head space SPME mode coupled with gas chromatography for dioxin in water. Extraction parameters were optimized by experimental design and estimated response surface methods. The calibration curves were linear at the $\mu g\ l^{-1}$ range with low detection limits for mentioned compounds. The high stability of the nano composite of ZnO-polyaniline nano plate coating is proved at relatively high temperatures (up to 300 ^{o}C) with a high extraction capacity and long lifespan (more than 100 times). The synthesized nano composite was proved by SEM and XRD results.

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Synthesis and Characterization of a Cobalt (II) Complex with N, $N^{/}$, $N^{//}$ -Tris (2-pyrimidinyl) Dimethylentriamine

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Cobalt complexes have been intensively studied during the last decade due to their huge impact in biological and catalysis applications. [1, 2] In the present work, [Co_3(PDMT)Cl_6] complex is synthesized in cyclohexanole under hydrothermal conditions using cobalt chloride and N, $N^{/}$,$N^{//}$ -Tris (2-pyrimidinyl) dimethylentriamine (PDMT) as ligand. The crystal structure of ligand and complex are solved using laboratory X-ray powder diffraction data and optimized molecular geometries of complex by B3LYP methods respectively. Crystallographic data of the ligand is shown crystal system and space group is monoclinic and P2/n respectively. The successful preparation of complex is confirmed by elemental analysis Mass, FT-IR, UV-Vis and TGA techniques. The formation of the complex is established by the observation of $[C_{14}H_{15}N_9Co_3Cl_6]^+$ fragment as a parent ion in the mass spectra, electronic absorption spectrum is shown Co (II) ions possessing tetrahedral symmetry and the TGA results approves the presence of ligand and after heating up to 400C°, Co_2O_3 is formed**.** Based on the theoretical method, three molecules of $CoCl_2$ in three directions are closed to the ligand, the conformation of PDMT as ligand due to the coordination is changed. Optimized structure of the [Co_3(PDMT)Cl_6] complex is given in Fig. 1.

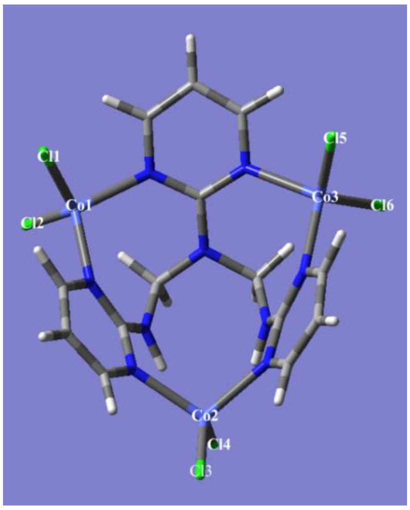

Fig. 1. Optimized structure of [Co_3(PDMT)Cl_6] complex by B3LYP method.

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Supramolecular assemblies of diphenylphosphinic acid and its triphenyltin(IV) complex: a combined experimental and theoretical study

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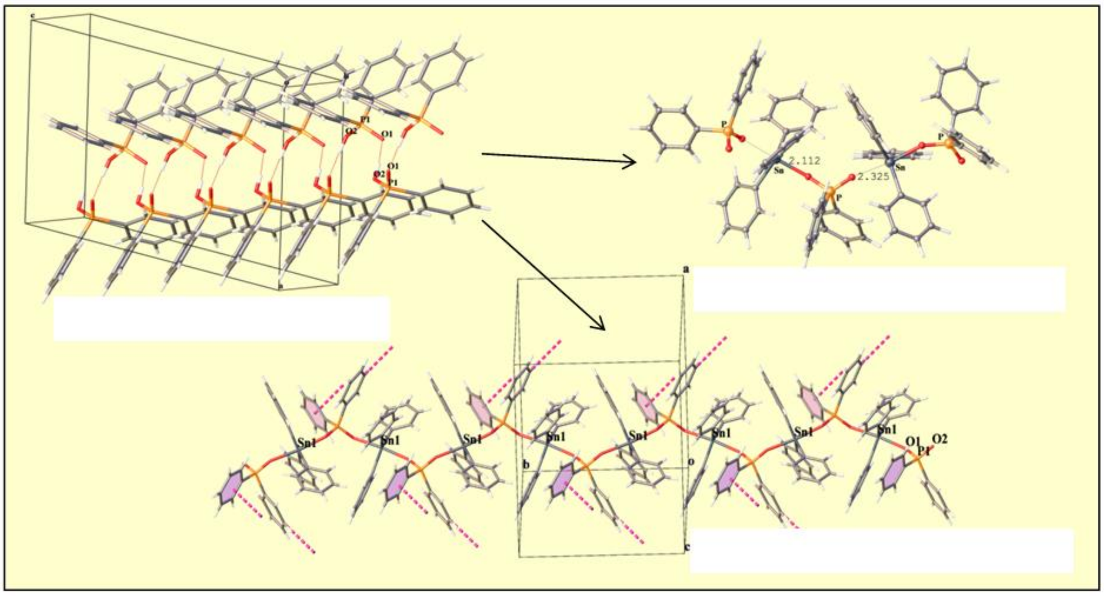
Extending our program in the design, synthesis and complexation of phosphoryl-containing ligands, we have focused on the coordination behavior of hetero- or homo-difuntional ligands (diphosphoryl compounds or *N*-pyridinilephosphoramides; respectively) toward organotins.[1, 2] Reaction of these neutral ligands with Ph_3SnCl afforded mono or binuclear tin adducts. In this work, interaction of bidentate ligand $Ph_2P(O)OH$ (**L**) with triphenyltin(IV) chloride is presented. The ligand is deprotonated toward tin centers and bridges between them; resulting in the polymeric coordination structure (**C**).Supramolecular frameworks of the ligand and its complex are discussed using geometrical analysis.Moreover, DFT calculation was performed to estimate binding energy of all non-covalent interactions (including hydrogen bonds, CH…π, π/π and coordination interactions). The P=O…H and P=O→Sn interaction along the *b*-axis, make a substantial contribution to directing the crystal packing of **L** and **C**, respectively. According to the NMR result, complex **C**is dissociated to the monomeric species in the solution, agreeing to the optimized structure in the gas phase.

$$Ph_2P(O)OH + SnPh_3Cl \xrightarrow{MeOH\text{-}CHCl_3} [Ph_2P(O)O{\rightarrow}SnPh_3]_n$$



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Tuning the dimensionality of hybrid inorganic-organic materials based on polyoxometalates

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Owing to potential applications in catalysis, photochemistry, magnetism, ion exchange, biological chemistry and medicine, much effort has been dedicated to exploring polyoxometalate (POM) chemistry.[1-3] In recent years, the design and assembly of hybrid inorganic–organic materials based on polyoxometalates has become an area of rapid growth due to the following developments: (i) advances in cluster chemistry, (ii) growth of organic synthesis pertinent to ligand preparation and post-synthetic modification, (iii) improvement in structure determination, particularly through X-ray crystallography. Up to now, the control of the dimensionality of the resulting hybrid compounds is still a great challenge, as the final structures are frequently modulated by various factors such as pH, reaction temperature, molar ratios of starting materials, the selection of POM anions and ligand molecules, among others. [4-7] In this review, we investigated the role of ligands in the synthesis of the hybrid inorganic–organic compounds with attractive topologies and different dimensionality such as entangled structures and related systems in terms of crystal engineering.

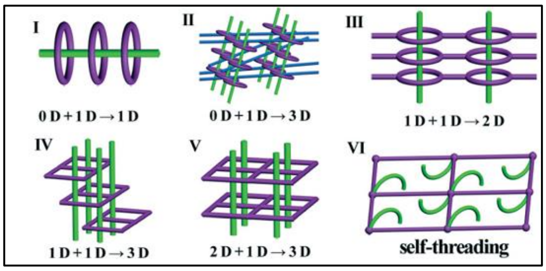

Fig. 1. Schematic representations of the reported POM-based polypseudorotaxanes.

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Feasibility predict physical and chemical properties of titanium organic compounds

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Today, the production and development of chemical compounds requires long time and a lot of financial costs. Therefore, it is very important to use the techniques of (QSAR) and (QSPR) to predict physical and chemical properties. Topological indices are constant of graph, used to study quantitative structure activity relationship (QSAR) and quantitative structure Properties relationship (QSPR) (Consonni, 2009; Van de Waterbeemd, 1992; Van de Waterbeemd, 1993). This graph describes the simplest connection of atoms in a molecule (Zarrabian, 2000). In this article we will randomly choose a number of organic compounds of titanium and calculating two topological indices: Harary and Balaban. Then we try to fit a model to predict the physical and chemical properties of some organic compounds of titanium. To offer this model, the physical and chemical properties of the samples were calculated using the Gaussian software. The results indicate good agreement on the application of topological index Harary, to predict the physical and chemical properties. The Log (P) and Exact Mass for these compounds versus Harary index (H), gives by:

$$\text{Log (P)} = 0.0797\ H + 0.2508$$

$$\text{Exact Mass} = 2.9213\ H + 135.06$$

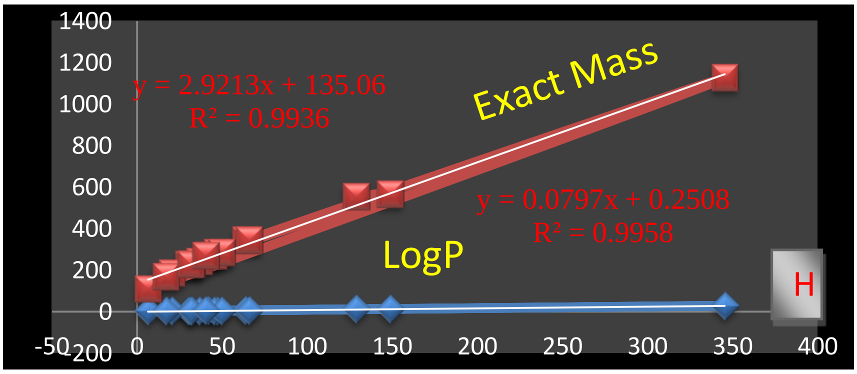

Fig.1.The Exact Mass and Log (P) versus Harary index

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Counter-cation effect on the liquid-phase sorption of C_1-C_4 normal alcohols in a set of new nanostructured polyoxometalate-based ionic crystals

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The construction of nanostructured materials with advanced functions by the self-organization of molecular building blocks is one of the key topics in modern materials chemistry. [1] These crystalline nanostructured solids have been studied from the viewpoints of gas storage, molecular sieve, shape-selective catalysis, and ion exchange. [2] Polyoxometalates (POMs) as transition metal macroanions can create microstructures in the ionic crystal lattice with the complexation of appropriate macrocations. [3] Herein, we reported three new ionic crystals, prepared by self-assembly of all ingredients, with the general formula of $A_3[Fe_3O(O_2CCH_2OCH_3)_6(H_2O)_3][\alpha\text{-}SiW_{12}O_{40}]\cdot nH_2O$ in which "A" is "Li, Na or K" and "n" is "3, 13.5 or 3" respectively (Figure 1). Every single-crystal was characterized by FT-IR, powder XRD, TGA, X-ray crystallography and N_2 adsorption/desorption analysis and finally was evaluated for alcohol sorption in liquid-phase by gas chromatography. Kinetic studies were performed for every single alcohol and resulting data were fitted on Lagergren's models. Observed changes in sorption capacity of the ionic crystals were related to their counter-cations.

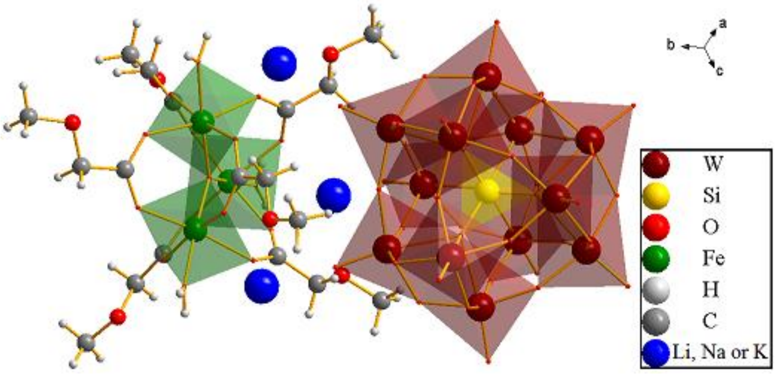

Fig. 1. Single-crystal structure of the ionic crystals.

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Effect of pH and template amounton synthesis and Crystallization of SAPO-34 nanostructured catalyst

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The production of light olefins from methanol (Methanol-to-Olefins or MTO process) is an interesting route for researchers of the petrochemical industry.[1] SAPO-34 molecular sieve with a pore size of 0.43–0.50 nm, relatively mild acidity and high thermal stability exhibits high selectivity for olefins in MTO.[2,3,] In the present work, the effect of pH on synthesis of SAPO-34 nano structured catalyst was investigated. The pH of samples precursor was controlled by template. Template as the space filling, structure-directing agent and charge compensating is one of necessary material for synthesis of SAPO-34.[4] The samples were synthesized in different pH by hydrothermal method. The synthesis catalysts were characterized by XRD and SEM techniques. The XRD data shown in (Fig. 1) indicate thatSAPO-34 zeolite has been prepared in pHranges of 7-8 and 9-10. The synthesised sample in pH=5-6 range was macro pore SiO_2, because of content of template wasn't enough for SAPO-34 phase formation. The crystallinity of samples was enhanced by the increasing of pH of precursor. It was found that the synthesisconditions affect the crystallinity, textural properties and crystallite size of catalyst.

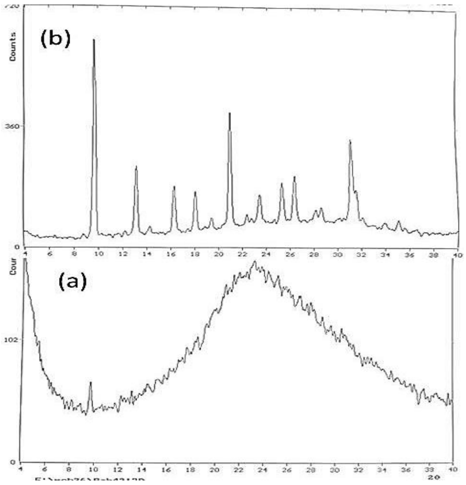

Fig. 1. XRD patterns of SAPO-34 samples fordifferentpH(a=5-6, b= 7-8)

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Synthesis, Characterization, and QSAR studies of some new phosphorus compounds having five and six-membered rings as anticancer agents

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Drug resistance and lack of selectivity are major problems in the treatment of diseases such as cancer and microbial infections. Considering this, the design and development of new bioactive agents to devoid of many of the unpleasant side effects has become a serious challenge to medicinal chemists. Due to steric, electronic, and conformational properties, structures of phosphorus derivatives allow them to interact easily with the biopolymers of the living systems.[1,2] Therefore, they inhibit acetylcholinestrase and butyrylcholinestrase enzymes and as such are useful for inhibiting of cell proliferation in the treatment of cancer .[3,4] Therefore, in this study, sixteen new desired derivatives with -NHC(O)NHP(O)- backbone were synthesized and characterized by IR, ^{1}H, ^{13}C, and ^{31}P NMR. Cytotoxic activities of these compounds and cyclophosphamide (standard drug) were assayed against HeLa, PC-3, and MCF-7 cancer cell lines. To understand the correlation between the anticancer activity and physicochemical properties of the synthesized compounds, the QSAR studies carried out. The QSAR models revealed that the presence of six ring of diazaphosphor may be favorable for higher antitumor activity, agreeing with result of *In vitro* anticancer activities. Besides, the QSAR models demonstrated the importance of electronic parameters like QN_2, QC and E_{L+1} in describing anticancer activity of the synthesized compounds.

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Structure, antimicrobial activity and interaction with a nucleotide/protein of trinuclear palladium (II) complex containing 9-Fluorenone oxime ligand and molecular docking investigation

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Over the past decades, oxime chemistry is one vital research field for inorganic and bioinorganic chemist, because of their simple preparation and their pharmacological applications. [1] Oxime derivatives are attractive synthetic goal because of their low toxicity to non-target organisms, antibacterial and antifungal properties and a high index of antitumor activity [2] via intercalation. The novel trinuclear Pd(II) complex with aryl oxime ligand, $[Pd_3(C_{12}H_9C=NO)_6]$ was synthesized and structurally characterized by elemental analysis, IR and resonance signals in the NMR, and single crystal X-ray crystallography. The DNA/BSA binding and antimicrobial activity of this complex were investigated. The interactions of the complex with calf thymus DNA has been explored by absorption, competitive, thermal denaturation and circular dichroism methods, which revealed that the compound could interact with DNA through groove binding. Further, the albumin interactions of complex were investigated using fluorescence quenching spectra and synchronous fluorescence spectra. The result of fluorescence titration suggested that the fluorescence quenching of BSA by complex was a static quenching procedure. The site marker displacement experiments suggested the location of complex binding to BSA was Sudlow's site I in the subdomain IIA. Finally, the molecular docking experiment supported the above results and effectively proved the binding of Pd(II) complex to BSA and DNA.

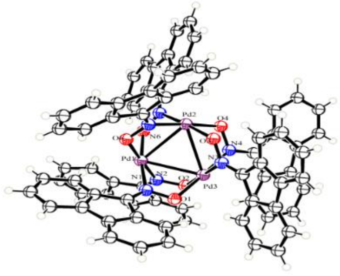

Fig 1. ORTEP diagram for Pd complex with ellipsoids drawn at the 50%probability level

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Structure determination from powder diffraction data (SDPD): X-ray polycrystallography of some organic and inorganic compounds

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The routine method for the crystal structure determination is still single-crystal X-ray analysis which require the single crystal sample with appropriate size and quality. However, there are many solids in which no suitable single crystals can be grown and only prepared as microcrystalline powders. In this regard, structure determination from powder diffraction data (SDPD) as a more challenging and more time consuming method than single crystal analysis, is widely and successfully used for organic and inorganic compounds.[1,2] Today, the reliability of structures which are carefully determined by SDPD is closely as high as from single-crystal analysis.[3]

In this study, I describe the SDPD method for crystal structure determination, and demonstrate its use to determine the crystal structures of our new synthesized carboxamide ligand as organic and mercury (II) halide complexes as inorganic compounds. The X-ray powder diffraction patterns of aforementioned compounds were recorded using a laboratory powder X-ray diffractometer. The structure solution has been performed by using a real space method with subsequent Rietveld refinement.

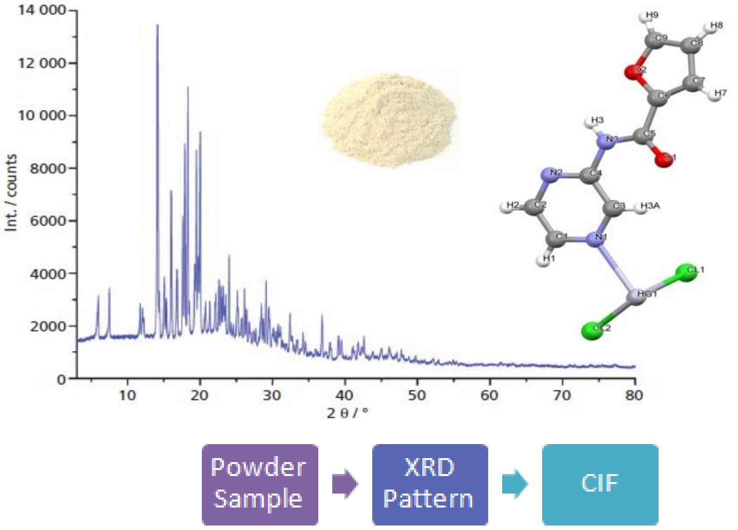

Fig.1 Schematic representation of SDPD for mercury (II) chloride complex

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Medicinal Properties of Photosensitizers Compounds, TPP, TCPP and TSPP

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Photosensitizers compounds could be excited by light of a specific wavelength [1], often by visible or near infrared light. A photosensitive drug absorbs photons which alter the drugs into an excited state. These excited drugs then pass their energy to oxygen to form free radicals (singlet oxygen) which oxidize cellular structures. [2] The structure of the new three porphyrin with Drug-Likeness are shown and compared in Table 1. In this study, some important activities extracted from PASS software that include three classes: pharmacological effects, molecular mechanisms and side effects and toxicity are given in Table 2. The main activity of the compounds 1-3 is their photosensitizer property,that PASS software was predicted it's; 1 > 2 >3, by the side effects (for example; ulcerogenic); 2 > 1> 3. One ideal photosensitizer would have the highest photosensitizer activity and the lowest side effect activities. Thus, our theoretical studies confirmed the compound 3 for experimental as an illustration for reporting antibacterial activity of this compound.

Table 1. The structure of the new threeporphyrin with Drug-Likeness.

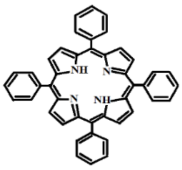
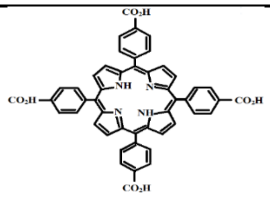
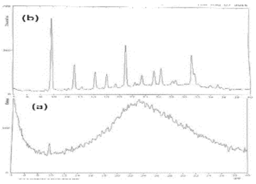
TPP	TCPP	TSPP
1. Drug-Likeness: 52.0%	**2. Drug-Likeness: 61.1%**	**3. Drug-Likeness: 26.6%**
		

Table 2.A portion of the predicted probability activity spectra of the title compounds.

Biological Activity		% PASS Activities		
		1.	2.	3.
Pharmacological Effects	**Photosensitizer**	**36.4**	**31.3**	**22.5**
	Antineoplastic alkaloid	42.6	35.8	15.4
	Antioxidant	36.5	35.9	19.4
	Antimycobacterial	36.0	32.8	19.4
	AntiinflammatoryLeumedin-like	10.7	46.4	3.60
	Antibacterial	2.90	15.4	3.90
MolecularMechanisms	**CYP1A1 human substrate**	**62.8**	**39.7**	**24.0**
	Anthranilate-CoA ligase inhibitor	4.40	73.3	38.9
	Squalene-hopene cyclase inhibitor	4.30	7.10	90.8
	Peptide deformylase inhibitor	19.6	35.8	80.6
Side Effects and Toxicity	**Ulcerogenic**	**51.4**	**55.7**	**14.5**
	Eye irritation, weak	5.90	13.6	25.4
	Skin irritation, weak	4.60	9.20	13.1

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Fabrication of a novel ZnO/MMO/CNT nanohybrid derived from CoMnAl/CNT layered double hydroxide for photocatalytic degradation of azo dye under visible light

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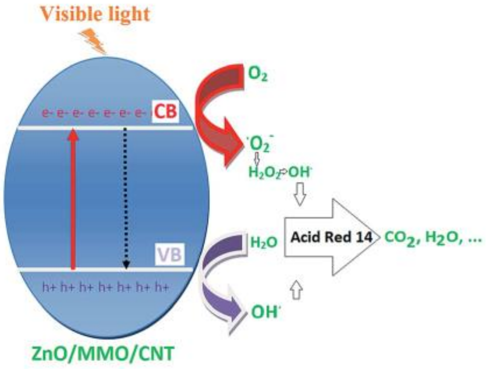
With the purpose of enhancement of photocatalytic performance in the visible region and efficient electron−hole separation, we reported a facile method for synthesis Co-Mn-Al-LDH/ZnO/CNT mixed metal oxide (ZnO/MMO) nanohybrid derived from ZnO/Co-Mn-Al layered double hydroxide (LDH) precursor. The physicochemical characteristics of the fabricated ZnO/MMO were surveyed by X-ray diffraction, scanning electron microscopy, UV/vis diffuse reflectance spectra and FT-IR spectroscopy. The photocatalytic activity of prepared ZnO/MMO/CNT nanohybrid was investigated by photocatalytic degradation of C.I. Acid Red 14, as a model pollutant, under visible light irradiation. The photocatalytic activity of ZnO/MMO/CNT was also compared with TiO_2- P25, ZnO and Co-Mn-Al-LDH/ZnO/CNT LDH. The experimental results shown that in comparison with other used photocatalysts, ZnO/MMO/CNT nanohybrid was an efficient photocatalyst under visible light irradiation. The effect of operational parameters including photocatalyst content, dye concentration, pH and intensity of light on the photocatalytic removal efficiency of dye was investigated. The result shown that efficiency decolonization was happened in the presence of ZnO/MMO/CNT nanohybrid, pH= 4.5, catalyst dosage = 0.01gr and light intensity = 45W.



Schematic representation of visible light photocatalytic process in the presence of ZnO/MMO/CNT nanohybrid

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Effect of Sorbitol/Oxidizer Ratio on Solution Combustion Synthesis of Copper-Based Nanocatalysts for Hydrogen Production

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In recent few years, the solution combustion synthesis of multicomponent metal oxides has been nominated as a promising straightforward preparation process to produce homogeneous, fine crystalline and unagglomerated powders.[1] Different parameters can affect on quality of synthesized nano material by the combustion synthesis such as fuel, fuel/oxidizer ratio, gas volume, flame and etc. Urea, glycine, and citrica acid are known as the conventional fuels for the solution combustion synthesis. [2] In this paper, sorbitol was chosen as the fuel to investigate its capability for synthesis of copper based nanocatalysts. To study the role of sorbitol/oxidizer, three samples were fabricated and their physicochemical properties were analyzed by XRD, FESEM, FTIR and BET analyses. Furthurmore, the efficiency of synthesized nanocatalysts for production of hydrogen through steam methanol reforming was tested in a U-type laboratory reactor which was connected to a gas chromatography analyzer. The results described that nanocatalysts which were syntheiszed by sorbitol via the solution combustion method showed acceptable methanol conversion and low carbon monoxide selectivity as the undesired product.

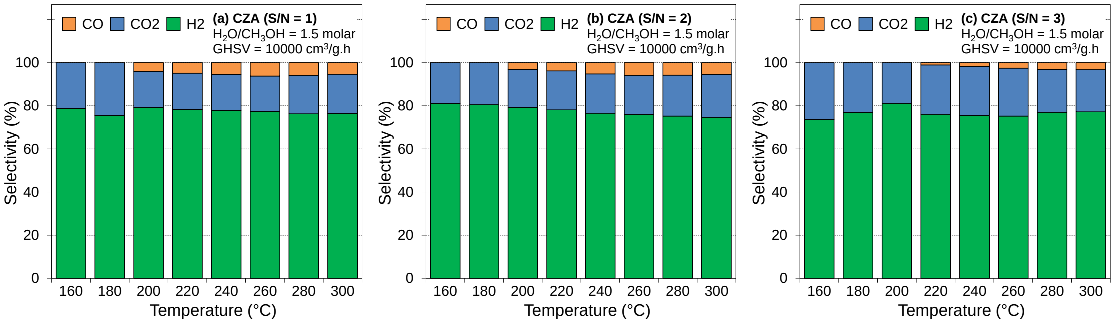

Fig. 1. Products selectivity over CuO/ZnO /Al_2O_3 nanocatalysts.

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Palladacycle complex of α-keto stabilizedphosphorous ylide; Synthesis, characterizationand high catalytic activity toward homogeneous Heck-Mizoroki reaction

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Application of palladacycles in coupling reactions such as Heck crosscoupling reactions have become an extremely useful method for the formation of C–C building blocks in organic synthesis.[1] Phosphorus ylides, due to their ready preparation and modification, highactivity and relative stability are very interesting ligands in organometallic chemistry[2] and Pd(II) complexes of these compounds are also can catalyzesome important organic reactions. [3] Sabounchei *et al.* reported the use of these complexes in the some cross-coupling reactions. [3] In this work, we report the synthesis, characterization and application of new Pd(II) complex [$PdCl_2(Ph_2PCH_2PPh_2C(H)C(O)Ph$-*m*-Br)] toward the Heck-Mizoroki cross-coupling reaction. Reaction of α-keto stabilizedphosphorous ylides [$Ph_2PCH_2PPh_2C(H)C(O)Ph$-*m*-Br] with $PdCl_2(COD)$in 1:1 ratios leads to mononuclear products of the palladacycle. Characterization of the complex by IR,^{1}H, ^{31}P and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom (**Fig. 1**). Moisture and air-stable, robust palladacycle phosphine–ylide complex was found to exhibit excellent catalytic activity in the Pd-catalyzed Heck-Mizoroki cross-coupling reactions. The ease of preparation of the catalyst precursors, its high solubility in organic solvents, low catalyst loading, and stability toward air make these complex ideal starting materials for the above transformations.

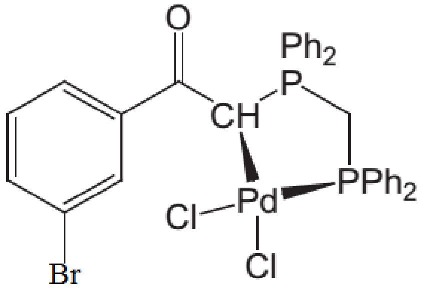

Fig. 1. The Pd(II) complex bearing phosphorous ylide .

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Posters

Molar Ratio of Copper/ MA to Control the Morphology of Copper nanoparticles Formed by Chemical Reduction Method

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For most application of nanoparticles, the size, shape and size distribution of metal nanoparticles found the key factors. As a consequence, attempts have been focused on the synthesis of metal nanoparticles with well-controlled morphology.[1] Copper, like other noble metals, performs thermal and electrical conductivity, which makes it a candidacy in electronic systems [2] and conductive. The properties of copper nanoparticles depend mainly on their preparation methods. Chemical reduction of copper salts in the presence anhydride maleic using ascorbic acid is a novel method. This method is nontoxic, economical and it can realize better morphology and size control by optimizing the experimental parameters. In this work, we attempted to study the effect of copper/MA molar ratio on the morphology of copper nanoparticles. Fourier transform IR spectra (FTIR), scanning electron microscopy (SEM-EDAX), X-ray diffraction (XRD) analysis have been used for the characterization of the samples. The FTIR results reveal that copper particles are well coated by the MA. Images SEM shows that the molar ratio Cu/MA played a crucial role in the morphologies of copper nanoparticles. X-ray diffraction results indicated that the nanoparticles are crystalline and mainly composed of face-centered cubic (FCC) Cu with average particle sizes were between 9.9 nm. Homogeneous flower like nanostructured copper–MA film was obtained for $CuSO_4.5H_2O$ /MA molar ratio of 100/1.

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Synthesis and spectroscopic studies for the determination of formation constants for Hg(II), Ag(I), Fe(II) complexes with ammonium 2-aminocyclopenten dithiocarbamate

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Transition metal complexes of dithiocarbamates continue to fascinate attention because of several industrial and biological application.[1] In this work, complexes were obtained at air stable composition at room temperature by the reaction of the ligand with their respective metal salts in 2:1 mole ratio. RNS and its complexation behavior with Hg(II), Ag(I), Fe(II) was investigated by examining the UV-Vis absorption spectra for determine the optimum conditions. Optimized conditions were instituted by studying effect of (1) solvent (2) reaction times (3) pH (4) temperature (5) ionic strength to correct the sensitivity of the present method. Formation constants of metal complexes determined by Likussar-Boltz method.

For complexes ML_2: $\log K_f = 0.3522 - 2\log K + \log Y_{Max} - 3\log(1 - Y_{max})$

In this equation: $K = C_M + C_L$ and $Y_{max} = A_{exp} / A_{max}$

Table1. Formation constants for Hg(II), Ag(I), Fe(II) complexes with RNS

Metals	Hg(II)	Ag(I)	Fe(II)
Formation constant	1.34×10^{11}	4.2×10^{6}	2×10^{4}

On the basis of experimental data of this complexes obtained by symbiosis principle. The sulfurs end of the RNS ligand is a soft electron donor and the nitrogen end is hard. In this ligand have two potential electron donor atoms. When bonding to metal ions, the bonding mode may be predicted by means of the symbiosis principle.

Table 2. Lewis acid

Borderline hard-soft	Soft	Softer
Fe^{+2}	Ag^{+}	Hg^{+2}

RNS ligand bonds through the sulfur atom, then: K_f $Hg^{+2} > Ag^{+} > Fe^{+2}$.

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Synthesis, characterization and crystal structure of a new silver(I) coordination polymer containing 3-methylthio-(1H)-1,2,4-triazole: A new precursor forpreparation of silver nanorods

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The reaction of 3- methylthio-(*1H*)-1,2,4-triazole (MTTz) with silver(I) nitrate in a molar ratio 2:1 in MeOH/CH_3CN led to the coordination polymer $\{[Ag_2(MTTz)_4](NO_3)_2\}_n$ (**1**). The coordination polymer (**1**) has been characterized by FTIR- and ^{1}HNMR- spectroscopy, ESI-MS spectrometry and elemental analysis as well as single crystal X-ray diffraction. According to the X-ray structure, the ligands in the cations of **1** exhibit two different tautomeric forms with two different coordination modes. While two of them act as *exo*-bidentate bridging agent between two metal centers via their nitrogen atoms and are responsible for the formation of a six-membered $(Ag–N–N)_2$ ring, the two other ligands coordinate unidentately to each silver atom. In addition, the metal centers of each six-membered ring are connected to the sulfur atoms of the consecutive ring, resulting in a coordination polymer along [001] (Fig 1. a). Photoluminescence associated with complex **1** upon excitation at 260 nm, exhibiting a weak emission at 324 nm at room temperature as a consequence of intraligand π-π* transitions. The slight red-shift in **1** as compared to the free ligands is due to the enhanced structural rigidity resulted by the existence of MTTz moieties coordinated to Ag(I) centers. Also, solventless thermolysis [1] of complex **1** at 600 °C under air atmosphere led to the formation of silver nanorods. The silver nanostructures were characterized by a series of techniques including X-ray powder diffraction (XRD), energy-dispersive X-ray (EDAX) and scanning electron microscopy (SEM) (Fig1. b).

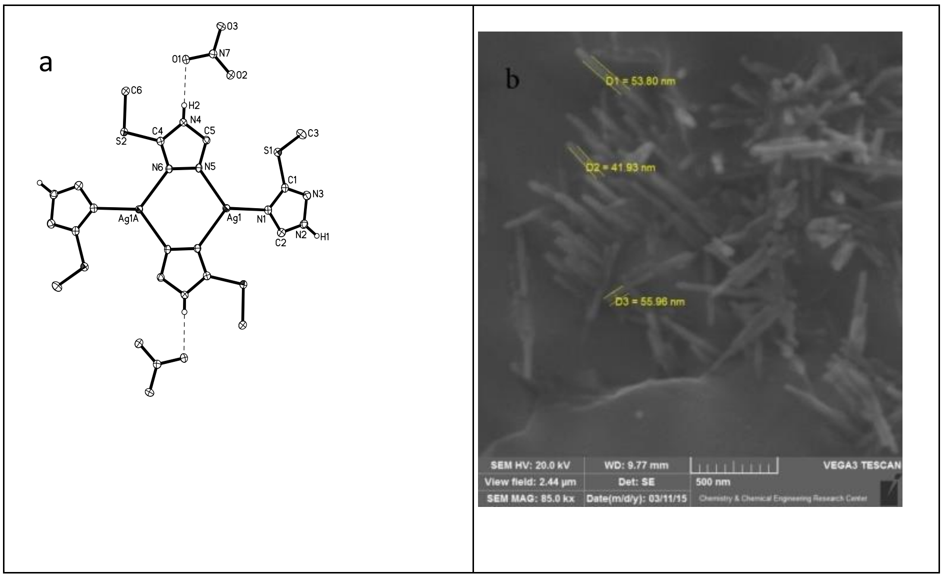

Fig. 1. (a) Molecular structure of **1**and (b)SEM images of silver nanorods

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Theoretical study of Oxaliplatine and carboplatine platinum (II) anticancer characteristics and comparison with cis-dichlorodiamino platinum (II) (CDDP) as a reference

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In this work, comparative hydrolysis of oxaliplatin and carboplatin has been studied quantum-mechanically using B3LYP method, with respect to cis-platin (cis diamino dichloro platinum II). The calculations of systems contain C, N, H and O described by the standard 6-31G (d) basis set. For Cl and Pt elements standard LANL2DZ basis set are used and described by effective core potential (ECP) of Wadt and Hay pseudopotential with a double-ξ valance using the LANL2DZ. Due to their symmetry, for these drugs, only one path is expected for approaching of water molecule to the complexes. The computed potential energy surfaces show that, for the neutral hydrolysis, the first step of reactions is the slower process, with activation barriers of about 29.94 kcal/mol (for oxaliplatin) and 33.98 kcal/mol (for carboplatin). Comparison of the hydrolysis barriers between two steps of reactions reveals that the rate-limiting process is the ring-opening reaction with the ligand release occurring quick. Therefore, oxaliplatin and carboplatin are more likely to bind to DNA in theirs completely hydrolysis forms. Also, the reactions are endothermic and the energies are +8.80, +28.86 kcal/mol for oxaliplatin and +7.84, +34.99 carboplatin in two step of hydrolysis reaction respectively.

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A theoretical study of Structure, properties and substituent effect on dialumenes

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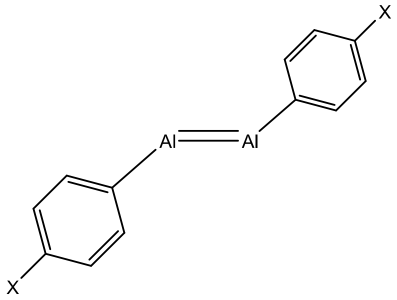
In this work, we report a theoretical study on molecular structure, and electronic properties of dialumene (ArAl=AlAr, Ar=aryl) and substituted dialumene. The structures and properties in these molecules have been studied utilizing Becke's hybrid three-parameter exchange functional and the nonlocal correlation functional of Lee, Yang, and Parr (B3LYP). All calculations were carried out with the Gaussian 03 suite of program using the 6-311G+ (d, p) basis set. The effects of the substituent groups on the structure, electronic properties, ionization potential (IP), electron affinity (EA), and reorganization energy has been studied. The most intensity electronic transition energy and oscillator strength of molecules calculated by Time-Dependent Density Functional Theory (TD-DFT) and shows λmax blue-shifted in withdrawing electron substituents. Quantum theory of atom in molecules has been used for explain of AlAl and AlC bonds in all molecules. QTAIM analysis indicated closed-shell interactions for AlC bonds and shared interactions AlAl bonds.



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A New and Highly Selective Fluorescent Chemosensor for Hg^{2+} based on N_2O_2-donor Naphthodiaza-crown Macrocyclic Ligand

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Determination of fluorescent probes which exhibit selective and sensitive signaling systems toward important chemical species is a very attractive research topic in the chemosensing and molecular imaging fields. In particular, versatile molecules that can be used to detect more than one metal ion facilitate multiple ion detection with a single device.[1,2] Thus, versatile molecules capable of detecting more than one metal ion are desired. Macrocyclicfluorescent chemosensors have received intense attention in recent years, owing to their selective metal ion recognition and sensitive signaling capacity. In this work a 19-membered N_2O_2-donor naphthodiaza-crown macrocyclic ligand (**L**) were synthesized and characterized employing IR, ^1H and ^{13}C NMR spectroscopy as well as microanalysis. The influence of metal cations such as Hg^{2+},Cd^{2+} ,Zn^{2+} ,Pb^{2+} ,Na^+ ,Ni^{2+} ,Co^{2+} ,Ba^{2+}, Fe^{3+}, Fe^{2+}, Cr^{3+} ,Co^{3+} ,Mn^{2+} ,K^+ ,Cu^{2+} ,Ag^+ ,Cr^{2+} ,Li^+ and Cs^+on the spectroscopic properties of chemosensor **L** in ethanol solution were investigated by means of fluorescence spectroscopy (Fig. 1.). The macrocycle was found to be as an effective fluorescence sensor for Hg^{2+} ions in the presence of other metal cations in solution by enhancement of the fluorescence emission of **L**.Hg^{2+} could selectively participatein complex formation with the receptor **L**.

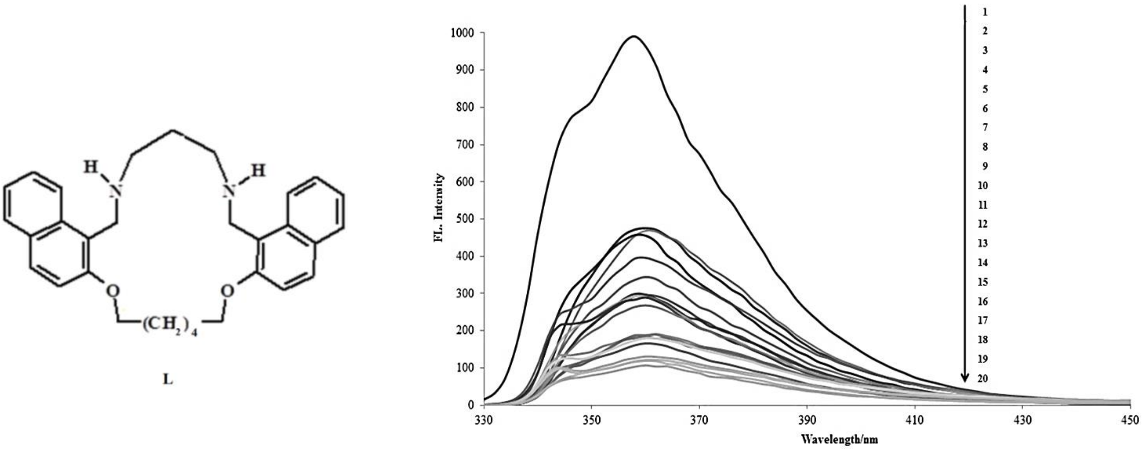

Fig.1. TheStructure of19-memberedN$_2$O$_2$-donor naphthodiaza-crown macrocyclic ligand(**L**) (left) and Fluorescence spectra of **L**(right) in the presence of various metal ions1.Hg^{2+}, 2.Cd^{2+}, 3.Zn^{2+}, 4.Pb^{2+}, 5.Na^+, 6.**L**, 7.Ni^{2+}, 8.Co^{2+}, 9.Ba^{2+}, 10.Fe^{3+}, 11.Fe^{2+}, 12.Cr^{3+}, 13.Co^{3+}, 14.Mn^{2+}, 15.K^+, 16.Cu^{2+}, 17.Ag^+, 18.Cr^{2+}, 19. Li^+, 20.Cs^+.

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Synthesis andstudy oftransition metalcomplexofcobalt (II)with Schiff base ligand derived from2-amino methylpyridineandSalicylaldehyde with azide

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In this scientific research the purpose is synthesis a complexes from the Cobalt (II) salt reaction with tridentate Schiff base ligand N2O donor from the reaction of Salicylaldehyde and 2-amino methyl pyridine with azide ligand. The aim in this research is to make a complex synthesis contains Sodium azide and cobalt transition metal. Since, in this research the resulted Schiff base ligand from density of Salicylaldehyde and 2-amino-methyl pyridine developed in liquid form so, the considered complex was obtained from the density of the desired metal salt, amine, aldehyde and sodium zide salt and refluxed action steps regarding stoichiometric ratio of ethanol solvent. Considered Synthesis of azide complex using molar ratio of1: 1: 1: 6 of Cobalt (II) salts, Salicylaldehyde, 2- Amino-methylpyridine and Sodium azide salt was carried out. This complex was examined using infrared spectroscopy, Ultraviolet, Elemental analysis, thermal analysis. In the IR spectrum absorption band region 2085/05 cm-1 resulted from coordination of Azide ligand into transition metal and also bifurcation of sharp peak of Azide is due to junction of one side of Azide ligand to central metal. The appeared peak in region 1558/48 cm-1 indicates adsorption related to safety stretching C=N and also adsorption band related to C-O phenolic in frequency of 1355/96cm-1.These evidence indicates formation of complex. High electrical conductivity of the electrolyte solution represents being Electrolyte of solution and Ionic complex structure.

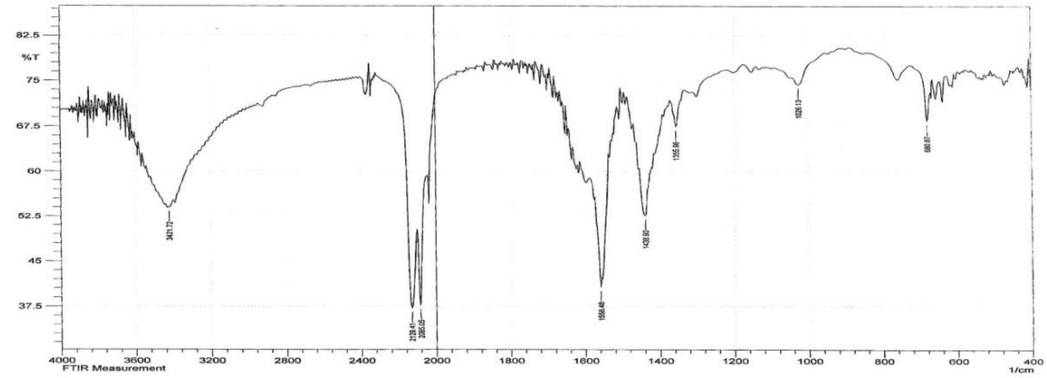

Fig.1. IR spectrum of Cobalt complex

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Photoelectrochemical properties of nano particles ZnO prepared by UPD on Au(III)

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ZnO nanowires were fabricated successfully using a new electrochemical approach based on underpotential deposition (UPD) and simultaneous oxidation Zn atomic layers from an oxygenated aqueous suspension of ZnO. Electrochemical UPD and the oxidation mechanism of the Zn atomic layers to ZnO were studied by cyclic voltammetry and potential-controlled electrochemical deposition techniques. These thin films were characterized by X-ray diffraction (XRD), X-ray fotoelectronspectroscopy (XPS), scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS).

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Electrochemically induced atom-by-atom growth of SnO/ZnOby co-deposition method

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Ultrathin films of SnO/ZnO were grown on Au(III) substrates using a novel, simple co-deposition method. These thin films were characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy(SEM), UV-visible spectroscopy and energy dispersive spectroscopy (EDS). Cyclic voltammograms were used to determine approximate deposition potentials for co-deposition. UV-vis spectra for the SnO/ZnO thin films with various thicknesses, which is related to deposition time, Shows that the band gap of the SnO/ZnO decreases as the film thickness increases.

Referesences

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Comparative Studieson Fluorescence and UV-Vis Spectroscopic Measurement of Binding Constantsfor N2O2-donor Naphthodiaza-crown Macrocyclic Ligands with Metal Cations

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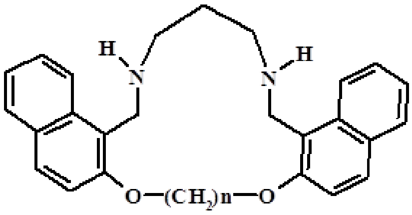
Macrocyclic ligands are well-known for binding to metal ions selectively, and they are accordinglyemployed as carriers in metal selective extraction, phase transfer catalysts, membrane transport and other related processes.[1] Although, the interaction of metal ions with the mixed nitrogen–oxygen-donor macrocycles have been studied in considerable depth, but related studies involving macrocycles incorporating naphthalene moieties are recently been received increasing consideration as interesting metal complexing reagents.[2]

In this work a series of N_2O_2-donor naphthodiaza-crown macrocyclic ligands, **L^1-L^5**, were synthesized and characterized applying IR, ^1H and ^{13}C NMR spectroscopy as well as microanalysis. Herein, we investigate the interaction of metal cations such as Co(II), Ni(II), Cu(II), and Zn(II) with a series of 15- to 19-membered mixed-donor naphthodiaza-crown macrocyclic ligands (Fig. 1.), each incorporating an O_2N_2-donor set. Employing fluorescence and UV-Vis spectrocscopy in ethanol using Job's method of continuous variation, it was established 1:1 stoichiometries for the interaction between Co(II), Ni(II), Cu(II) and Zn(II) and the macrocyclic ligands. For instance, Table 1 typically shows the respective *K* valuescalculatedfor these complexes with **L^1**. Measurement of their binding constants(*K*) withthe mentioned metal ions applying Benesi–Hildebrand equation revealed well-established correlation between the fluorescence and UV-Visresults.



n	compound
2	L^1
3	L^2
4	L^3
5	L^4
6	L^5

Fig.1. The general structures of theN_2O_2-donor naphthodiaza-crown macrocyclic ligands

Table1. The comparison between K (M-1) values of metal ions With L1 obtained by fluorescence and UV-vismethods

Metal ion	Fluorescence emission (at 358 nm)	UV-Vis [λ_{max} (nm), ε L mol^{-1} cm^{-1})
Co^{2+}	876 (± 75)	668 (± 98), [640 nm, = 19.69]
Cu^{2+}	5650 (± 87)	4238 (± 353), [780 nm, 29.49]
Ni^{2+}	1700 (± 95)	1483 (± 423), [663 nm, 22.47]
Zn^{2+}	7812 (± 76)	-

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Theoretical investigation of pyrrole in photocatalyst reaction of metylene blue

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The conductively filled conducting polymers were first made in 1930 for theprevention of corona discharge. The potential uses for conductively filled polymershave since been multiplied due to their ease of processing, good environmentalstability and wide range of electrical properties. Being a multi-phase system innature, however, their lack of homogeneity and reproducibility has been an inherentweakness for conductively filled polymers. Therefore, controlling the quality of dispersion to obtain homogeneous conducting polymer composites is critically important.

In this study the ionization energy of photocatalyst surface TiO_2 which modified by pyrrole used to degradation of methylene blue calculated by B3LYP/6-311G method and the intraction band gap decreased to better role as photocatalyst.

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The HOMO and LUMO energy structure of Asparaguic Acid

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Organosulfur compounds are organic compounds that contain sulfur. They are often associated with foul odors, but many of the sweetest compounds known are organosulfur derivatives, e.g., saccharin. Nature abounds with organosulfur compounds—sulfur is essential for life. Two of the 20 common amino acids are organosulfur compounds, and the antibiotics penicillin (pictured below) and sulfa drugs both contain sulfur. While sulfur-containing antibiotics save many lives, sulfur mustard is a deadly chemical warfare agent. Fossil fuels, coal, petroleum, and natural gas, which are derived from ancient organisms, necessarily contain organosulfur compounds, the removal of which is a major focus of oil refineries. Asparagusic acid is the organosulfur with the formula $S_2(CH_2)_2CHCO_2H$. The molecule contains both carboxylic acid and disulfide functional groups. It is present in the vegetable asparagus and may be the metabolic precursor to other odorous thiol compounds.[

In this study the structure energy surface of asparagusic acid were established by B3LYP/6-311G method and the HOMO and LUMO orbitals distingued. The graphical counters presented to shown the band gap of energy.

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Immobilization of a molybdenum complex on IRMOF-3 as a heterogeneous catalyst for selective epoxidation of olefins

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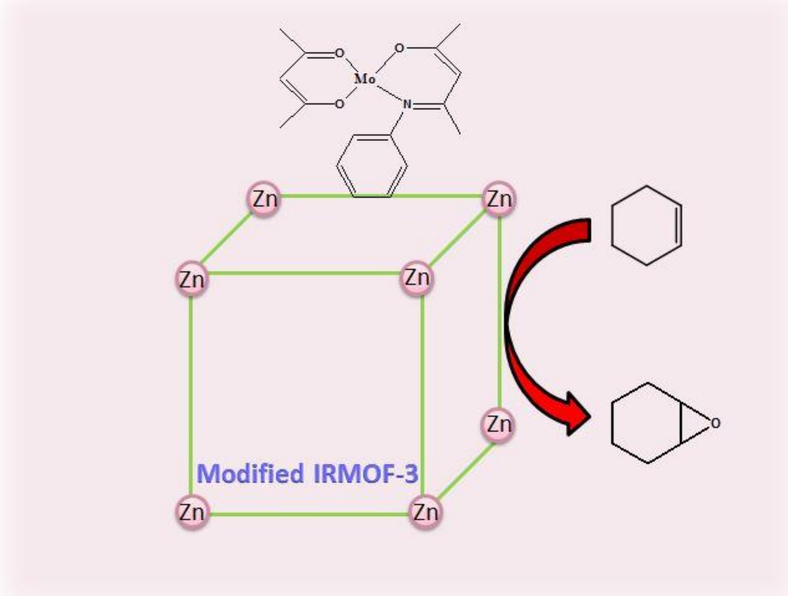
Metal-organic frameworks (MOFs), as a new class of functional materials, are nanoporous crystalline organic-inorganic hybrid solids constructed from inorganic metal nodes connected to organic linkers.[1,2] Chemical modification of nanoporous IRMOF-3 metal-organic framework afforded enhanced catalytic activity in epoxidation reaction. Post-synthetic modification of the MOF was conducted through the covalent attachment of the bis(acetylacetonato) dioxomolybdenum(VI) complex to the free amine groups in the IRMOF-3. The resulting molybdenum containing MOF was characterized by Fourier transform infrared, atomic absorption spectroscopies, powder X-ray diffraction, scanning electron microscopy, thermogravimetric analysis and nitrogen adsorption/desorption techniques. The resulting catalyst was highly active in epoxidation of different olefins as well as allylic alcohols, while the unfunctionalized IRMOF-3 showed low catalytic efficiency. The immobilized molybdenum complex can be reused for successive runs with no leaching during the epoxidation reaction.



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Mo(VI) Schiff base Complexes supported ontoMulti wallCarbon Nanotubes as Green, Reusable and Selective catalyst for Oxidation of Sulfides

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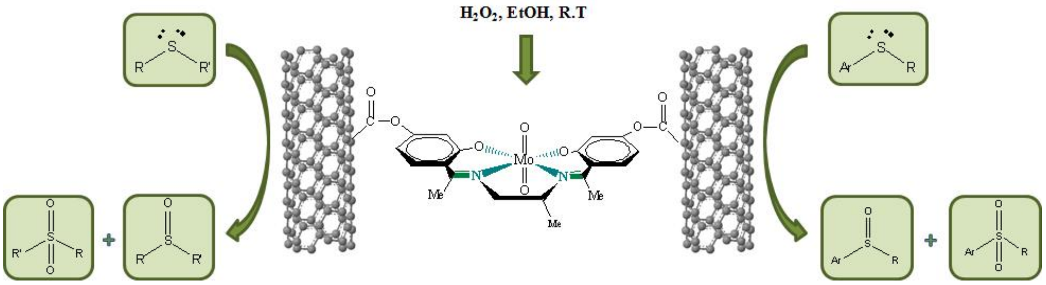
Oxidation of sulfides is among the most important reactions in chemistry and different publications exist to describe new methods in oxidation reactions. Increasing concern about rapid accretion of pollutants, environmental degradations and the danger of chemicals, create an important challenge for the future in the scientific community and scientists would prefer replacement of traditional processes by "cleaner" catalytic alternatives. In this aspect in the past decades, lots of catalytic reactions were presented not only to improve conversion of the reactions, but also to green chemistry approach such as employing renewable and green feed stock.

In the present research, MoO_2L_1 Schiff base nanoparticleshave been prepared under ultrasonic irradiation and also MoO_2L_1Schiff base complex has been supported on chemically modified multi wall carbon nanotubes (MoO_2L_1@MWCNT). The prepared heterogeneous catalysts have been characterized by IR, NMR, Raman and UV-Vis spectroscopy, Field Emission Scanning Electron Microscopy (FESEM) and Dynamic Light Scattering (DLS) for particle size measurement as well as Transition Electron Microscopy (TEM) and Thermal Gravimetry Analysis. Catalytic activities of the prepared catalysts in green oxidation of sulfides with aqueous 30% H_2O_2 as an environmentally friendly oxidant in ethanol at room temperature were studied. Repeated runs of both complexes were carried out three times and the results represented their stability and excellent catalytic activity in oxidation of sulfides.



Synthesis, structural characteristic, antimicrobial and spectral properties of new Cu(II) complexewith an ONO Schiff base ligand

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The new complexes of Cu(II) metal ions with a Schiff base ligand (H_2L) (E)-2-(5-bromo-2-hydroxybenzylideneamino)phenol have been prepared and characterized. The characterization of the newly formed complexes has been done by using UV–Vis, IR spectroscopy and Elemental analysis. The crystal structure of Cu(II) have been determined by X-ray diffraction study. The single crystal X-ray diffraction analyses revealed that copper(II) cation is five-coordinated and the coordination polyhedron is a slightly distorted square pyramid. A series of three coordinated transition metal(II) complexe have been synthesized by the reaction with the tridentate Schiff base H_2L, which was prepared by the condensation of 5-bromosalicylaldehyde with 2-aminophenol. The synthetic procedure in this work resulted in the formation of complexes in the molar ratio (1:1) ($M:H_2L$) with tree drop of MeIm. The newly synthesized Schiff base participated in bonding to copper as square pyramidal ligand through the azomethine nitrogen and phenolic oxygen atoms and nickel as squar planner and cobalt as tetrahedral were also synthesized and characterized by the spectral and analytical techniques the UV–Vis, IR and X-ray data are showned. The ionization constants of the investigated H_2L–Schiff base-ligand have been determined potentiometrically. The complex formation equilibria were investigated to ascertain the composition and stability constants of the complexes.

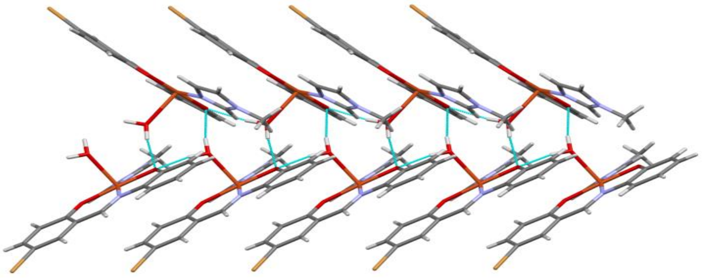

Fig. 1. The fragment of hydrogen-bonded chain in Cu(II).

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Nanolayered manganese oxide/carboxylated multi walled carbon nanotubes composite: a good water-oxidizing catalyst for artificial photosynthetic systems

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The finding of an efficient, cheap and environmentally friendly water-oxidizing compound is highly desirable for artificial photosynthetic systems because water oxidation is a bottleneck for water splitting into H_2 and O_2.[1] H_2 production by water splitting is currently much discussed as a promising route for the conversion of sustainable, but intermittent energy.[2] Mn compounds are very interesting because they are not only cheap and environmentally friendly but also efficiently used by nature for water oxidation.[2]

Herein, we report nano-sized nanolayered manganese oxide/carboxylated multi walled carbon nanotubes composite as water oxidizing compounds in artificial photosynthesis. The composites are synthesized by different and simple procedures and characterized by a number of methods. The water-oxidizing activities of these composites are also considered in the presence of cerium(IV) ammonium nitrate. We conclude that synthesis of nanolayered manganese oxide/carboxylated multi walled carbon nanotubes composite as oxidizing catalyst is possible by very simple method.

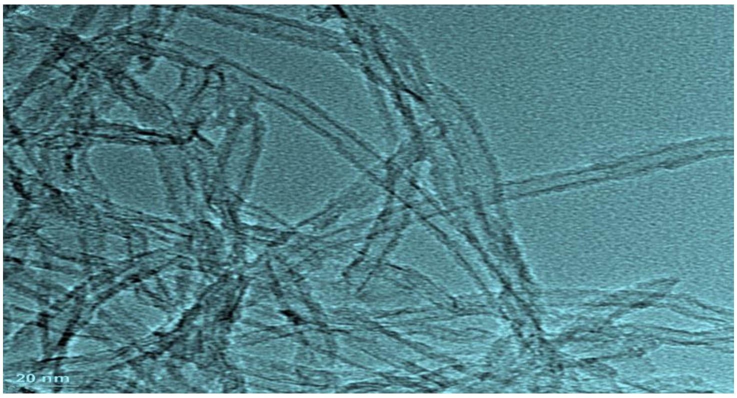

Fig. 1. TEM images from nanolayered manganese oxide/carboxylated multi walled carbon nanotubes composite

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Synthesis and characterization of some spinel oxide nanoparticles using sol-gel method

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In this project one group of nanosized Spinel-type oxides contain are prepared from nitrates of the constituent metal ion, citric acid (CA), using a sol-gel method. A series of common analytical techniques are used to characterize the crystallinity, morphology, specific surface area, and grain size of the nanopowders. Thermal decomposition process of the complex precursor is examined by means of differential thermal analysis–thermal gravimetric analysis (DTA/TGA). X-ray diffraction (XRD) patterns show that single spinel phase is completely formed after calcination treatment. The surface morphology and composition of these nanopowders are also investigated using scanning electron microscopy (SEM) and energy dispersive X-ray spectrometer (EDX). The Fourier transform infrared (FTIR) spectra and the ultraviolet-visible (UV-Vis) spectra are also measured for studying of structure of prepared nanopowders.

Moreover, the ability of spinel nanoparticles to remove **e**nvironmental pollutant from aqueous solutions is assessed. The adsorption studies are carried out at different pH values, different adsorbate concentrations, various adsorbent dosages, different temperature, and contact time in a batch experiments to find the optimum conditions.

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Synthesis and Characterization of new Ba(II) Complex based on Pyridine-2,6-dicarboxylicAcid and 2-Amino

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supramolecular architectures based on metal and organic building blocks have attracted interest because of their novel topologies and also potential applications in host–guest chemistry and magnetism[1]. Pyridine-2,6-dicarboxylic acid is one of the suitable substances for designing self-assembly of metal ions and bridging organic ligands.[2,3] On these bases After the synthesis of (2-apyH_2)(pydc) [2-apy: 2-aminoand pydc: pyridine-2,6-dicarboxilate) as a proton transfer compound, we synthesized and characterized the structure of $[2\text{-apyH}]_2[Ba(pydc)_2(H_2O)_3]$. $5H_2O$. This complex crystallizes in Monoclinic system and $P2_1/c$ space group. The Ba(II) ion is coordinated by four O atoms and two N atoms from two (pydc) $^{-2}$ ligands and three water molecule in a distorted three capped trigonal prism geometry (fig.1). The cell parameters are as follows: a=13.457(3)Å, α=90°, b=13.193(3)Å, β=95°, c=17.948(4)Å, γ=90°.

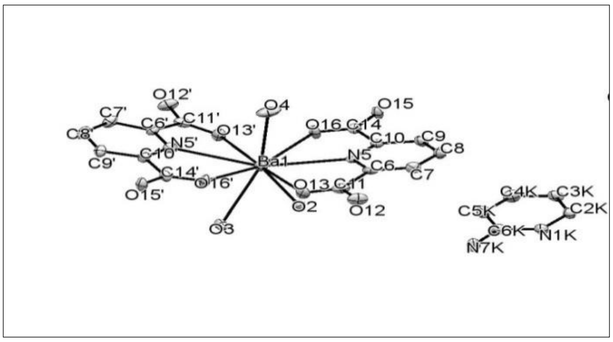

Fig. 1. ORTEP view of $[2\text{-apyH}]_2[Ba(pydc)_2(H_2O)_3].5H_2O$

A wide range of non-covalent interactions consisting of hydrogen bonding and C-H….π, π-π stacking are effective in its stabilizing.

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Synthesis and characterization studies of new P-coordinated mercury (II) complexes formed by the ligand, [$Ph_2PCH_2CH_2Ph_2PC(H)C(O)C_6H_4NO_2$]

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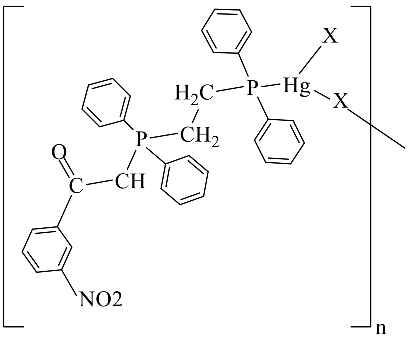
The reactivity of metal complexes toward phosphorusylides has attracted the interest of chemists due to the versatility of its reaction pathways and the variety of the resulting products and their different applications[1]. Much of the interest in the coordination properties of resonance stabilized phosphorusylides stemming from their bond versatility due to the presence of different functional groups in their molecular structure[2]. In this work, the reaction of bifunctionalized ylide, [$Ph_2PCH_2CH_2PPh_2{=}C(H)C(O)C_6H_4NO_2$] with mercury(II) halides in equimolar ratios using dry methanol as solvent yielded the P,P-coordinated monomeric complexes [$HgX_2(Ph_2PCH_2CH_2Ph_2PCH_2C(O)C_6H_4NO_2)$] (X = Cl (**1**), Br (**2**), I (**3**)). Characterization of the obtained compounds was also performed by elemental analysis, IR, ^{1}H, ^{31}P, and ^{13}C NMR. Elemental analysis indicate a 1:1 stoichiometry between the yilde and Hg(II) halide in each of complexes. On the basis of the physicochemical and spectroscopic data we propose that ligands herein exhibit monodentate P-coordination to the mercury(II) centre (Fig. 1).[3] The antifungal activities of free ligand and their corresponding mercury(II) complexes are also evaluated. The results show that the mercury(II) complexes are more active than the title ligand.



X = Cl (**1**), Br (**2**), I (**3**)

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Synthesis and characterization of new diphosphine ligand and its palladium(II) complex

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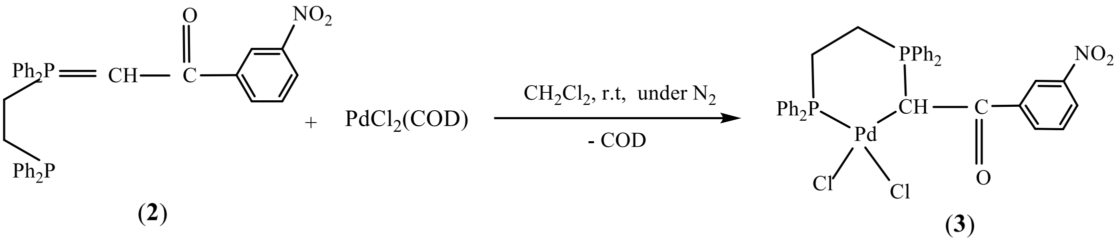
The organometallic chemistry of phosphorous ylides has undergone a great growth in the last few years[1], mainly due to their interesting application as reactants in organometallic and metal-mediated organic synthesis. [2] In this work, the reaction of $Ph_2PCH_2CH_2PPh_2$ (dppe) with $BrCH_2C(O)C_6H_4NO_2$ in acetone produces the phosphonium salt $[Ph_2PCH_2CH_2Ph_2PCH_2C(O)C_6H_4NO_2]Br$ (**1**). Further, by reacting the phosphonium salt with appropriate base the new bidentate phosphorus yielde, $[Ph_2PCH_2CH_2Ph_2P{=}CHC(O)C_6H_4NO_2]$ (**2**) was obtained. The reaction of entitle ligand with $PdCl_2(COD)$ [COD = dichloro(1,5-cyclooctadiene)] in dichloromethane under mild conditions formed the P,C chelated complexes with the composition $[(Ph_2PCH_2CH_2Ph_2P{=}CHC(O)C_6H_4NO_2)PdCl_2]$ (**3**) (scheme 1).[3] Characterization of these species was also performed by elemental analysis, IR spectroscopy and ^1H, ^{31}P, and ^{13}C NMR techniques. The results of MTT indicated that the complex (**2**) has a cytotoxic effect on CaCo 2 cells line (colon cancer). MTT assay at 24 hours showed cell viability hah decreased about 50% compared with the control ($p < 0.05$). Results indicate that palladium(II) complex could inhibit the growth of colon cancer cell through direct cytotoxic effects.



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Binding studies of Acetylacetonato propylendiamine palladium(II) Chloride with CT-DNA

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A novel palladium (II) complex has been synthesized with propylendiamine(pn) andacetylacetonato(acac) by the reaction of $[Pd(pn)Cl_2]$ with sodium salt of acetylacetonat. Thus a complex of the type [Pd(pn)(acac)]Cl has been obtained. This complex has been characterized by spectroscopic methods such as UV-vis, FT-IR and ^{1}H-NMR and non-spectroscopic methods such as elemental analysis and conductivity measurements.

The interaction of the complex has been studied with DNA of calf thymus (CT-DNA) at 300K and 310 K using UV-vis isothermal titration method in 25 Mm Tris-Hbuffer of pH=7.0. This complex can denature CT-DNA at very lower concentrations.The concentration of this complex in the midpoint of transition, $[L]_{1/2}$, at 300 K and 310 K are 0.065 and 0.067 respectively.

In the interaction studies between above complex with DNA, several thermodynamic parameters such as m (a measure of the metal complex ability to denature DNA), ΔG^{o}_{H2O} (conformational stability of DNA in the absence of metal complex), ΔH^{o}_{H2O} (the heat needed for DNA denaturation in the absence of metal complex) and ΔS^{o}_{H2O}(the entropy of DNA denaturation by metal complex) and binding parameters such as ***g*** (the number of binding sites per 1000 nucleotides), ***K*** (the apparent binding constant), ***n*** (the Hill coefficient) and **ν** (the ratio of the concentration of bound metal complex to the total DNA concentration) have been determined. The result of these studies indicate that [Pd(pn)(acac)]Cl exhibit cooperative binding with DNA.

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Interaction studies of CT-DNA and Acetylacetonato ethylenediamine palladium(II) nitrate

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A new Palladium(II) complex of the type [Pd(en)(acac)]NO_3 (where en is ethylenediamine and acac is acetylacetonato) have been synthesized and characterized by UV-Vis, FT-IR, ^{1}H NMR spectroscopic techniques and elemental analysis and conductivity measurements. It has been interacted with calf thymus DNA using UV-Vis isothermal titration method in Tris-HCl buffer solution containing 10 mmol/L sodium chloride (PH=7) at 27 °C and 37 °C.

The above complex can denature DNA and the concentration of this complex in the midpoint of transition, ($[L]_{1/2}$), is very low. In the interaction studies between the [Pd(en)(acac)]NO_3 complex with DNA, several binding parameters such as g (the number of binding sites per 1000 nucleotides), K (the apparent binding constant), n(the Hill coefficient) and m(a measure of the metal complex ability to denature DNA) have been determined. Thermodynamic parameters such as $\Delta G^{\circ}_{(H2O)}$ (conformational stability of DNA in the absence of metal complex), $\Delta H^{\circ}_{(H2O)}$ (the heat needed for DNA denaturation in the absence of metal complex) and $\Delta S^{\circ}_{(H2O)}$ (the entropy of DNA denaturation by metal complex) have been determined.

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Interaction Enthalpy of Zinc Cation with Serine-Serine Dipeptide with DFT Calculation

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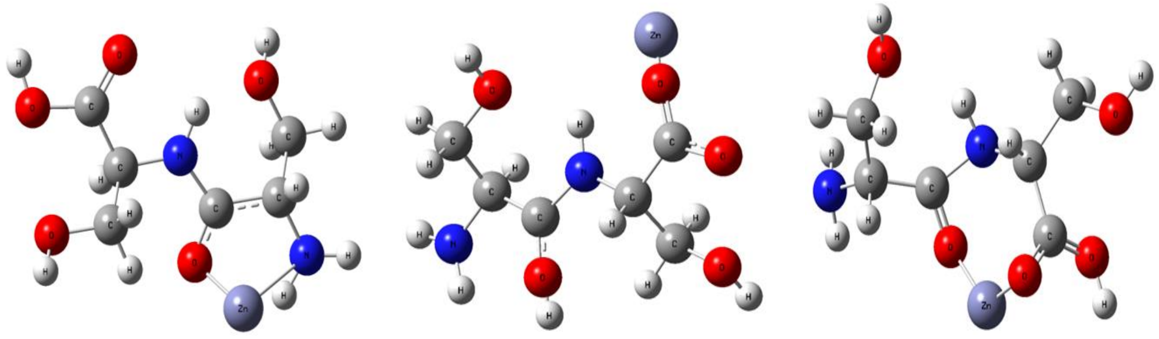
In view to better understand the interactions of aminoacids and peptides with metallic cations, in the isolated state, the model system serine-serine–Zn^{2+} has been theoretically studied .[1,2] Structures and energetic of complexes between serine-serine dipeptide and zinc cation were investigated applying density functional theory (DFT). Zn^{2+}cation was allowed to interact with different sites of serine-serine and three stable isomers were obtained. Calculation for three different cerincerin-Zn^{2+} isomers were performed at B3LYP level of theory using 6-31G* and 6-31G** basis sets. Relative energy calculations at different levels indicated that the most stable complex holds the structure, in which zinc cations are bound to the oxygen sites of carbonyl groups and the dipeptide of serine-serine which acts as a bidentate ligand that has a structure of three-membered ring. Vibration frequency of most stable isomer is calculated by B3LYP/6-31G** level and enthalpy, entropy and Gibbs energy of reaction was obtained.



1 **2** **3**

Fig.1. Optimized structures of the serine-serine – Zn^{2+}complexes

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Synthesis of functionalized magnetic nanoparticles as a precursor for preparation of nanodrug

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Nanomaterials have attracted much attention in the areas of biomedical due to the unique properties of the respective material at the nanoscale level. Numerous chemical methods can be used to synthesize magnetic nanoparticles for medical imaging applications[1]. The most common method for the production of magnetite nanoparticles is the chemical co-precipitation technique[2]. In recent reports, some nanoparticles such as magnetic nanoparticles have been introduced as drug delivery systems to enhance the related drug delivery efficiency to cancer cells. The particles, loaded with the drug, are concentrated at the target site with the aid of an external magnet. The drugs are then released on the desired area. Functionalization of MNPs with amino group, silica, polymer, various surfactants or other organic compounds is usually provided in order to achieve better physical and chemical properties[3].One way to overcome the limitation caused by the release of the drug from the carrier is to use a system in which the therapeutic agent remains coupled to the magnetic carrier throughout the duration of the treatment. [4] Based on this idea, the possibility of targeting radionuclides *via* magnetic carriers has been investigated.

In this study the magnetic iron oxide nanoparticles were prepared *via* co-precipitation method. The nanoparticles were functionalized with hydroxyl functional group. Then the molecule as a linker is attached to the surface because of chelating agent binds. Y-90 is connected for the radio-therapeutic purposes and therapeutic effects on mice with tumor were studied in presence and absence of magnetic field.

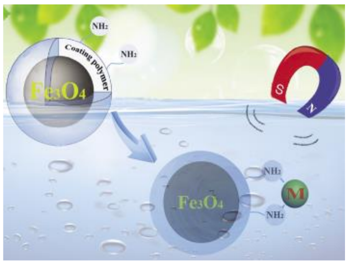

Figure.1. Functionalized magnetic nanoparticlesand adsorption of heavy metals.

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Synthesis of functionalized Iron oxide nanoparticles as a targeted drug delivery system

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The major disadvantage of most chemotherapeutic approaches to cancer treatment is that most are non-specific. Therapeutic drugs are administered intravenously leading to general systemic distribution.[1] The non-specific nature of this technique results in the well-known side effects of chemotherapy as the cytotoxic drug attacks normal, healthy cells in addition to its primary target, tumor cells. To overcome this great disadvantage magnetic nanoparticles (MNP) can be used to treat tumors.[2] A potential benefit of using magnetic nanoparticles is the use of localized magnetic field gradients to attract the particles to a chosen site, to hold them there until the therapy is complete and then to remove them.[3] Superparamagnetic nanoparticles (SPIONs) are currently used as contrast agents for magnetic resonance imaging. These particles can also be used as drug carriers for local chemotherapy, called magnetic drug targeting. A suitable coating should be applied on the SPIONs in order to achieve NPs with hydrophilic surfaces that have high colloidal stability without deterioration of their magnetic properties.[4] Moreover, the core/shell structures of MNPs have the advantages of good dispersion and appreciable amount of drug can be loaded to the coating shell (Fig.1).

In this work magnetic nanoparticles are functionalized with silica by post-modification method. Then chelator molecules attach to the nanoparticles surface for two purposes: 1) As a chelator of Ga-68 for PET imaging. 2) As a linker between Core-shell structure and drug. Finally drugs are loaded on chelator surface *via* steric binding.

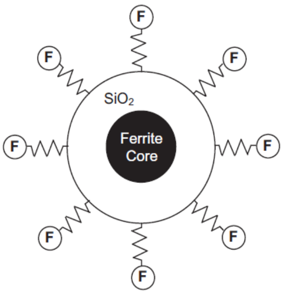

Figure1. Functionalized magnetic nanoparticles with shell of silica and functional group attached to the shell.

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New precursor for preparation of nano zinc oxide

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Zinc oxide, an inexpensive material, has a direct wide band gap of 3.37 eV at room temperature with an excitation binding energy of 60 meV. Since last several years, ZnO is a subject of renewed research interest because of its potential application, in many devices, such as, solar cells, laser diodes, ultraviolet lasers, thin film transistors [1] optoelectronics and lithium ion batteries. Controlled manipulation of ZnO structure at the nano scale can result in enhanced chemical, electrical and optical properties. Hierarchical nano materials can be synthesized by many methods such as seeding, ionic liquids, hydrothermal, ultrasonic and etc.[2] A nano-sized Zn complex was synthesized by sonochemical irradiation and compared with its crystalline structure. Compound 1 was characterized by X-ray powder diffraction (XRD) and IR spectroscopy. To prepare the nano structure of compound 1, two different concentrations of initial reagents, 0.01 and 0.005 M, were tested. Appropriate nano-sized particles of compound 1 were obtained at both concentrations. Particle sizes of the nano particles depend on the concentrations of initial reagents. Results show a decrease in the particles size as the concentrations of initial reagents is decreased. Calcination of compound 1 at different sizes produced nano particles of ZnO. SEM images show the complex with smaller size resulted residue with less size and better morphology. The XRD pattern of the residue obtained from calcination of compound 1 shows the obtained pattern matches with the standard pattern of ZnO with the lattice parameters (a = 3.24982 Å C = 5.20661 Å and z = 2) which are same with the reported values, (JCPDScard number 36–1451).

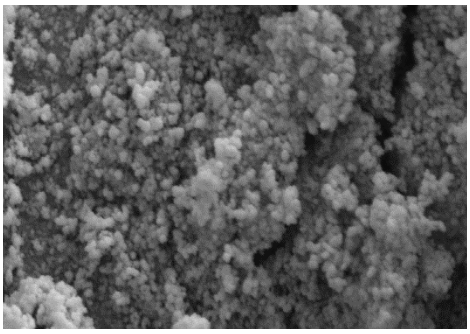

Fig.1. nano particles of Zno

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Synthesis, characterization and DNA binding studies of palladium(II) complex containing 1,10-phenanthrolin and acetylaceton ligands

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Studies of the interaction between metal complexs and DNA in terms of understanding of how to target DNA sites with specificity may lead to developing highly sensitive chemotherapeutic agents.[1-3]

[Pd(phen)(acac)]NO_3 (where, phen=1,10-phenanthroline, acac=acetylacetonato) have been synthesized. This complex have been characterized by elemental analysis, molar conductance, ^{1}H NMR, FT-IR and electronic spectroscopic studies. In this water soluble complex, both 1,10-phenanthrolin and acetylaceton ligands coordinates with Pd(II) center as bidentate.

Partial interaction of the complex to calf thymus DNA, were investigated by ultraviolet difference spectroscopy. Absorbance titration experiments imply the interaction of Pd(II) complex molecule with DNA and exhibits cooperative binding. The concentration of this complex in the midpoint of transition, $[L]_{1/2}$, is 0.038 and 0.049mM at 300 and 310K respectively. In the interaction studies between the [Pd(phen)(acac)]NO_3 complex with DNA, several binding parameters such as g (the number of binding sites per 1000 nucleotides), is 5 at 300 and 310K, K (the apparent binding constant), are 22.59 and 18.33mM^{-1} at 300 and 310K respectively, n (the Hill coefficient), are 3.96 and 4.60 at 300 and 310K respectively, m (a measure of the metal complex ability to denature DNA), are 229.4 and 152.1(kJ/mol)(mM^{-1}) at 300 and 310K respectively.

Thermodynamic parameters such as $\Delta G^0_{H_2O}$(conformational stability of DNA in the absence of metal complex) are 9.78 and 8.21kJ/mol at 300 and 310K respectively, $\Delta H^0_{H_2O}$(the heat needed for DNA denaturation in the absence of metal complex), is 56.78kJ/mol and $\Delta S^0_{H_2O}$(the entropy of DNA denaturation by metal complex), is 0.156 at 300K have been determined.

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Synthesis, crystal structure of a three-dimensional copper azido polymer

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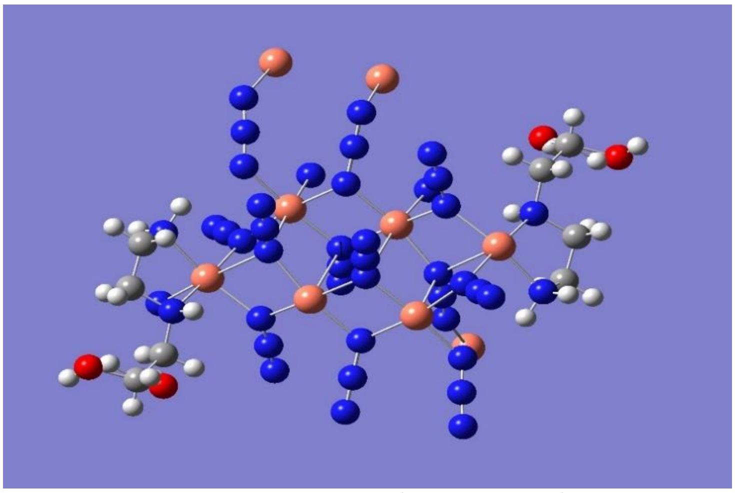
The design and construction of coordination polymers have attracted tremendous attention in the field of crystal engineering due to their novel and diverse topologies and promising applications in many fields such as catalysis, gas adsorption and separation, optics, and magnetism.[1] In this work, the self-assembly reaction of $Cu(NO_3)_2.3H_2O$ with blocking ligand: 2-(2-aminoethylamine) ethanol (aeae) in the presence of NaN_3 lead to the formation an novel three-dimensional coordination polymer $[Cu_6(N_3)_{12}(aeae)_2]_n$. The title complex is characterized by IR and single crystal X-ray diffraction. Single crystal X-ray structure reveales that this compound contains Cu_6 building block, where the Cu(II) atoms are connected each other through different types of bridging modes of Azide ligands: $\mu_{1,1}$, $\mu_{1,1,1}$, $\mu_{1,1,3}$, $\mu_{1,1,1,3}$. The hexanuclear cluster is further assembled via $\mu_{1,3}$, $\mu_{1,1,3}$, $\mu_{1,1,1,3}$ azido groups a into 3D framework. Each Cu(II) ion was surrounded by six nitrogen atom in a distorted octahedral geometry.



The molecular structure of the basic unit of 1

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Metal–organic framework based on terephthalic acid: synthesis, crystal structure

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Organic–inorganic hybrid materials, which contain metal centers connected by organic spacers, have attracted much attention in recent years. In particular, coordination polymers (CPs) or metal–organic frameworks (MOFs) are of considerable interest owing to their potential applications including gas storage, catalysis, luminescence, magnetism and electrochemical activity. [1-3]

In the present work, Two new metal organic framework (MOF) structures have been obtained from the M–terephthalic acid (H_2BDC)–dimhethylformamide ($M=Zn^1$, Pb^2) system and characterized by IR and single crystal X-ray diffraction. The crystals were obtained by solvothermal synthesis at 393 K. Structure 1 consists of three zinc cations linked by terephthalic groups in 2D layers stacked in an offset manner to accommodate H_2O moieties coordinated to Zn^{2+} within voids in adjacent layers. Structure 2 consists of a 3D network constructed from Pb^{2+} ions bridged by deprotonated terephthalic acid moieties and DMF.

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Synthesis, Characterization and Crystal Structure of Zn (II) Coordination Polymer with O-, N-donor Ligands

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Construction of coordination polymers, also called metal–organic frameworks, by combining appropriate linking bipyridyl-type ligands and transition metals is currently under intensive study due to their desirable properties applicable to magnetism, photoluminescence, catalytic properties and gas storage [1-4]. In designing these polymers, the properties of linking ligands such as various coordination modes, variable lengths, and relative orientation of donor atoms play a fundamental role in determining the structural outcomes of target polymers. In this study, The long and rigid spacer of N, N'-bis-pyridin-4-ylmethylene-naphthalene-1,5-diamine(L) exhibit a self-assembly reaction with zinc (II) salt and acethylacetone to produce a new coordination polymer of $[Zn(acac)_2(L)]_n$. The X-ray crystallography results show one-dimensional polymeric chains with an octahedral geometry around the zinc (II) metal center which is coordinated with two nitrogen of bipyridyls and 4 oxygen atoms from two acac ligands.

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Some Novel Iron Complexes of salophene Schiff bases Derivatives: Synthesis, Characterization and crystal structures

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Schiff bases have played an important role in development of coordination chemistry; because of their distinct advantages. A lot of attention has been recently devoted to the tetradentate Schiff bases and their complexes such as their ability to reversibly bind oxygen, catalytic activity in the hydrogenation of olefins and photochromic properties applications. [1–3] In the present work, four Fe(III) complexes of [Fe(S1)Cl].MeCN(1), [Fe(S2)(Cl)(H_2O)].MeCN(2), [Fe(S2)(Cl)].MeCN(3), [Fe(S3)(Cl)(H_2O)].2H_2O(4) and one dinuclear [Fe(S4)Cl]$_2$ (5) where, H_2S1=N,N'-bis(salicylidene)phenylediamine,H_2S2=N,N'-bis(3-methoxysalicylidene)cyclo-hexyldiamine, H_2S3=N,N'-bis(3 methoxysalicylidene)ethylenediamine and H_2S4= N,N'-bis(salicylidene)ethylendiamine, have been prepared and characterized by IR, UV–Vis spectroscopy and single crystal X-ray diffraction studies. In compounds 1 and 3, Fe (III) has five-coordinated square pyramid geometry from deprotonated Schiff base in equatorial plane and Cl^- in the axial position. Compounds of 2, 4 and 5 have six coordinated geometry which equatorial positions are same as 1 and 3. In 2 and 4 the axial ones are occupied by Cl^- and water molecule, meanwhile, in 4 is occupied by Cl^- ion and other is bridging oxygen atom from salen ligands.

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Synthesis and characterization of a new Cu(II) complex containing 1,2,4-triazole derivative; A precursor for preparation of CuOnanosheets

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1,2,4-Triazoles are aromatic five memebered heterocycles containing three nitrogen atoms, which appear in the structure of various natural products.1 Among the 1,2,4-triazole derivatives, the coordination chemistry of mercapto- and thionesubstituted 1,2,4-triazoles has attracted considerable attention since they contain soft (S) and hard (N) donor atoms, simultaneously. In the present work, we wish to report the synthesis and characterization of a new Cu(II) complex containing 3-mercapto-1,2,4-triazole as ligand and an organic diacid as co-ligand. We have found that this new Cu(II) complex can be used as precursor for the preparation of copper oxide nanostructure. The complex has been characterized by NMR, FTIR spectroscopy, UV-Vis, elemental analysis and mass spectrometry. The formation of copper oxide resulting from solventlessthermolysis of copper complex has been confirmed by powder X-ray diffraction (XRD), EDX and thermal gravimetric analysis (TGA). According to the SEM images of the residue from solventless thermolysis of the complex (Fig. 1)at 900 ° C (under N2) exhibits nanosheet morphology.

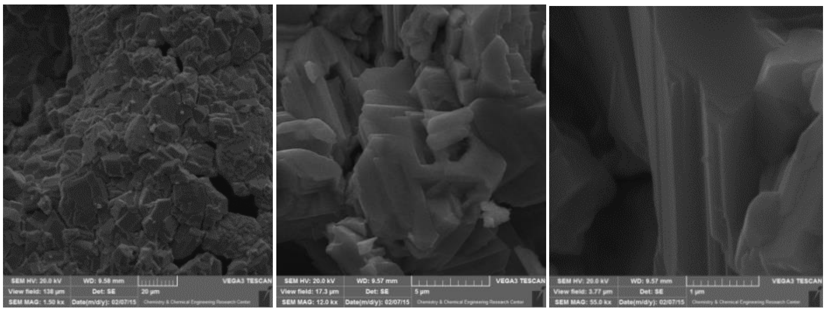

Fig. 1. SEM images of CuOnano sheets.

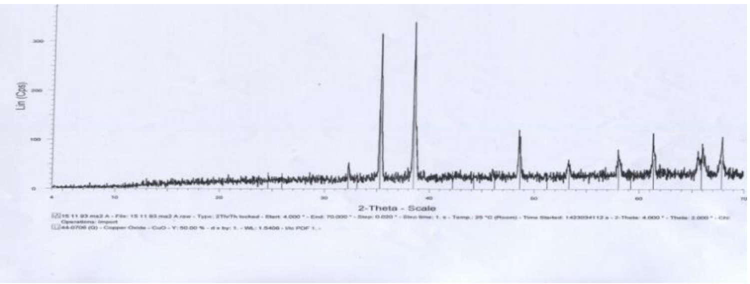

Fig. 2. Powder X-ray diffraction of CuO.

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Preparation, characterization, calculated studies of crystal structure of monodantate organophosphorus complex of Mercury(II) Iodide and bidentate heterocyclic metal complexes

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Phosphorus ligands are known to demonstrate rich coordination chemistry.1 They are effective nucleophiles, because of their value for a variety of industrial, biological and chemical synthetic uses.2 It is the requirement to satisfy this need that has provided the impetus for our work, which has been directed towards evaluating the ligating behavior of phosphorus ligands. In the compounds reported to date, the chemical behavior of the α-keto phosphorus ligands has been clearly dominated by the C-coordinated form3 The complexation behavior of the α-keto-stabilized phosphorus ligand 1-(3-nitrophenyl)-2-(triphenylphosphoranylidene) ethanone, (Ph3P=C(H)C(O)PhNO2) towards the transition metal ions such as mercury(II) was investigated. Crystals of 3 were obtained from a ethanol/diethyl ether solution by solvent diffusionwhich is demonstrated by single crystal X-ray analyses3 Fig.1. The theoretical studies for [Ph3P=C(H)C(O)PhNO2Hg(Cl)2]2(1), [Ph3P=C(H)C(O)PhNO2Hg(Br)2]2 (2) and Ph3P=C(H)C(O)PhNO2Hg(I)2]2(3) also indicated that, for these compounds, the observed trans-like structures are more stable than the possible cis-like structures. 4

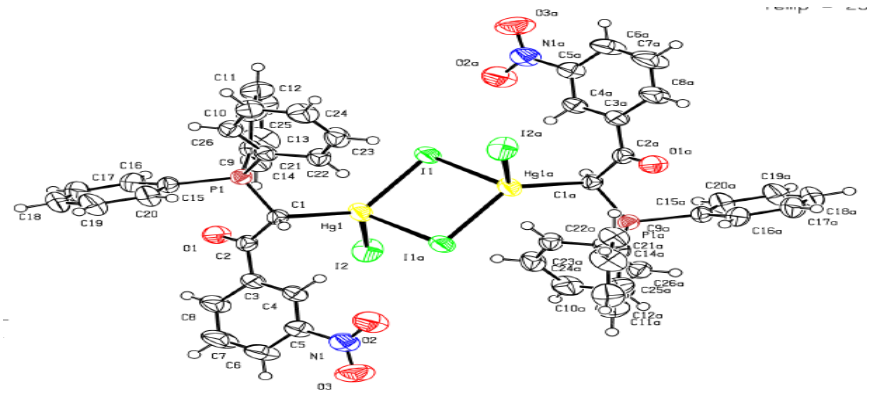

Fig.1. Molecular structure of the complex 3

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Synthesis, characterization, physic-chemical, antifungal activity of mixed-ligand complexes of Fe(II), Ni(II) and Cu(II) salts

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Much attention has been paid to the studies of mixed ligand complexes of metals in recent years because of their wide application in various field of chemical activity and more particularly because of their presence in biological, environmental and other systems. [1] In fact, many naturally occurring metals complexes are mixed-ligand complexes[2] containing two or more different ligand molecules, or if the ligand is a single macromolecule having two or more different kinds of donor atoms.[3] The present work shows, reaction of metal salts such as Fe (II), Cu (II) and Ni (II) with Some mixed-ligand complexes of the general formula $[M(Hdmg)_2B]$, where Hdmg = dimethylglyoximato monoanion, B = triethylamine. All synthesized compounds were analyzed and characterized by melting points, solubility, infrared, CHN and UV/VIS electronic spectra. The antifungal activities of the complexes were tested using penicilium and Aspergillus flavus. The complexes melted/decomposed at 140-298°C and, most of them dissolved only in polar solvents. The recovered data of this project may have important applications in biology and biochemistry.
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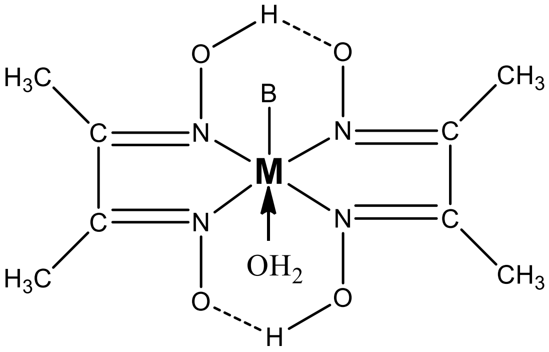

Fig.1. Suggested structure for sample complexes.

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^{31}P NMR study of the stoichiometry and stability of several HgX_2-Acetylemethylentriparatolylphosphorane complexes in various Ionic liquid - Acetonitrile mixtures

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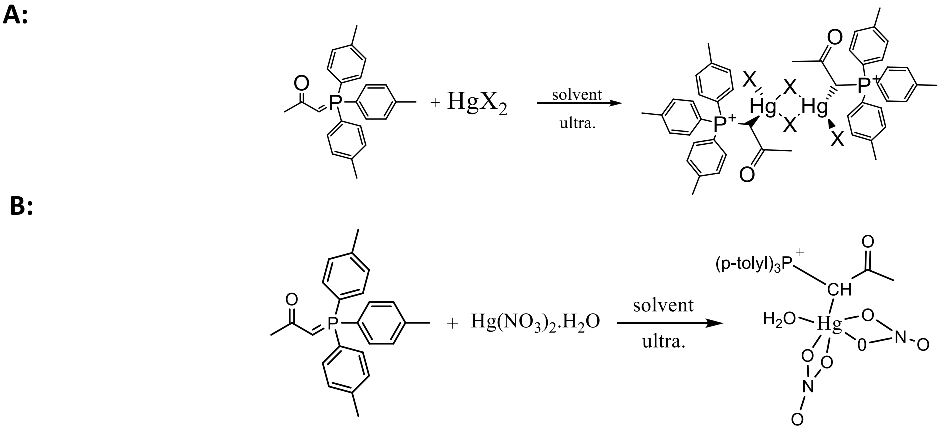
The reaction of phosphorus ylide, $CH_3COCHP(p\text{-tolyl})_3(L)$ with HgX_2 (X = Cl, Br and I) and $Hg(NO_3)_2.H_2O$ in equimolar ratios using Ionic liquid [BMIM][PF_6] and acetonitrile (AN) as solvent leads to binuclear and mononuclear products, respectively. [1,2] ^{31}P NMR spectroscopy was used to investigate the stoichiometry and stability of the HgX_2 complex with p-methylbenzoylemethylentriparatolylphosphorane (L) in binary [BMIM][PF_6] and AN mixtures of varying composition. In all cases studied, the variation of ^{31}P NMRchemical shift with the [HgX_2]/[ylide] mole ratio indicated the formation of 1:1 complexes (Scheme 1). The formation constants of the resulting complexes were evaluated from computer fitting of the mole ratio data to an equation that relates the observed chemical shifts to the formation constant. In all mercuric salts used, the stabilities of the resulting 1:1 complexes varied in the order $Hg(NO_3)_2 > HgCl_2 > HgBr_2 > HgI_2$. It was found that, in the case of all complexes, an increase in the percentage of Ionic liquid in the solvent mixtures significantly decreased the stability of the complexes.



Scheme 1. Purposed structures of (A): HgX_2 (X= Cl^-, Br^-, I^-) and (B): $Hg(NO_3)_2.H_2O$-L complexes in solution.

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Synthesies and characterization of some new heptaazaCd(II) , Zn(II) and Mn(II) macrocyclic Schiff base Complexes containing two pyridyl unit as pendant arms

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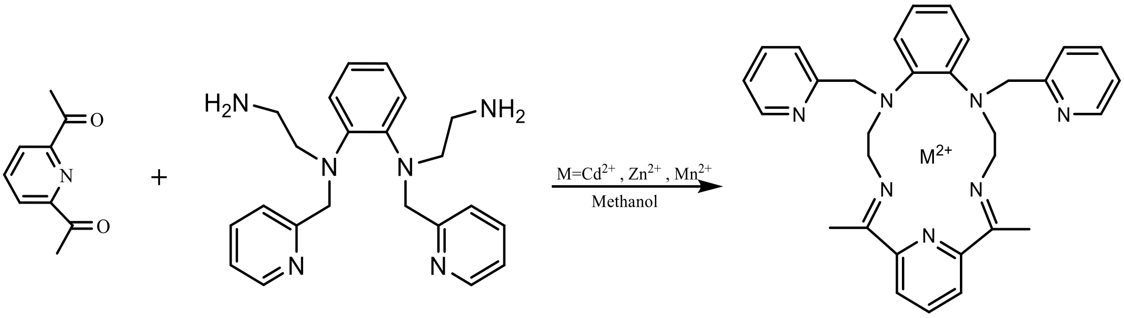
The development of the so-called Schiff base compounds has attracted a lot of interest in the fields of coordination chemistry and material science. [1] The presence of ion pair on the nitrogen atom of imino group enables the coordination of numerous metal cations. [2] Recently, we reported the synthesis and characterization of some octaazaMn(II) macro-cyclicShiff base complexes. [3] In this work, we describe the Mn(II), Cd(II) and Zn(II) templated [1+1] cyclo condensation of 2,6-diacetylpyridine with branched hexadentate amine ligands, N1,N1'-(1,2-phenylene)bis(N1-(pyridin-2-ylmethyl)ethane-1,2-diamine), that produ-cing three complexes countaning two 2-methylpyridine pendant arms.



All the complexes have been characterized by IR, elemental analysis and FAB-Mass spectroscopy and in the case of Zn(II), Cd(II) complexes by 1H and 13CNMR spectra. In the IR spectrum, a band at 1652 and 1653 cm-1 (for Zn(II)), 1645 and 1669 cm-1 (for Mn(II)) and 1652 and 1687 cm-1, (for Cd(II)), indicated the formation of C=N double bonds, no piaks attributed to NH2 and carbonyl groups implied that the condensation reaction had been completed. A complex show a strong non-split absorption at 1078-1094 cm-1, indicating the presence of non-coordinated perchlorate anions.

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Synthesis of some New Cadmium(II) , Zinc(II) and Manganese(II) octaazaMacroacyclic Schiff base Complexes containing the pyridine-2-carbaldehyde and two pyridyl units as pendant arms

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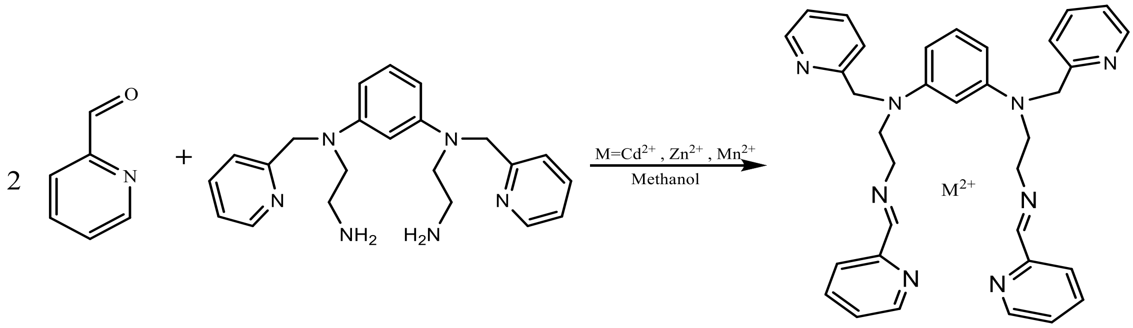
Schiff-base ligands are of significant importance in chemistry, because Schiff base ligands are potentially capable of forming stable complexes with metal ions [1]. A large number of Schiff-base and their complexes had been studied for their interesting and important properties e.g. their ability to reversibly bind oxygen, catalytic activity in hydrogenation of olefins and transfer of an amino group, photochromic properties, and complexing ability towards some toxic metals[2]. Schiff-base ligands, as a variety of compounds with the imine group, have gained importance because of physiological and pharmacological activities associated with them. They constitute an interesting class of chelating agents capable of coordination methal ions, which serves as models for biological system [3].



In this work three complexes were prepared with direct [1+1] condensation of pyridine-2-carbaldehide with 4,7-bis(2-pyridylmethyl)-4,7-diazadecane-1,10 diamine in methanol followed by addition of $Cd(NO_3)_2.4H_2O$, $MnCl_2.2H_2O$ and $ZnClO_4$. After on solution was filtered whilst hot and $NaClO_4$ added to the filtrate.The resultant complexes were characterized by FT-IR, Mass, CHN, ^{1}H and ^{13}CNMR spectroscopy.

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Synthesis of the Platinum(II) Hydride Complex $[PtH(CH_3CN)(^tBu_3P)_2]PF_6$ by Oxidation of the Platinum(0) Complex $[Pt(^tBu_3P)_2]$ with $[Cu(CH_3CN)_4]PF_6$

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Transition metal hydrides have potential technological application as hydrogen storage materials, smart windows, sensors and Catalysis.[1,2] Oxidation of the bis-phosphineplatinum(0) complex $[Pt(^tBu_3P)_2]$, **1**, by$[Cu(CH_3CN)_4]PF_6$ give the platinum(II) hydride complex $[PtH(CH_3CN)(^tBu_3P)_2]PF_6$, **2** .The hydride platinum(II) complex, **2**, characterized by multi nuclear NMR spectroscopy. ^{31}P NMR spectrum of $[PtH(CH_3CN)(^tBu_3P)_2]PF_6$, shows a singlet signal at δ= 80ppm with platinum satellite ($^1J_{PtP}$= 2810 Hz)(Figure.1). The signal of the hydride ligand appeared as a singlet at δ= -19.5 ppm ($^1J_{PtH}$=992 Hz) (Figure 1) indicating formation of the hydride complex.These data confirmed by solid state structure of $[PtH(CH_3CN)(^tBu_3P)_2]PF_6$that determined using X-Ray crystallography.The solid state structure of Complex $[PtH(CH_3CN)(^tBu_3P)_2]PF_6$shows planner geometry around the Pt center.

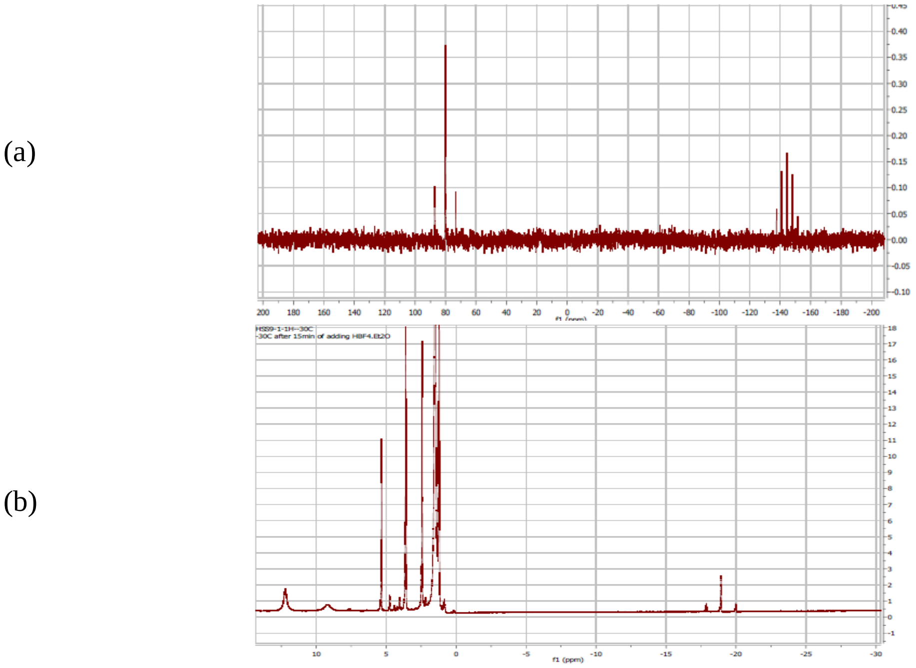

Figure 1 (a) The ^{31}PNMRspectrum and (b) the ^{1}H NMR spectrum of$[PtH(CH_3CN)(^tBu_3P)_2]PF_6$

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Quantum chemical studies on molecular structure, spectroscopic analysis, NLO, and NBO analysis of carboplatine

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This work deals with quantum chemical studies on molecular structure, spectroscopic analysis, NLO, and NBO analysis of carboplatine. Carboplatin, the second-generation platinum drug, is much less nephrotoxic and neurotoxic than cisplatin. The Modified Perdew-Wang Exchange and Correlation (MPW1PW91) method has been used in these calculations. The calculations of systems contain C, N, H and O described by the standard 6-311G (d,p) basis set. For Pt element standard Def 2-TZVPPD basis set are used and Pt described by effective core potential (ECP) of Wadt and Hay pseudopotential with a triple-ξ valance using the Def2-TZVPPD. Time dependent density functional theory (TD-DFT) is used to calculate the energy, oscillatory strength and wavelength absorption maxima (λ_{max}) of various electronic transitions and their nature within molecule. Thermodynamical properties like entropy heat capacity, zero point energy have been calculated for the title molecules. Non linear optical (NLO) behavior of title compound is investigated by the computed value of first hyperpolarizability (β_0).

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Synthesis and characterization of perovskite – type nanoparticles by sol – gel processing

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Uniform nanoparticles (NPs) of $Gd_xSr_{1-x}FeO_3$ (GSFO) were synthesized via sol–gel method.[1] The obtained product was characterized by thermal gravimetric analyses–differential thermal analyses (TGA/DrTGA), X-Ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), dispersive analysis of X-Ray (EDAX), Brunauer-Emmett-Teller (BET) and fourier transform infrared (FT-IR). The single perovskitephase could form completely after sintering at the temperature of 700 °C. In addition, TEM images show that the average particle size of GSFO approximately 35 nm. Based on SEM image, porosity of the surface is evident and it seems that the particles have not grown with uniform size. The EDAX analysis attached to SEM was used for further studies ofthe obtained product composition. EDAX spectra showed the presence Gd, Sr, Fe and O in the adsorbent. BET results showed that the average of specific surface area (SSA) of GSFO NPs was $8.7 m^2.g^{-1}$. FT-IR spectra were measured for the xerogel and powder sample after calcination and the results were in agreement with XRD results. The TGA/DrTGA result showed that the optimum calcination temperature is about 700 °C.[2]

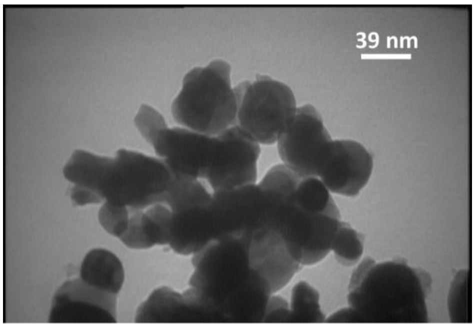

Fig.1. TEM imageof the GSFO NPs obtained at 700°C.

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Synthesis, characterization and catalytic behavior of multifunctional copper coordination polymer capped with sodium tungstate

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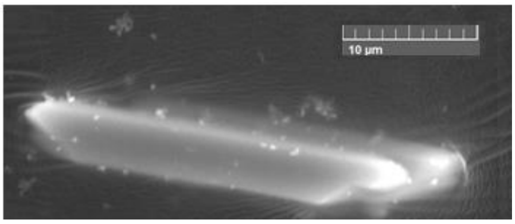
Coordination polymers (CPs) are infinite crystalline lattice that consist of metal ions and organic ligands linked via coordination bond. The design of bridging ligands are to be the most effective ways to manipulate the versatile structure of coordination polymers. Among multifunctional organic ligands, pyridine derivatives such 4,4 ´ -bipy and 2,2 ´-bipy are useful neutral organics for the Construction coordination compounds due to their two binding sites and rigid structure. In this study, organic-inorganic hybrid materials based on sodium tungstate and copper coordination polymer was prepared and designated as CuWCP and characterized by various techniques including elemental analysis (ICP), x-ray powder diffraction XRD, FTIR, and TGA. It was found that Cu W CP can be used as efficient Lewis base heterogeneous catalyst For knovenagel condensation reactions at 60 ℃. obtaining the corresponding knovenagel condensation reaction products in moderate to excellent yield in less than 1 hour is promising. The catalyst can be easily recovered from the reaction mixture and reused several timeswithout significant loss of activity.



CuWCP as catalyst

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Green synthesis and characterization of Fe_3O_4-TiO_2-$H_3PMo_{12}O_{40}$ polyoxometalate nano catalysts for the oxidation of tricyclic aromatic organic compounds

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Syntheses of Fe3O4 nanoparticle have gained much interest in recent years. Due to its catalytic activity, magnetic property and easy separation. Polyoxometalates are inorganic compounds with metal-oxygen binding that demonstrated electrochemical and catalytic effects due to their structural variety. Recently, Fe_3O_4 magnetic nano particles have been used as polyoxometalates support. Indeed, the catalyst can be separated by external magnetic field.[1,2] In this study Fe_3O_4-TiO_2-$H_3PMo_{12}O_{40}$ (Fe-Ti-POM) synthesized by sol-gel method. Characterization of all products was analyzed by SEM, XRD, FT-IR and UV-Vis techniques. Polycyclic aromatic hydrocarbons (PAHs) are toxic and carcinogenic. The oxidation of PAHs are simple, green and cost effective method.[3] Activity of synthesized nano catalysts (Fe-Ti-POM) was tested for oxidation of tricyclic organic compounds. Products are characteraized by FT-IR, UV-Vis. The effect of various parameters such as temperature, solvents, dose of catalyst is studied. The reaction was also investigated under ultrasound condition, reflux and uv irradiation conditions.

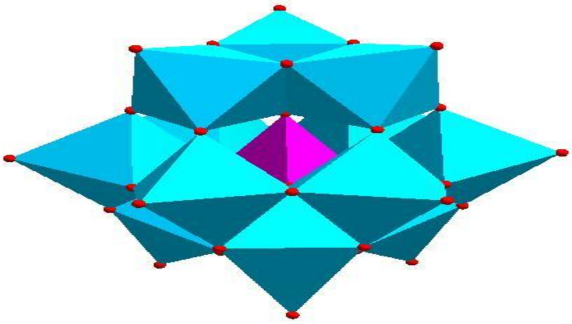

Fig. 1. Keggin Structure of $H_3PMo_{12}O_{40}\cdot 30H_2O$

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4,7-Phenanthroline as a monodentate ligand in *trans*-[$PtCl_2(SMe_2)$(4,7-phen)]

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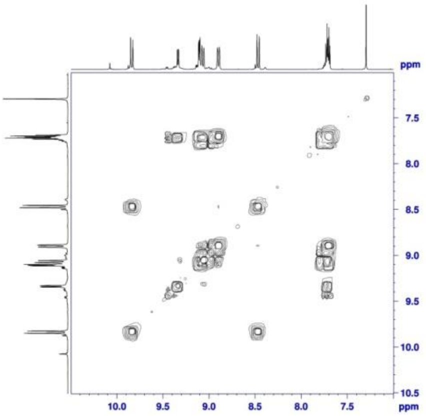
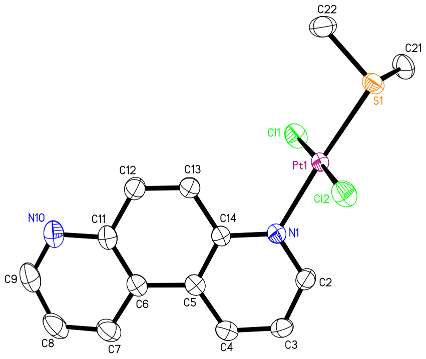
The N-donor bidentate ligands containing exo nitrogen atoms such as 4,4′-bipyridine, 2,2′-bipyrine are widely used for the preparation of dinuclear and polynuclear compounds 1. On the other hand, there is continuing interest in the photophysical and chemical properties of diimine platinum(II) complexes.2 Phenanthrolines are a class of diimine ligands which show different mode of activities. Many new platinum(II) complexes have been developed with the aim of obtaining the anticancer activity with reduced solubility.3 It has been shown that phenanthroline derivative of platinum displays activity against cancer, bacterial and fungal infections .4 Therefore, we report the preparation and characterization of the novel complex trans-[PtCl2(SMe2)(4,7-phen)] (4,7-phen = 4,7- phenanthroline). The product has been fully characterized by elemental analysis, 1H, 13C{1H}, HHCOSY, HMBC and HSQC NMR spectroscopy. The crystal structure of trans-[PtCl2(SMe2)(4,7-phen)] reveals that platinum adopts a slightly distorted square planar geometry.





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Immobilization of Fe, Mn and Cu tetraphenylporphyrin complexes in mesoporous MCM-41 and their catalytic activity in oxidation of sulfide

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Different biomimetic approaches to cytochrome P450 activity have been reached with metalloporphyrins and variousoxidants.[1] Recently, mesoporous materials have been studied as supports because they present high specific surface area, better dispersion and regeneration properties.[2]

In this research, Fe, Mn and Cu tetraphenylporphyrin complexes has been prepared and characterized by IR , ^{1}H NMR and UV-Vis spectroscopy. Then, these metalloporphyrins have been encapsulated in the nanocavity of mesoporous MCM-41 and characterized by different spectroscopic methods.Also Catalytic activity of these complexes have been studied for the oxidation of various sulfids.The effects of different reaction parameters such as solvent, the amount of oxidant, amount of catalyst and reaction time have been optimized.

Also a comparison of the effect of metal ion in the catalytic activity has been studied. Also homogeneous and heterogeneous catalytic systems were compared.

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Selective oxidation of sulfides to sulfoxides with urea hydrogenperoxide (UHP) catalyzed by Fe, Mn and Cu complexes of non-, partially and fully β-brominated *meso*-tetraphenylporphyrin

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Metalloporphyrins have been investigated intenselyas biomimetic models of cytochrome P450s, catalasesand peroxidases or as transmembrane electron transportagents.[1] The use of chemical model systems willhelp scientists for overcoming the difficulties in workingwith enzymes *in vivo* and *in vitro*. Halogenated metalloporphyrins are more active as catalysts and more resistant to oxidative degradation than their β-unsubstituted analogues.[2] Biomimetic oxidation of organic compounds in the presence ofmetalloporphyrins has been studied from different points of view.[3] In the present research, non-, partially and fully β-brominated *meso*-tetraphenylporphyrins (H_2TPPBrx(OAc) (x = 0, 4, 8)) and their manganese, copper and iron complexeshave synthetized and characterized. Also catalytic activity of these complexes has been studied for the oxidation of sulfideswith urea hydrogen peroxide (UHP). Then the effects of different reaction parameters such as solvent, the amount of oxidant, amount ofcatalyst and reaction time have been optimized. A comparison of the effect ofmetal ion on the catalytic activity has been investigated.

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Synthesis and controlled release properties of kanamycin-zinc oxide nanocomposite

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Zinc oxide nanoparticles are a very interesting material because of their practical applications in a series of cosmetic perpetrates, sun protection cream, acne treatment or as a wound dressing .[1] Also, zinc oxide and zinc oxide nanoparticles exhibit high strong inhibitory and antibacterial effects as well as a broad spectrum of antimicrobial activities.[2] In this study, zinc oxide nanoparticles were synthesized using a simple precipitationmethod without calcination step. The zinc oxide nanoparticles were coated with a known Gram-negative antibiotic, kanamycin, and nanocomposite material was characterized by FT-IR, XRD, SEM, PLS, TGA/DTG. The antibacterial activity tests such as disk diffusion and minimum inhibitory concentration (MIC) were performed in different concentrations of zinc oxide and nanocomposite by a standard microbial method on Escherichia coli, Staphylococcus aureus. The biological tests show a synergic activity of kanamycin-zinc oxide nanocomposite. The release of kanamycin from the kanamycin-zinc oxide nanocomposite was also verified. We have proved that zinc oxide nanoparticles can greatly improve and increase the antibacterial activity of kanamycin.

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Synthesis and characterization of some organoplatinum(IV) complexes containing phosphine ligands

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There is continuing interest in the oxidative addition reaction of organoplatinum(II) complexes.The synthetic chemistry of alkylplatinum(IV) compounds containing nitrogen ligands has been thoroughly studied. In these reactions, the electron rich platinum center attacks alkyl halides usually by an S_N2 mechanism, however, there are few reactions which proceed by a radical mechanism or concerted three-center addition. [1-3] On the other hand, there has been agrowing interest in the preparation of platinum complexes containing polydentate phosphine ligands such as 1,1'-bis(diphenylphosphino) ferrocene(dppf),bis(diphenylphosphino) -methane(dppm) and bis(diphenylphosphino)ethane(dppe).In this context, we have investigated the reaction of dimethylplatinum(II) complex $[PtMe_2(phen)]$ (phen = 1,10-phenanthroline) with some primary alkyl halides.Then, the reaction of resulting products with mono and bidentate chelating phosphine ligands having different length of chain resulted in the formation of Pt(IV) complexes $[PtMe_2R(phosphine)(NN)]X$ (X = halide). The resulting products have been characterized by elemental analysis, ^{1}H, ^{13}C and^{31}PNMR spectroscopy.NMR data indicated that the products exist as a mixture of *trans* and *cis* isomers but the *cis* isomer exists as the minor product.

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Synthesis and catalytic property of complex of Cu (II) with o-hydroxy-benzophenone for oxidation of olefines

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Olefin oxidation is especially interesting because of the industrial importance of this type of reaction. Oxidation of alkenes to give oxygen containing value added products like alcohols, aldehydes, ketones, acids, epoxides, etc. is an extremely important and useful reaction in both chemical and pharmaceutical industries.[1] Benzophenones (BPs) which exhibit the structure of diphenylketone, are compounds of great interest due to their biological and physicochemical properties.[2] In this study the homogeneous Cu(II) complex with o-hydroxy-benzophenone has been synthesized and employed as catalyst for the oxidation of olefines. This complex characterized by IR, UV-vis spectra and CHN analysis. The catalytic performance of homogeneous complex was evaluated in the liquid phase oxidation of styrene, α-methyl styrene and cyclohexene in acetonitrile with tert-butyl-hydroperoxide (TBHP) as oxidant. This complex was active in oxidation under mild condition in which the highest yield of styrene oxidation was about 100% with two main product: benzaldehyde and epoxy styrene. The influence of the various reaction parameters in oxidation of styrene such as: time, solvent, amount of catalyst and amount of oxidant has been studied.

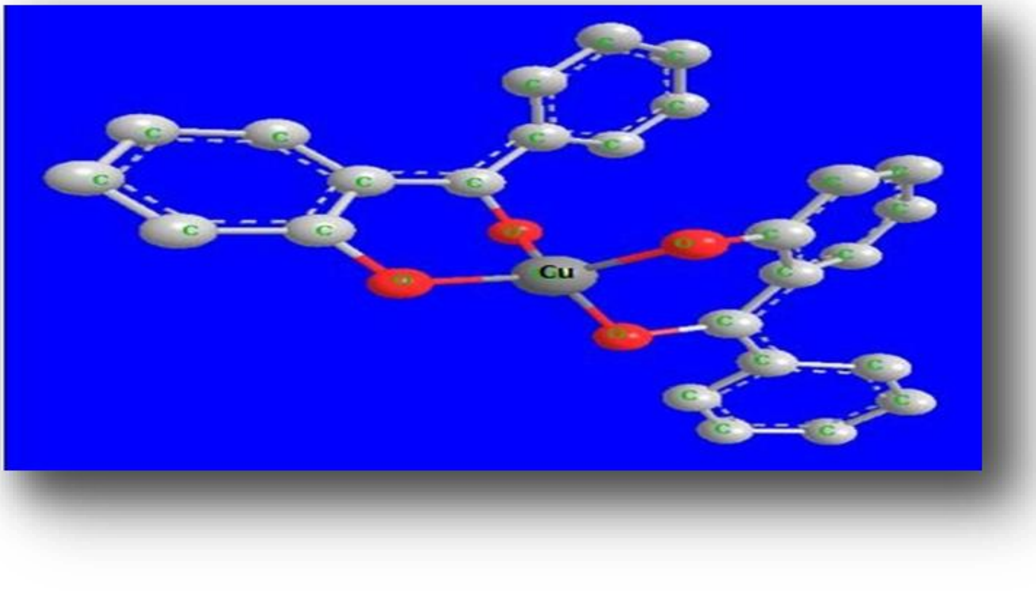

Fig.1.structure of Cu (II) complex with o-hydroxybenzophenon

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Synthesis of different nano crystals, ZnO nano-flower like, nano-cones and nano-rods

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In this study, simple and robust chemical deposition methods were proposed in order to synthesize the ZnO nano-crystals. The nano-cones, nano-flowerlike and nano-rods are the produced forms of ZnO.

Synthesis of nano-flower like: First, the amount of 1.788 g of Zn(NO3)2.6H2O was dissolved in 25 ml of deionized water (solution A). Also, 3.9 g of NaOH was dissolved in 25 ml of deionized water (solution B).[1] Solution B was added drop wise to solution A. Then, the mixture was refluxed for 2 h at 50 ℃ in an oil bath. The precipitate was centrifuged and washed three times with deionized water and ethanol, and finally was dried for 4 h at 60 ℃ in an oven.

Synthesis of ZnO nano-cones: First 50 ml of 0.1 M $Zn(NO_3)_2.6H_2O$ was mixed with 50 ml of 0.1 M Hexamethylene tetra-amine, and were stirred for 20 minutes at room temperature.[2] Few drops of 1.0 M NaOH solution were added to adjust pH of solution about 10. Final solution was filtered and washed three times with deionized water and absolute ethanol, and then dried for 8h at 100 ℃ in an oven.

Synthesis of ZnO nano-rods: First, 1.5 g of $Zn(CH_3COO)_2.6H_2O$ and 0.45 g of polyethylene glycol 2000 (PEG 2000) was dissolved in 210 ml of distilled water, then 2.25 ml of 25% ammonia was added drop wise to above mentioned solution.[3] The resulting mixture was refluxed for 6 h at 60 ℃.Then, the mixture was cooled, centrifuged and the precipitate was rinsed twice with distilled water and absolute ethanol. 135 ml of distilled water was added and the precipitate was refluxed for 9 h at 60˚C. Finally the precipitate was dried for 8 h at 100 ℃ in an oven.

Morphology of the samples was studied using scanning electron microscope (SEM) and XRD results. The XRD analysis confirms the wurtzite structure of all samples.

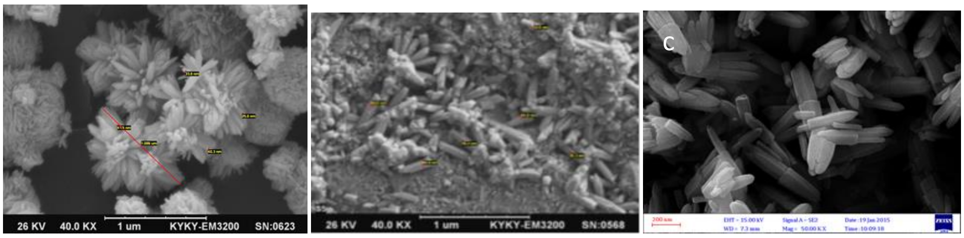

Fig.1. a) SEM photographs of the ZnO nano-flower like, b) ZnO nano-cones, c) ZnO nano-rods

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Inorganic-organic hybrid based on β-octamolybdatenanocluster as catalyst for cyclooctene epoxidation

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Polyoxometalates (POMs) are metal-oxygen clusters with various structures and application in catalysis. Many inorganic-organic hybrid compounds are prepared based on polyoxomolybdate anions including $\{Mo_2O_7\}$, $\{Mo_4O_{13}\}$, $\{Mo_5O_{15}\}$, $\{Mo_8O_{26}\}$, $\{Mo_{15}O_{47}\}$. The POM anions in these materials can act as ligands, compensating counter ions or as templates to create porous structures [1-4].

An inorganic-organic hybrid material based on β-octamolybdatenanocluster and 4,4´-bipyridine ligand,$Mo_8O_{26}(C_{10}H_{10}N_2)_2(C_{10}H_8N_2)\cdot 2(H_2O)$(**1**), was synthesized under solvothermal conditions and characterized by single crystal X-ray diffraction, powder X-ray diffraction (PXRD), thermogravimetric analysis (TGA) and FT-IR spectroscopy. The structure of **1** is presented in Fig. 1. The prepared hybrid was applied as heterogeneous catalyst for the epoxidation of cyclooctene using *Tert*-butyl hydroperoxide (TBHP) as oxidant and dichloromethane as solvent. Compound **1** showed good catalytic activity and selectivity in the epoxidation reaction and can be easily recycled and reused after three successive catalytic cycles without losing either activity or selectivity.

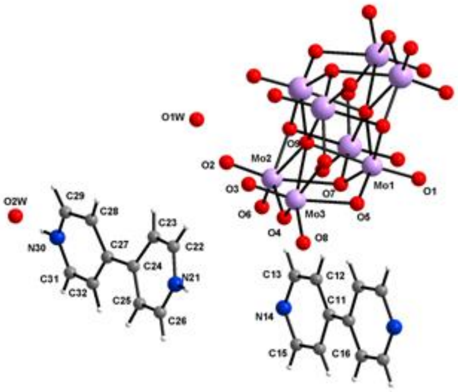

Fig. 1. The structure of inorganic-organic hybrid**1**

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Synthesis, structure and thermal stability of Lanthanum (III) 2D coordination polymer with 2,3-pyrazinedicarboxylic acid

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Coordination polymers, formed by metal cations linking with organic bridging ligands, have promising applications in catalysis, nonlinear optics, gas storage and medicine.[1] Lanthanide ions have larger radii and higher coordination numbers than the transition metals, therefore, they may generate coordination polymers with distinctive molecular structures and unusual properties.[2] In this work,atwo-dimensional Lanthanum(III) coordination polymer, namely, $[La(pzdc)(pzdcH)(H_2O)_3]_n$, (**I**), ($H_2pzdc$, pyrazine-2,3-dicarboxylic acid) has been synthesized andcharacterizedby X-ray crystallography.The coordination polymer crystallizes in orthorhombic crystal system with*Pbca* space group. The unit cell parameters are *a*=7.9321(2)Å, *b*=14.7305(3) Å,*c*=27.7895(6)Å. The La(III) center has nine-coordination geometries (Fig. 1). Non-covalent interactions such as hydrogen bonding and π-π stacking are responsible for the extending of the coordination polymerinto the three-dimensional supramoleculararray. Furthermore, the IR, CHN, XRD and TGA properties are also investigated in this work.

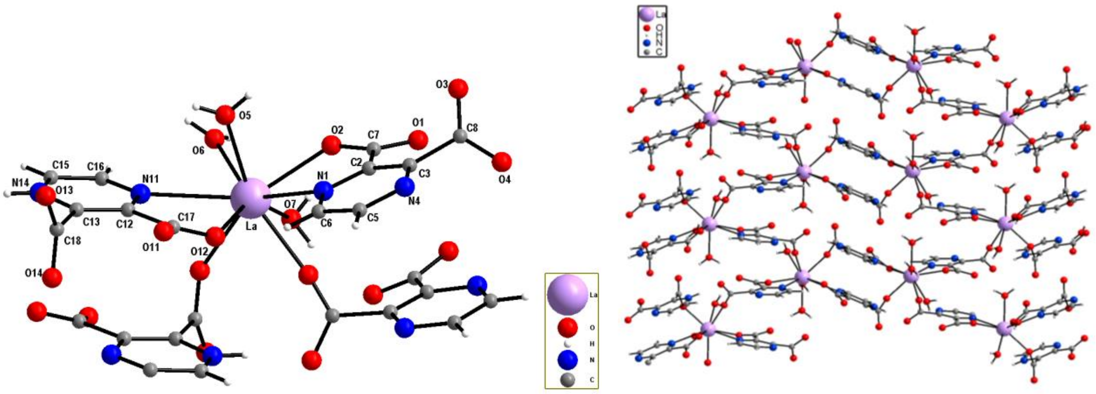

Fig. 1.(a) Representation ofthe coordination polyhedron around La atom in (**I**)and (b) the two-dimensional network of (**I**) along the baxis.

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Synthesis, characterization and X-ray crystal structure of manganese(II) complex of thiosemicarbazone based schiff base ligand with N and S donors

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Thiosemicarbazones are now well established as an importantclass of sulfur donor ligands particularly for transitionmetal ions. [1] This is due to remarkable biological activities observed for these compounds, which has since been shown to be related to their metal complexing ability. These compounds present a great variety of biological activity ranging from antitumour, fungicide, bactereocide, antiinflammatory, and antiviral activities .[2,3] The presence of amide, imine and thione groups makes them potentially polydentate ligands [4] and it is not surprising that numerous thiosemicarbazone complexes have been prepared and characterized.

New complex of manganese(II) with thiosemicarbazone based schiff base ligand was synthesized and characterized by FT-IR and UV-Vis absorption spectroscopy. The single crystal X-ray diffractions of the complex shows that the Mn(II) ion is in a distorted octahedral geometry coordination of N_4S_2. The complex crystallizes in monoclinic, space group $P2_1/c$ with a = 13.9782(2) Å, b = 19.2445(3) Å, c = 10.8004(2) Å, β = 104.505(2) and Z=4 (Fig 1).

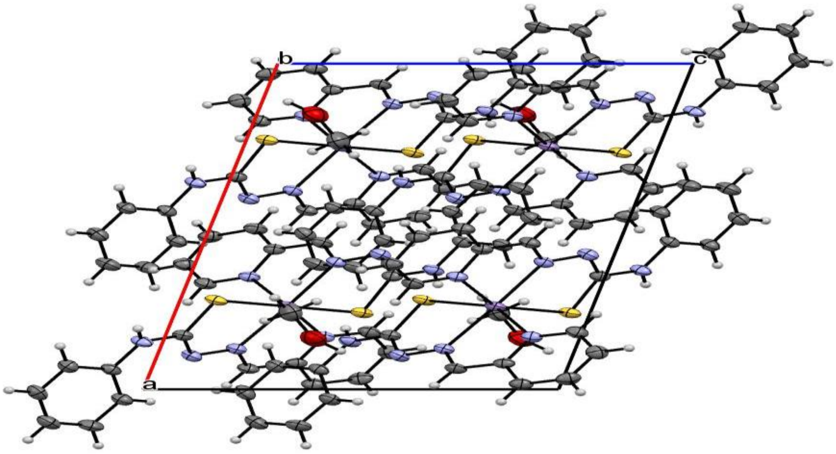

Figure1.Crystal packing structure diagram of the manganese (II) complex.

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Dinuclear cadmium(II) complex with Schiff base ligand: Synthesis, characterization and crystal structure

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The investigation of metal complexes with sulfur containing schiff bases is a subject of current andgrowing interest and it has been shown that many ofthem present anticancer activity .A particular important group of such ligands includes those containing thiosemicarbazon-emoieties, because their complexes formed with many of the transition metals showa wide range of biological properties.[1] These biological activities are often attributed to their chelating ability with metalions. [2] Thiosemicarbazones typically form coordination compounds in neutral or anionic forms, and they can act in various coordination modes due to their geometricalflexibility and polydentatenature.[3]

The dinuclear complex of cadmium (II) with N(4)-phenyl-2-formyl pyridine thiosemicarbazone was synthesized and characterized by FT-IR , UV-Vis absorption spectroscopy and X-ray diffraction techniques.The complex crystallizes in P 2_1/cspace group with a = 9.6976(4)A ° ,b = 2.2739(11) A ° ,c = 15.7149(6)A ° , β = 95.069(4) and Z=4 (Fig 1).

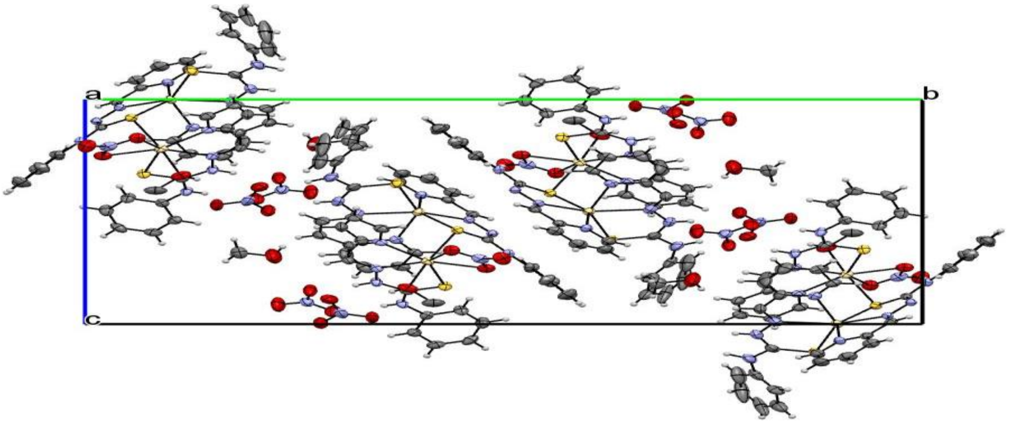

Figure1.Crystalpacking structure diagram of the cadmium (II)complex.

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Zinc Oxide Nanoparticles on Bioinspired Porous Silica: Photocatalytic Degradation of Congo red

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In this study, we have demonstrated a simple low-cost method to grow ZnO nanoparticles on the surface of porous silica which was prepared from rice husk biomass. The rice husk ash is a massive byproduct of rice milling. The silica content of the rice husk ash can be as high as 90-98%, so it can be a good source of silica. First, the sample of rice husk was washed thoroughly with distilled water to remove adhering soil and dust. Then an adequate process of acid leaching was carried out to remove metal ions, chlorides, phosphates, etc. Uniformly sized ultrafine silica powder can be obtained by thermal decomposition of rice husk in an oxidizing atmosphere. The properties of product have been investigated by SEM/EDX, XRD, FTIR, and BET/BJH. This method can conveniently provide preparation of silica with high surface area and nanometer grade. Zinc oxide nanoparticles embedded on the surface of porous silica by sonochemical reaction and then thermal treated of ethanol solution of zinc acetate with bioinspired silica. The resulting structures were confirmed by characterizations of XRD, SEM, and UV-Vis spectroscopy. Finally, the photocatalytic activity of prepared ZnOnanocatalyst was investigated by degradation of Congo red.

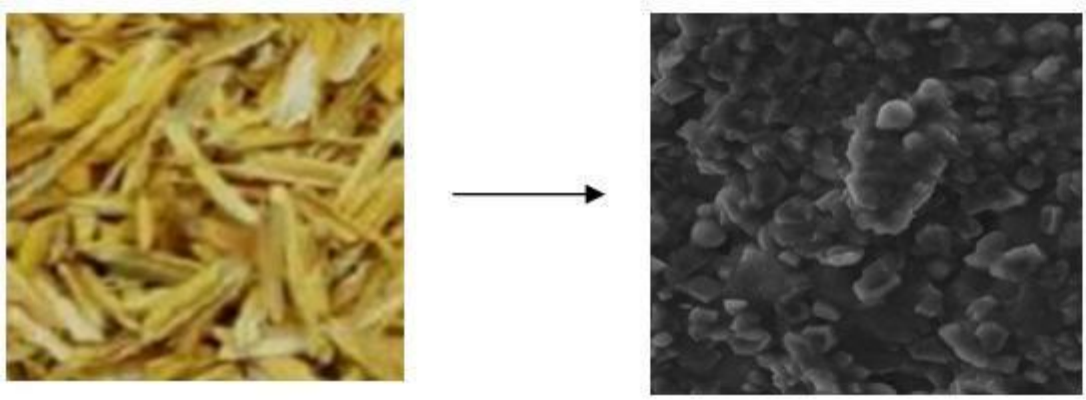

Figure1: Bioinspired silica from Rice husk

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Synthesis of Three new Cadmium(II), Zinc(II) and Manganese(II) heptaaza Macrocyclic Schiff base Complexes containing two pyridyl units as pendant arms

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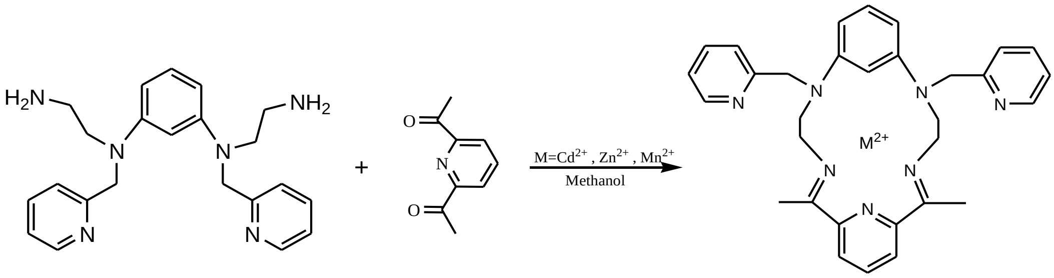
The capability of metal ions to promote the template synthesis of macrocyclic ligands has been studied extensively and depends on several factors related to the ligand characteristics, as well as on the nature of the metal ion. [1] The stability of macrocyclic metal complexes depends upon a number of factors, including the number and type of donor atoms presenting in the ligand and their relative positions within the macrocyclic skeleton, as well as the number and size of the chelate rings formed on complexation. For transition metal ions, features such as the nature and magnitude of crystal-field effects play also an important role.[2] One of the features of non-rigid large ring macrocyclic ligands is their ability to fold to give, have involved the synthesis of ligands with rigid backbones to prevent the folding which can otherwise occure.[3]

In this work,three complexes were prepared with direct [1+1] condensation of 2,6-diacetylpyridine with branched hexadentate amine ligands, N^1,N^3-bis(2-aminoethyl)-N^1,N^3-bis(pyridin-2-ylmethyl)benzene-1,3-diamine in methanol followed by addition of $Cd(NO_3)_2.4H_2O$, $MnCl_2.2H_2O$ and $ZnClO_4$. After on solution was filtered whilst hot and $NaClO_4$ added to the filtrate. The resultant complex was characterized by IR, Mass, CHN, ^{1}H and ^{13}CNMR spectroscopy. In the IR spectrum, a band at 1660.7 cm^{-1} indicated the formation of C=N double bonds, no picks attributed to NH_2 and carbonyl groups implied that the condensation reaction had been completed. A complex show a strong non-split absorption at 1094 cm^1, indicating the presence of non-coordinated perchlorate anions.



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Synthesis and Characterization of Copper,Cobalt,Nickel and Zinc complexes with new ligand basedon Thiosemicarbazone

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Thiosemicarbazone ligands can coordinate in a number of different manners. In general, they are in two tautomeric forms; a neutral thione form and thiolate form .[1,2] Metal complexes with an ONS donor set are of much interest because of their potential applications in fundamental and applied sciences. In the present work (2-(2,2 phormyl phenoxy)etoxy) benzaldehyde was prepared from reaction of salcylaldehide with 1,2-dibromoetane.then H2L ligand was prepared from the reaction of dialdehyde with thiosemicarbazide and characterized by the FT-IR, UV-Vis, Elemental Analysis, 1H NMR and 13C NMR. Complexes of the ligand with copper(II), cobalt(II) ,Nickel(II) and Zinc (II)were prepared and characterized by using FT-IR, UV-ViS and Elemental analysis. FT IR.

Spectra of complexes indicated that H2L ligand is change to the thiolate form and proton on the nitrogen atom of the ligand is lost during coordination and connect to the metal as an uni-ionic ligand. Elemental analysis of complexes confirms proposed structures.

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Synthesis and characterization of Co(II) and Cu(II) complexes of a new unsymmetrical bis-thiosemicarbazone ligand

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Thiosemicarbazones are an interesting group of multidentate ligands because of their mixed hard-soft donor character and versatile coordination behavior. These compounds have become a subject of intense research interest since the discovery of their cytotoxic activity against cancer cell and bacteriostatic effects. The biological properties of thiosemicarbazones are often increased by metal ion coordination, for example lipophilicity which controls the rate of entry into the cell is modified by coordination and some side effects may decrease upon complexation. This observation further encouraged detailed studies on coordination chemistry involving thiosemicarbazoes. [1-2]

In this research work, cobalt(II) and copper(II) complexesof a new unsymmetrical bis-thiosemicarbazone ligand (H_2L) had been synthesized.Thesecomplexes were prepared from $Co(CH_3COO)_2.4H_2O$ and $Cu(CH_3COO)_2.4H_2O$ salts (with 1:1 ratio) under reflux for about 4h in chloroform-methanol mixture. Copper(II) and cobalt(II) complexes have been characterized with IR and UV-Vis spectrum. Comparison of IR and UV-Vis spectrum of the Schiff-base ligand with its metal complexes confirms that the ligand is coordinated with metal ions. Electrochemical studies showed that copper(II) complex was reversibly reducible.

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Application of CNT/MnO_2 synthesized as Catalyst for the O_2 Electrode in lithium-Air battery

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Li–O_2 batteries, as a promising eco-friendly electrochemical power system [1.3] have recently attracted great attention becauseof their ultra-high theoretical specific energy .[4.6] Alithium-air battery that uses non-aqueous electrolytes was first reported in 1996.[7] The discharge reaction in a Li-air battery is the reductionof oxygen with lithium ions to form lithium (per) oxide at 2.91V. In this work, Manganese dioxide nanoparticles on carbon nanotubes synthesized and optimized using chemical methods. After optimization, the samples were used as the cathode catalyst inlithium-air battery. Figure 1 shows the discharge curve oflithium-air battery. The synthesized compound had the capacity of about 5300 mA.h/g with current density of 500 mA.h/g.FESEM, EDS-SEM, XRD, FT-IR, and BET studies of the sample were performed. Cycle ability of the battery was performed in 20 cycles.

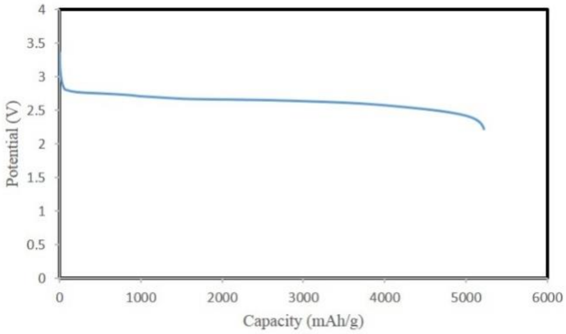

Fig. 1. the discharge curve of lithium-air battery

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Synthesis and characterization of a new unsymmetrical bis(thiosemicarbazon) ligand and its complexes with zinc(II) and cadmium(II) transition metals

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Thiosemicarbazones ($R_1R_2C=N-N(H)-C(=S)NR_3R_4$) constitute an important class of N, S-donor ligands, and their coordination chemistry was initially explored during the early sixties.[1]Thiosemicarbazones are of considerable pharmacological interest since a number of derivatives have shown a broad spectrum of chemotherapeutic properties. The wide range of biological activities possessed by substituted thiosemicarbazones includes cytotoxic, anti-tumour, anti-bacterial, and anti-viral properties. The biological properties of the ligands can be modified and in fact enhanced by the linkage to metal ions.[2]

In this work research, a new type of unsymmetrical bis(thiosemicarbazone) ligand has been synthesized and characterized by FT-IR, ^{1}H NMR and ^{13}C NMR spectroscopy. Zinc(II) and cadmium(II) complexes of unsymmetrical bis(thiosemicarbazone) ligand have been prepared and characterized by a range of techniques including elemental analysis, FT-IR spectroscopy, UV-Vis and fluorescence emission spectroscopy. In comparison with the ligand, emission wavelength of Zn and Cd complexes has shifted to higher ones. Elemental analysis showed that both complexes are mononuclear, and the ligand acts as dianionic.

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Selective oxidation of alcohols to aldehydes and ketones with hydrogen peroxide catalyzed by copper(II) Schiff base complex containing isatin

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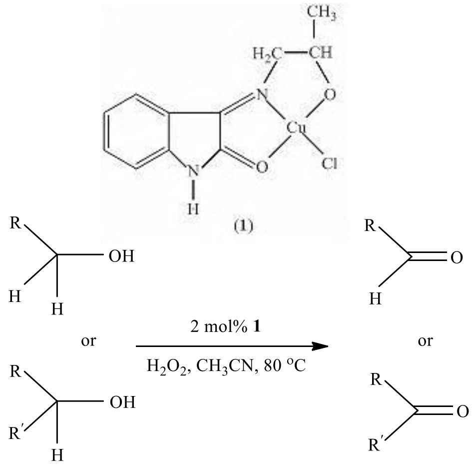
Aldehydes and ketones are important intermediates in the synthesis of other organic compounds both at laboratory and industrial level. Therefore selective oxidation of alcohols toward carbonyl compounds by transition metal catalysts is a broadly studied field and various catalytic methods have been developed.[1] Catalytic oxidation using transition metal Schiff base complexes is attractive, in view of their accessible synthesis and versatile coordination structures and various examples of such transition metal complexes have been reported.[2] Oxidizing agents that are traditionally used for these oxidations are often toxic or hazardous and produce heavy metal waste.[3] Consequently to overcome these shortcomings, a substantial amount of research has been directed toward developing new and efficient catalytic systems based on the use of aqueous 30% H_2O_2 as a final green oxidant.

In this work, the tridentate Schiff base ligand containing isatin was prepared by the standard procedure of refluxing ethanolic solutions of 1-amino-2-propanol and isatin in a 1:1 molar ratio and metallated with $CuCl_2.2H_2O$ to obtain complex **1**.The prepared Schiff base ligand and catalyst **1** were characterized by FT-IR andUV-vis spectroscopic techniques and elemental analysis. The synthesized catalyst **1** was successfully applied as a new homogeneous catalyst for oxidation of various alcohols to the corresponding aldehydes or ketones (scheme 1). Good to high yields, short reaction times, use of hydrogen peroxide as a green oxidant and no by-product formation make this method attractive and a useful contribution for oxidation of alcohols.

Scheme 1. Oxidation of alcohols to corresponding carbonyl compounds



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Density functional theory studies on the N_2-CNTand B_2-CNT supported cobalt nanocatalysts

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Fischer–Tropsch (FT) synthesis is of paramount significance in the utilization of natural resources, such as natural gas and coal. It has attracted wide interest since it was discovered about 80 years ago .[1,2] The FT synthesis is a process for transforming CO and H_2, which can be obtained by treating natural gas, into long-chain hydrocarbons. Only Fe, Co, Ru, and Ni have sufficient activity in FT synthesis for industrial applications. Fe and Co are the metals used as catalysts commercially. Fe is more than 200 times less expensive than Co, but Co is more active and more resistant to deactivation .[3] In this work, the twoN_2-CNT and B_2-CNT supported Co nanocatalystswere used for the hydrocarbon synthesis by DFT computations in order to evaluate the stability of the catalyst.For this purpose, the structures of cobalt nanocatalysts supported on nitrogen and boron substituted armchair (4,4) carbon nanotube abbreviated as N_2-CNT-Co (**1**) and B_2-CNT-Co (**2**) were optimized using Gaussian 98 program at B3LYP/LANL2DZ level of theory (Fig. 1). The binding energies were measured from the equation E(bind) = E(complex) – Σ E(molecule). It was found that catalyst **1** is 1.02 times more stable that catalyst **2** indicating it is more suitable for application in the gas to liquid (GTL) process using the FT synthesis. The dipole moment values of compounds **1** and **2** are 2.4788 and 5.9907 Debye, respectively, reflecting much higher polarity of **2** than that of 1 that is due to the effect of boron on the system polarization. Therefore, the N_2-CNT supported Co catalyst is considered as an active and appropriate nanocatalyst for the FT synthesis of hydrocarbons.

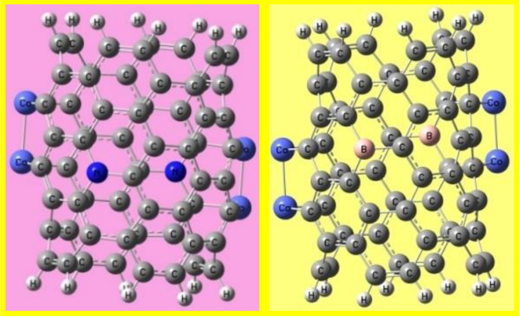
(**1**) (**2**)

Fig. 1. The optimized structures of N_2-CNT-Co (**1**) and B_2-CNT-Co (**2**) nanocatalysts.

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The NBO analysisof the N_2-CNTand B_2-CNT supported cobaltnanocatalysts

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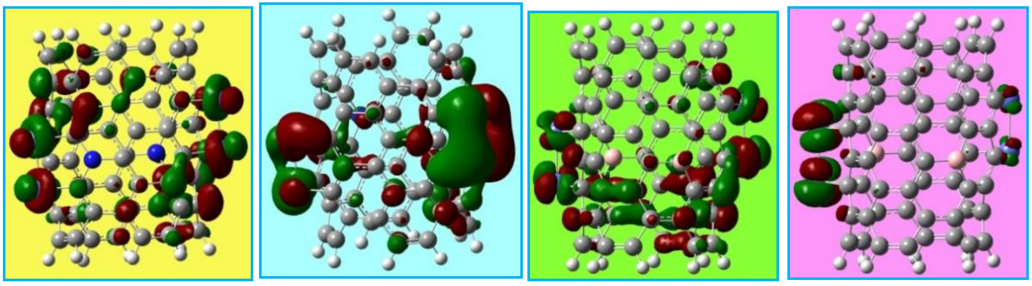
As a gas-to-liquid (GTL) reaction, Fischer–Tropsch (FT) synthesis can produce hydrocarbons using syngas (CO and H_2) derived fromcoal, natural gas, or biomass.[1] Supported cobalt catalysts are preferred due to their high activity, high selectivity to long-chain paraffins, low water–gas-shift activity and high resistance to deactivation. [2] For these catalysts, the support not only provides a large surface area for the cobalt dispersion, but also has significant effects on the FT performance due to metal–support interactions, porosity and mass transfer limitations .[3] Carbon has an inert surface and can enhance the reducibility of cobalt oxide .[3] In this research, the twoN_2-CNT and B_2-CNT supported Co nanocatalystswere used for the hydrocarbon synthesis by DFT computations in order to evaluate the stability of the catalyst.For this purpose, the structures of cobalt nanocatalysts supported on nitrogen and boron substituted armchair (4,4) carbon nanotube abbreviated as N_2-CNT-Co (**1**) and B_2-CNT-Co (**2**) were optimized using Gaussian 98 program at B3LYP/LANL2DZ level of theory. The binding energiesrevealed that catalyst **1** is 1.02 times more stable that catalyst **2** indicating it is more suitable for application in the gas to liquid (GTL) process using the FT synthesis. The natural bond orbital (NBO) analysis exhibited that the HOMO-LUMO band gaps of compounds **1** and **2** are 0.9538 and 1.1135 eV, respectively indicating superior electron conductivity in **1**.The HOMO and LUMO orbitals of catalysts **1** and **2** are shown in Fig. 1. It is seen that both of the HOMO and LUMO orbitals are mainly located on cobalt active centers and there are small amounts of LUMO orbitals on the nitrogen atoms in **1**. The LUMO orbitals of **2** are almost totally placed on the Co centers and they are not observed on the B_2-CNT carbon and boron atoms. Thus, the presence of Co atoms is necessary in order to perform the FT synthesis.



(HOMO of **1**) (LUMO of**1**)(HOMO of **2**) (LUMO of**2**)

Fig. 1. The HOMO and LUMO orbitals of N_2-CNT-Co (**1**) and B_2-CNT-Co (**2**) nanocatalysts.

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Synthesis, characterization and investigation of photocatalytic activity of polymer/suppoted porous ceramics-TiO_2 nanocomposites under UV light irradiation

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Titania appears to be a promising and important prospect for using in environment purification due to its strong oxidizing power, nontoxicity, considering cost and photochemical stability.[1] Conjugated polymers act as stable photosensitizer combined with wide band gap TiO_2 was an emerging area of research for photocatalytic activity applications.[2] Porous ceramics play an active role in the photocatalytic reaction by preventing electron hole recombination and providing hydroxyl groups for hole capturing.[3] In this study, a series of Polymer-modified porous ceramics TiO_2 nanocomposites containing SiO_2-M-TiO_2 (M: Fe, Ca, Mg,….) were successfully prepared in different concentrations by in situ chemical oxidative polymerization. The SEM images revealed agglomeration and sphere morphology of the nanocomposites before and after coating with polymer. The formation of anatas and rutil crystals were determined by XRD and the obtained data were used to calculate the particle sizes that were about 50-70 nm. The FT-IR analysis of these nanocomposites showed specific bands at 1300 $cm^{-1}$and 1399 cm^{-1} that have been attributed to C-N stretching mode for benzenoidand quinonoid units of polymer, subsequently. The prepared nanocomposites were used as an efficient photocatalyst for the degradation of Rhodamine B (RhB) under UV light irradiation. The experimental parameters such as initial concentration of Pollutant, catalyst loading, pH, solution temperature, light intensity and the reaction flask distance to lamp were optimized for maximum degradation efficiency. The obtained results show that nanocomposites exhibit significantly higher photocatalytic activity than that neat TiO_2 on degradation of RhB under UV light irradiation.

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The use of Co-B/Fe_3O_4 nano catalyst for reduction of bromate in water under hydrogen gas

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The association of bromate in drinking water with several public health risks, namely related to its carcinogenic potential and its toxic nature, has led to an interest in the development of sustainable alternatives for its removal from water. The hydrogen reduction of bromate over suppurted heterogeneous catalysts has already been shown to be an interesting alternative for the reduction of bromate into less hazardous species, without formation of additional sludge.[1]

In this study Co-B/Fe_3O_4 catalyst, synthesized by ultrasound condition. Characterization of product were analyzed by SEM, XRD and FT-IR techniques.

Activity of synthesized nano catalysts (Co-B/Fe_3O_4) was tested for reduction of bromate under hydrogen. The effect of various parameters such as temperature, hydrogen gas flow, pH, initial concentration of bromate and dose of catalyst, was studied .

The roles of the nano catalyst and of the reducing agent were assessed, and it was proposed that the reaction mechanism on the surface of the nano catalyst comprised the dissociative adsorption of hydrogen and subsequent reaction with adsorbed bromate.[2]

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Molybdenum complex supported on ɣ-Fe_2O_3 magnetic nanoparticles: A new catalyst for C-C bond formation *via*Knoevenagel reaction

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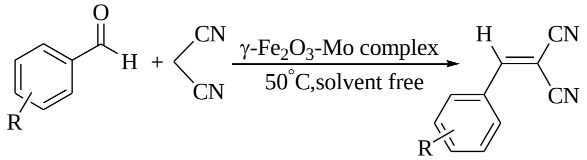
C–C-bond formation reactions are one of the important reactions in synthesis. The classical Knoevenagel reaction[1] is a well-known example for C–C-bond formation wherein the end products are generally α,β-unsaturated carbonyl compounds or α,β-unsaturated malonates. These adducts are good Michael acceptors and can be used directly in the various chemical reactions. The importance of Knoevenagel adducts has led to exploration of several methods to promote Knoevenagel condensation. It is also worth mentioning, most of the methods suffer from limitations such as tedious work-up procedures and using hazardous solvents or unrecyclable catalysts. Magnetic nanoparticles (MNPs) are receiving increasing interest as supporting material for the synthesis of heterogeneous catalysts because of their unique properties.[2] MNPs have advantages including easy preparation and functionalization, large ratio of surface area to volume and low toxicity.[3] The catalyst supported on magnetic nanoparticles can be easily separated from the reaction mixture and products by an external permanent magnet and reused. Here we report an efficient method for the synthesis of a new molybdenum complex immobilized on ɣ-Fe_2O_3 magnetic nanoparticles. The prepared catalyst characterized by different techniques (CHN, ICP, TGA, FTIR, XRD, VSM, TEM). It was successfully applied as amagneticaly recyclable heterogeneous catalyst for C–C-bond formation reaction under solvent free condition. Good to high yields, short reaction times, simple work-up, ease of catalyst recovery, no by-product formation and re-usability of the catalyst without appreciable loss of activitymake this method attractive and a useful contribution to the present methodologies.



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Preparation and characterization of nanohydroxyapatite (nHAp) co-doped with Zn/Ag

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The hydroxyapatite, $Ca_{10}(PO_4)_6(OH)_2$, presents a good pattern of biological apatite especially when it is modified by the presence of many other ions (Mg^{2+}, Zn^{2+}, CO_3^{2-},HPO_4^{2-},etc.)[1,2]. In the present work, as eriesofhydroxyapatite samples co-doped with Zn/Ag were synthesized using precipitation method[3]. The effect of different amounts of Zn and Ag on average size and degree of crystalline was investigated.

The formation of nHA particle was investigated by X-ray powder diffraction spectroscopy (XRD) and alsoindicates the affectation of crystallinity of hydroxyapatite as function of dopant content. The fourier transform infrared spectroscopy (FT-IR) shows the typical peaks of carbonate vibration at 872 and 1382 cm^{-1}, these observations also indicated the formation of nHA. The unique particle morphology were observed by scanning electron microscope (SEM) equipped with an energy dispersive X-ray (EDX) analyzer. The EDX spectra investigated the elemental compositions and (Ca+dopants)/P molar ratios, and all samples were pure. The binary combination of the co-dopants and their amount significantly affect thevaluesof the crystallitesize and crystallinity degree.For each samples, the sevalues gradually decrease with increasing the amount of the co-dopants.

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A new study on the improving the catalytic activity of magnetically recoverable schiff base nanocomplexes in the presence of chitosan

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In recent years, heterogenization of homogeneous catalyst by different methods and various material hassignificantly developed. One of these methods,is using various supports such as clays, silica, polymers and so on.[1,2] In this study,firstly the Fe_3O_4 nanoparticles were synthesized and modified by chitosan biopolymer. In the next step, schiff base complexes were immobilized on to these particles.[3] The FT- IR analysis of these nanoparticles showed specific bands at 1627 and 1620 cm^{-1} that depicts the efficient coating of chitosan on the Fe_3O_4 nanoparticle and the formation ofimin bonds, subsequently. The SEM images revealed agglomeration and sphere morphology of the nanoparticle before and after coating with chitosan. The obtained data of XRD pattern were used to calculate the particle size that was about 23 nm. The M-H curvesfrom analysis VSM indicated the superparamagnetic behavior of these nanoparticles before and after surface modification that a negligible decrease is observed after coating with chitosan.Finally, these nanoparticles were used as catalyst in biginelli reaction that showed high activity as long as easy separation and recyclability.

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The use of carbon nanotubes as a catalyst in the air cathode of lithium-air battery

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The lithium-air batteries which has the potential to provide 5–10 times higher capacity than Li-ion cell have attracted numerous attention recently.[1] The cathode active material O_2 obtained from theair reacts with Li from lithium anode to form insoluble discharge products in nonaqueous electrolyte, and they will block the diffusion paths of oxygen and cause dramatic capacity reduction.[2] Research activities on various aspects of lithium-air batteries havebeen intensified following the pioneer work by Abraham and Jiang, [3] while the structure designing of carbon materials used in the air cathodes holds the majority .[4-6] In this work, multi-walled carbon nanotubes (MWNTs)as cathode materials without catalysts for lithium-air batteries in nonaqueous electrolyte. Also, the heat treatment was used to improve the cathode. Figure 1 shows the discharge-charge curve of lithium-air battery. It demonstrated that MCNTs, not only increased the discharge capacity but also exhibited higher reaction activities. Cycle ability of the battery was performed in 20 cycles.

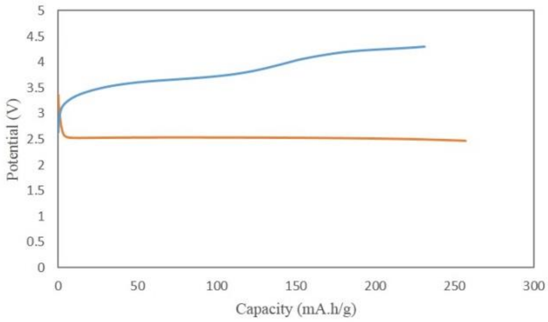

Figure 1: The discharge-charge curve of lithium-air battery

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Synthesis and Characterization of a new Organotin(IV) Complex with iminopyridine Ligand

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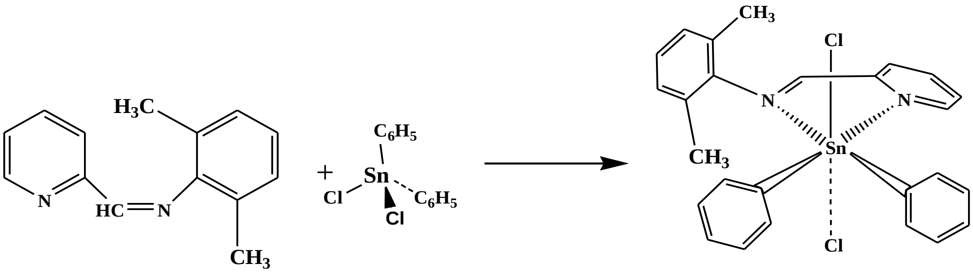
In recent years, a new interesting applications found in the field of pesticides and medicine, the metal complexes with tridentate O, N, N types of alternative structures have attracted the attention of chemist. Various metal complexes with bi- and tridentate Schiff bases containing nitrogen and oxygen donor atoms play important role in biological system and represent interesting models for metalloenzymes, which efficiently catalyze the reduction of dinitrogen and dioxygen.[1] In recent years metal compounds, which have a stable d^{10} electronic configuration, have received a lot of attention in the fields of inorganic chemistry, biochemistry and environmental chemistry.

Compared with organotin compounds, inorganic compounds of tin are also important in industry applications, for example, electroplating, ceramic glazes and pigments, heterogeneous catalysts, gas sensors, and so on. [2] Perhaps the most important recent development in tin (IV) chemistry has been the increase in studies of the solid state properties of tin (IV) compounds. [3]

In the present first Schiff base iminopyridine ligand has been prepared by the condensation between primary amine and active carbonyl group, then related complex synthesized in normal hexane solution. The novel complex derived from Sn(IV) containing chloride, phenyl and iminopyridine ligands were synthesized and characterized by elemental analysis, ^{1}H NMR, ^{13}CNMR, IR and UV–Vis spectroscopy.



Scheme 1. Synthesis of the title compound

References:

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Synthesis and Characterization of novel Lead (II) Complexes with bidendateiminopyridine Ligand

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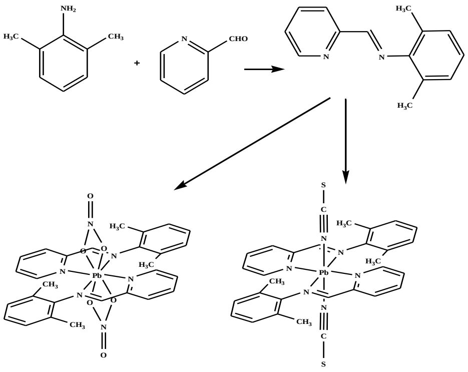
Schiff base metal complexes have been known since the 19th century. Investigation on metal organic complexes represents one of the most active areas of material science and chemical research. Schiff base metal complexes play a key role in the development of coordination chemistry. [1-3]

The coordination chemistry of Pb(II) with N- and O- donor ligands has been investigated in the past decade and frequently discussed in regard of the stereochemical activity of the lone pair of electrons. [4]

To further investigate this area, first Schiff base iminopyridine ligand has been prepared by the condensation between primary amine and active carbonyl group, then related complexes synthesized in methanol solution. The ligand and metal complexes have been characterized by elemental analysis, UV, IR, ^{1}H NMR and ^{13}CNMR spectroscopy. The spectroscopic data of metal complexes indicated that the metal ions are complexed with azomethine and pyridine nitrogen atoms. The ligand acts as bidentate with two N sites and can coordinate with metal ion.



Scheme 1. Synthesis of ligand and related lead complexes

References

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Performance of nanostructure Fe-Ag ZSM-5 catalysts for the degradationof MR and Optimization using RSM

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Photocatalytic degradation of methyl Red was investigated using Fe-Ag-ZSM-5 nanocatalysts under UV light irradiation in aqueous dispersions. The effect of important parameters such as Ag loading, Fe loading, calcinations temperatureand irradiation time was investigated and the process conditions were optimized using response surface methodology (RSM) based on central composite design (CCD). The optimum condition for Ag loading, Fe loading, calcination temperature and irradiation time was 5.17 wt%, 2 wt%, 580° C and 60 min, respectively. A maximumof 96% of Methyl red was removed under the optimum experimental conditions. The proposed model equation using RSM has shown good agreement with the experimental data, with a correlation coefficient (R^2) of 0.952.

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Synthesies and characterization of three new octaaza Mn(II), Zn(II), Cd(II) and macroacyclic Schiff base complexes containing two pyridyl unit as pendant arms

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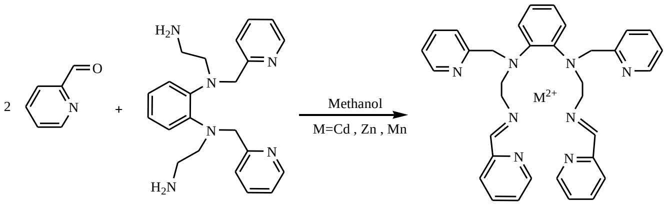
The Schiff base ligands are one of the most widely used ligands due to the ease of formation and remarkable versatility, and therefore they have played an important role in the development of coordination chemistry as they readily form stable complexes with most of the transition metals. The research 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]. Recently, we reported the synthesis and characterization of some octaaza Mn(II) macrocyclic Shiff base complexes.[1] In this work, we describe the Mn(II), Cd(II) and Zn(II) templated [1+1] cyclocondensation of picolinaldehydeand branched hexadentate amine, N1,N2-bis(2-aminoethyl)-N1,N2–bis(pyridine–2–ylmethyl)benzene -1,2-diamine,that producing three complexes containing two 2-methylpyridine pendant arms (Scheme1).



Scheme 1.

All the complexes have been characterized by IR, elemental analysis and in the case of Zn(II), Cd(II) complexes by ^{1}H and ^{13}CNMR spectroscopy.

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Theoretical Study of the solvent effects on the molecular structure, molecular orbital, ^{1}H and ^{13}C NMR and hyperpolarizability of $(NHC)_2Ru(=CHPh)Cl_2$

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In this work, the solvent effect on the structural parameters, UV, IR and electronic spectra of $(NHC)_2Ru(=CHPh)Cl_2$ was investigated by Modified Perdew-Wang Exchange and Correlation (MPW1PW91) method. The calculations of systems contain C, N, H and O described by the standard 6-311G (d, p) basis set. For Ru element standard Def 2-TZVPPD basis set are used and Ru described by effective core potential (ECP) of Wadt and Hay pseudopotential with a triple-ξ valance using the Def 2-TZVPPD. The solvent effect on structural parameters, frontier orbital energies, and properties of complex has been carried out based on Polarizable Continuum Model (PCM). This complex is an excellent yardstick structure and an olefin metathesis catalyst which exhibits both types of carbenes. These calculations show that Ru-C(NHC) bond distances increases with increasing of solvent polarity. ^{1}H and ^{13}C NMR chemical shifts were calculated by using the gauge-invariant atomic orbital (GIAO) method. The dependence of the first hyperpolarizability of the studied compound both on the dielectric constant of the media and the Onsager function were studied.

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Theoretical Study of Sialbenzenes containing chromophores for DSSC materials

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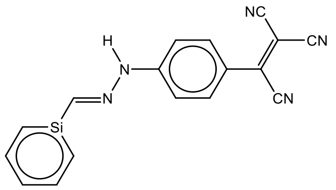
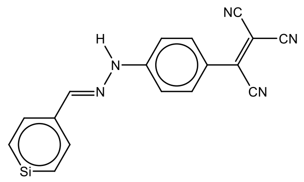
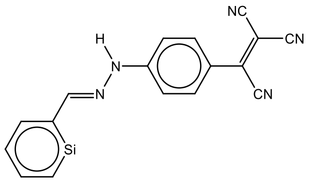
The ground state geometries of Sialbenzenes containing chromophores (Figure 1) have been computed by using density functional theory (DFT) at B3LYP/6-311++G (d,p) level of theory. Quantum chemical calculations were carried to investigate the electron coupling, electron injection, electronic and photophysical properties of these molecules. The lowest HOMO and LUMO energies have been observed for ones. The HOMOs of the dyes are below the redox couple and LUMOs are above the conduction band of TiO_2. The calculated results of these dyes demonstrate that these dyes can be used as potential sensitizers for TiO_2 nanocrystalline solar cells.



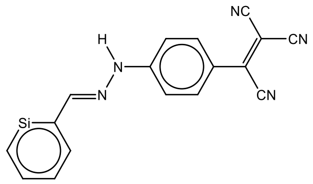
Si



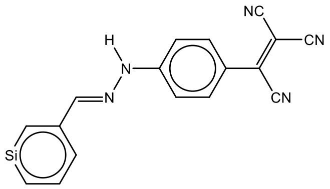
p-Si



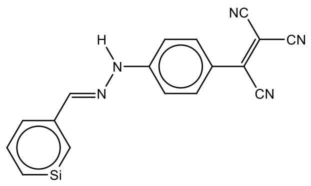
O2-Si



O1-Si



M2-Si



M1-Si

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Synthesis and Spectral Characterization of Copper(II), Nickel(II) and Zinc(II) Complexes with 2-Aminobenzoic Acid and 2-amino-3-methylpyridine as the Ligand

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Anthranilic acid (or o-amino-benzoic acid) is an organic compound with the molecular formula $C_7H_7NO_2$. The molecule consists of a benzene ring, hence is classed as aromatic, with two adjacent, or "ortho-" functional groups, a carboxylic acid and an amine. [1] The mixed ligand complexes of Ni(II), Cu(II) and Zn(II) with Anthranilic acid have shown profound activity against Staphyl ococcus, Klebsiella SPP. and Bacillas bacteries. Several other mixed ligands complexes with anthranilic acid were reported to have antifungal and antibacterial potential. [2] 2-Amino-3-methylpyridine is used as an intermediate for manufacturing pharmaceuticals. It is usually prepared by the Chichibabin reaction between 3-methylpyridine and sodium amide in an organic solvent. [3] The pyridine substructure is one of the most prevalent heterocycles found in natural products, pharmaceuticals, and functional materials. [4] In this report, Synthesis, spectroscopic and magnetic characterization of Cu(II), Ni(II) and Zn(II) complexes is described. All compounds have been prepared with Anthranilic acid and 2-amino-3-methylpyridine as the ligand and $Cu(NO_3)_2.3H_2O$, $Ni(NO_3)_2.6.H_2O$ and $Zn(NO_3)_2.4.H_2O$ as metal salt. Methanol was used as solvent. Alcohol as the solvent can acts as a bridging ligand and produces alkoxo-bridged complexes. The complexes have been characterized by FT-IR, UV-Vis, elemental analysis and magnetic moment methods. The FT-IR spectra indicate M-O and M-N vibrations in the range of400-580cm^{-1}. We have examined d-d transition, Ligand → metal charge transition and $\pi\rightarrow\pi^*$ and $n\rightarrow\pi^*$ transition of ligand in these complexes by using of UV-Vis method. Magnetic moments measurement shows that complexes are dimeric and monomer.

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Adsorption of cathionic dye from aqueous media by one of the mixed metal oxide nanosized

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In the present investigation, a porous $Gd_xSr_{1-x}FeO_{3-\delta}$ (GSFO) nanopowder was synthesized by sol-gel method and tested for the removal of methylene blue (MB) dye from aqueous solution. The size of the GSFO NPs was about 35.23 nm, with an average specific surface area (SSA) of 8.70 $m^2.g^{-1}$. Adsorption of MB was conducted to the model of thiazine dye at various GSFO NPs dosages, dye concentrations, solution pHs and contact times in a batch reactor. Experimental results indicate that the prepared GSFO nanopowder can remove above 87% of dye under optimum operational conditions of a dosage of 0.02 g, pH = 12 and a contact time of 30 min for initial dye concentration of 50 $mg.L^{-1}$. The isotherm evaluations revealed that the Redlich-Peterson model attained better fits to the experimental equilibrium data than the Langmuir, Freundlich, Temkin and Dubinin-Radushkevich models. In addition, adsorption kinetic data followed a pseudo-second-order rate rather than pseudo-first-order and intra particle diffusion models.

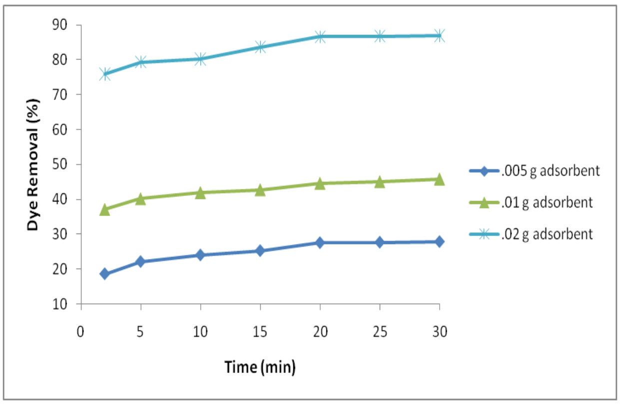

Fig. 1. Effect of stirring time on removal of MB in different dosages, (■) 0.05g, (▲) 0.01g, (∗) 0.02g of GSFO (initial dye concentration = 50 mg/L, initial pH=12).

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Study of the oxidative addition of organoplatinum(II) complexes containing diimine and phosphine ligands

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Oxidative addition reactions are recognized as a fundamental step in many catalytic processes. The synthetic chemistry of alkylplatinum(IV) compounds containing nitrogen ligands have been thoroughly studied [1]. Halogenoalkyl complexes of transition metals are classified as functionalized alkyl complexes of transition metals [2]. These complexes can be precursors for the preparation of homo and heteronuclear complexes. However, less is known about the reactions of organoplatinum(IV) complexes containing diimine ligands with phosphine ligands. In this context, we undertook a study of the reaction of a related series of alkyl and haloalkyl complexes of dimethylplatinum(II) complexes with the simultaneous presence of diimine and phosphine ligands. The reaction of the dimethylplatinum(II) complexes $[PtMe_2(NN)]$ {NN = bpy (2,2'-bipyridine);phen (1,10-phenanthroline)} with a series of alkyl halides and dihaloalkanes led to the formation of the organoplatinum(IV) complexes $[PtMe_2RX(NN)]$. Then, the reaction of the resulting organoplatinum(IV) complexes with monodentate and chelating phosphine ligands in the presence and absence of the tin(II) have been investigated. The resulting products were fully characterized by elemental analysis, ^{1}H, ^{31}P and ^{13}C NMR spectroscopy.

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Immobilized [Co_3(N, N$'$, N$''$ -Tris (2-pyrimidinyl) Dimethylentriamine)Cl_6] complex on modified Fe_3O_4 nanoparticles as magnetically separable catalyst for Oxidation of alkenes and alkanes

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Catalytic oxidation is an important technology that finds applications in all kinds of chemical industry [1, 2]. The [Co_3(PDMT)Cl_6] complex, where PDMT is N, N$'$,N$''$ -Tris (2-pyrimidinyl) dimethylentriamine was prepared in cyclohexanol under hydrothermal condition . In order to heterogenized the copmplex, Fe_3O_4 nanoparticles are prepared and modified with (3-aminopropyl) trimethoxysilane (APTMS) followed by immobilization of the complex designated as Fe_3O_4@Si2@APTMS@[Co_3(PDMT)Cl_6] (compound **1**). The prepared nanocatalyst is characterized by FT-IR, XRD, VSM and TEM techniques. The TEM results show that the formation of Fe_3O_4 nanoparticles with about 15 nm diameter with spherical morphology (Fig. 1a). The particles diameter varies between 30 and 40 nm after coating and functionalization (Fig. 1b). It was also found that immobilization of [Co_3(PDMT)Cl_6] complex on modified MNPs, the nanoparticle size increases to 45-50 nm (Fig. 1c). Observing core and shells of iron oxide, modified and immobilized one is also considerable.

The prepared compound catalyzes the oxidation of alkenes; cyclooctene, styrene, cyclohexene, norbornene, trans-stilbene, and alkanes; flourene, diphenylmethane, ethylbenzene, adamantane, cyclohexane, cyclooctane with TBHP as an oxidant with 25–100 % conversion and 40–100% selectivity. No desorption is observed during the course of reactions.

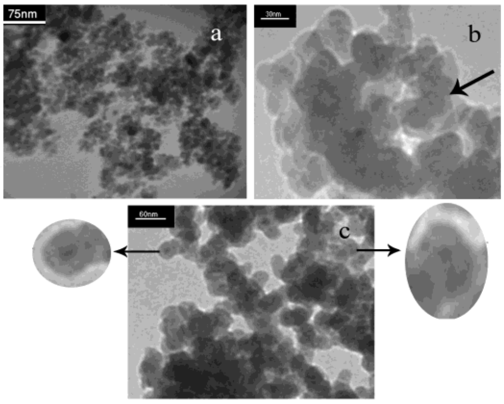

Fig. 1. TEM micrograph of a) Fe_3O_4, b) Fe_3O_4@ SiO_2-APTMS and c) compound (1).

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Synthesis and characterization of transition metal complexes containing new tetrapodal base on 3-mercapto-1, 2, 4-triazole

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In recent years the synthesis of ligands with several active center has attracted considerable attention[1]. 3-mercapto-1,2,4-triazole is an aromatic five membered heterocycle, containing three nitrogen atoms and one sulfur atom. we wish to report synthesis and characterization of anew tetrapodal ligand base on 3- mercapto-1,2,4-triazole and its behavior against late transition metals ,such as silver and copper. The tetrapodal ligand is prepared by the reaction of 1,2,4,5-tetrakis(bromomethyl) benzene and 3-mercapto-1,2,4-triazole as an air-stable solid mass and has been characterized by IR,NMR spectroscopy, Mass spectrometry as well as X-ray diffraction. The molecular structure of the tetrapodal ligand is shown in figure 1. The behavior of the ligand against silverion has also been studied.

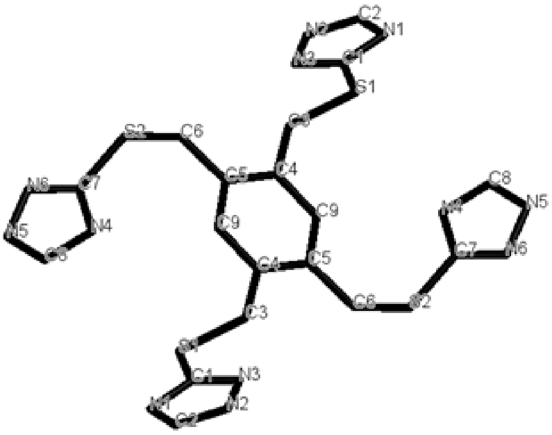

Fig. 1. Tetrapodal ligand

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Preparation of gold nanoparticles and application as biosensors for detection of cancer cells and optimization parameters by central composite design

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Most biomarker testing is taking place at centralized dedicated laboratories using large, automated analysers, increasing waiting time and costs. Smaller, faster and cheaper devices are highly desired for replacing these time-consuming laboratory analyses and for making analytical results available at the patient’s bedside use of miRNA -functionalized gold nanoparticles as a way to detect secreted miRNA in a patient's blood has increased in recent decades. [1,2] Gold nanoparticles exhibit several interesting physical and chemical properties that have made them an integral part of research in nanoscience. In this research we report the high sensitivity of this assay stems from the indirect amplification of the target sequence by the sizable number of miRNA strands that can be loaded on a single gold nanoparticle. Therefore, the amount of miRNA on each nanoparticle directly correlates to the amount of amplification possible and therefore the sensitivity attainable in this system. Also, we investigated the variables that influence miRNA coverage on gold nanoparticles by central composite design. The effects of salt concentration, spacer composition, nanoparticle size, and sonication time have been evaluated. Maximum loading was obtained by salt aging the nanoparticles to 0.5 M NaCl in the presence of miRNA spacer. In addition, miRNA loading was substantially increased by sonicating the nanoparticles during the surface loading process. The advantages provided by higher miRNA loading have the potential to dramatically impact biodetection. Size and shape of gold nanoparticles was proved by SEM image. UV-Vis spectrum was used for identification of target for detection of prostate, breast, vagina and colorectal cancers.

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Biginelli three component cyclocondensation reaction for preparation of dihydropyrimidinones using phosphated zirconia as novel solid acid catalyst

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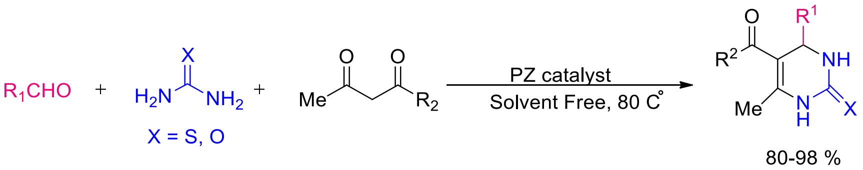
Dihydropyrimidinones are an important class of compounds that show biological activities such as antiviral[1], antitumor[2], antibacterial and anti-inflammatory actions.[3,4] They are routinely synthesized in a Biginelli three component cyclocondensation reaction between CH-acid carbonyl compounds, aldehydes and urea (or thiourea) under strongly acidic conditions[5]. Since dihydropyrimidinone-based drugs exhibit significant biological activity, their synthesis has been the focus of much interest from organic and medicinal chemists. There are many improved procedures for the preparation of dihydropyrimidinone based on metal (and ammonium) salts with nucleophilic anions, ionic liquids, natural HEU type zeolite, polyaniline-bismoclite complex, heteropoly acid, sulfated zirconia and others, are reported.[6] However, many of these protocols suffer from disadvantages like use of hazardous and toxic catalyst, poor yields, long reaction time, low recovery and cost involvement. Phosphated zirconia(PZ) is a stable, homogeneous, neutral, non-volatile, nearly cheap and safe reagent which is prepared from $Zr(OH)_4$ and NaH_2PO_4 flowing with calcinations of the mixture in 600-700 °C[7]. It has been little studied as a catalyst inorganic chemistry, i.e. Biginelli reaction.We wish here to report a one-pot facile and improved protocol for preparation of dihydropyrimidinones under nearly neutral reaction conditions with and without solvent, using PZ as catalyst.



A summary of the optimized experiments considering the amount of PZ catalyst and urea, effect of temperature and the nature ofon the yield has been preformed. Our results show that: i) the reaction does not proceed if no catalyst is employed, ii) the insolvent, temperature and amount of the catalyst and urea affect the yield of the reaction, iii) under optimized conditions, the yield of Biginelliproduct is increased to 80-98% with the addition of PZ in 20-50 minutes, iv) Various types of substituted benzaldehydes containing either electron-withdrawing or electron-donating substitutions successfully afforded the Biginelli products in high yields.

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Tungstophosphoric acid supported on γ-Fe_2O_3@SiO_2 nanoparticles catalyzed oxidative amid bond formation

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Amide bond formation is a common reaction because of the importance of this functional group in synthesis of polymers, natural products, pharmaceuticals and fine chemicals. Amide synthesis can be occurred in both catalytic and no catalytic conditions. No catalytic classic methods are incorporated with carboxylic acid activation by altered reagents such as phosgene or thionylchloride which is limited with different problems. In the most of catalytic methods, transition metals or their involving compounds are used as a homogenous catalyst. On the other hand, heteropolyacids and their salts are used as an efficient, practical and green acid, they have catalytic role as an oxidative reagent in different reactions with many workable applications, too[1]. According to our attempts, tungestophosphoric acid is catalyzed the strategy for amide synthesis from benzyl alcohols and amines (hydrochloride salts). In this method, γ-Fe_2O_3@SiO_2@HPW applied as catalyst and TBHP as external oxidant, respectively. In this situation, different derivatives of benzamides were synthesized in good yields.

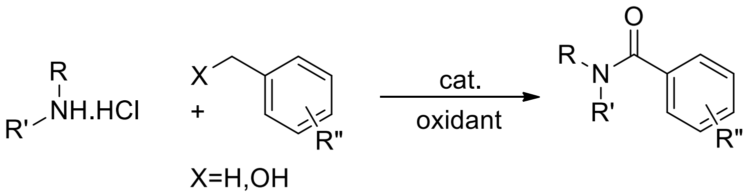

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Fig. 1: the model reaction of oxidative amidation by applying γ-Fe_2O_3@SiO_2@HPW

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Electrochromic aspects of multilayer phosphotungstic acid and tungsten oxide nanoparticles on graphene nanosheet

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Chromism is a reversible change in a substance's color resulting from a process caused by some form of stimulus. Many materials are chromic, including inorganic and organic compounds and conducting polymers. There are also several types of chromism.[1].Electrochromism, a reversible and optical change, is associated with an electrochemically induced oxidation–reduction reaction after applying an appropriate potential on the electrochemical active materials.[2] These are metal oxide films, molecular dyes and conducting polymers. The key properties of electrochromic materials are the switching times, the contrast ratios, coloration efficiency, electrochromic memory and long term stability.[2] They have a number of potential uses, including displays, smart mirrors and windows, active optical filters and computer data storage.[3,2] Electrochromism was discovered in tungsten trioxide.[4] In this work FTO-glass modified with graphene nanosheets. Using graphene nanosheets help to formation of uniform layers and enhanced the electrochromism properties. In the second step the tungsten trioxide nanostructures formed by electrode postion under constant potential (-0.45 V vs. Ag/AgCl). The results indicated the uniform film formation on the FTO/Gr. Finally, the phosphotungstic acid (PWA) film deposited on the FTO/Gr/WO_3 applying repetitive cyclic potential from 1 to -1 V vs. Ag/AgCl. The electrochemical and optical properties of constructed multilayer films were evaluated by voltametric methods and UV-Vis spectroscopy. The results implies to good electrochromism activity for fabricated multilayer film. Long term stability, reversible optical change, and good switching time are some properties of FTO/Gr/WO_3/PWA.

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Synthesis, characterization and antibacterial study of cadmium selenide quantum dots doped by lanthanium and cerium

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Quantum dots as semiconductor nanocrystals have been used extensively in the medical and biological system. Although quantum dots are known as nanoparticles, toxicity and biological negative effects of particles cannot ignore. Antimicrobial activity of nanoparticles is due to increased levels of exposure to micro-organisms. Small size and high surface to volume ratio and will enhance their interaction with microbes to antimicrobial activity. Metal and metal oxide nanoparticles antimicrobial activity, and its mechanism were investigated; the results showed that the presence and size of nanoparticles in antimicrobial activity are effective.[1,2] In the present work, cadmium selenide quantum dots was prepared from the reaction of sodium seleno sulfate with cadmium chlorideand doped by lanthanium and cerium.[3] Then characterized by IR and SEM.(Fig. 1.) The antibacterial activity of these compounds as been tested against some Gram (+) bacteria such as Staphylococcus Aureus, BacillusSubtilis and Gram (-) bacteria such as Escherichia Coli and Pseudomona Aeruginosa. The results showed that the synthesized compounds have antibacterial activity.

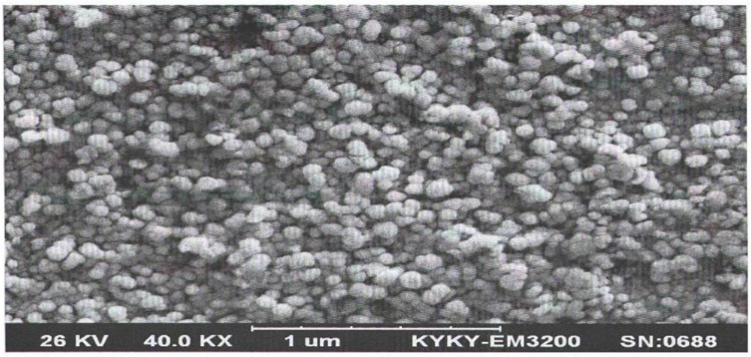

Fig. 1. SEM of cadmium selenide quantum dots doped by cerium

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Investigation of chemiluminescence properties of cadmium selenide quantum dots doped by lanthanium and cerium

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Quantum dots are semiconductor nanocrystals (2–100 nm) with unique optical properties.[1] most of chemiluminescence reaction due to low quantum efficiency have weak chemiluminescence property. This weak emission can been hanced by compounds with high quantum efficiency. The investigation of chemiluminescence of QDs explores their applications, for example, detection of blood sugar and atropine in pharmaceutical formulation.[2,3] The most popular types of quantum dots include CdTe, CdSe, ZnSe, and ZnS.[4] Recently, quantum dots doped by transition metal ions have been attention because they have interesting phenomena.[5] Lanthanide ions such as lanthanum and cerium, with spectral characteristics are widely used fluorescent research.[2] The chemiluminescence properties of luminol – hydrogen peroxide reaction was studied in aqueous medium with different catalysts ($CuSO_4.5H_2O$, $K_3Fe(CN)_6$ and $CrCl_3$).[6] (Fig. 1.) In the present article, our attention is focused on the investigation of the chemiluminescence in the luminal system in the presence of Mn or Cr with QDs CdSe doped by lanthanium and cerium. QDs CdSe doped by lanthanium quenched, and QDs CdSe doped by cerium enhanced the chemiluminescence of these systems.

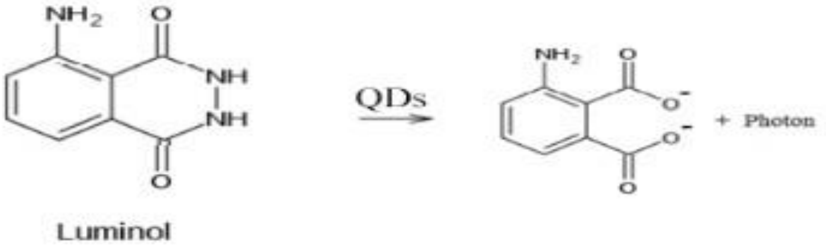

Fig. 1. Chemiluminescence reaction of luminol in presence of QDs

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Nano Molybdenum (VI) Schiff base complex as a mild and selective catalyst for oxidation of alcohols

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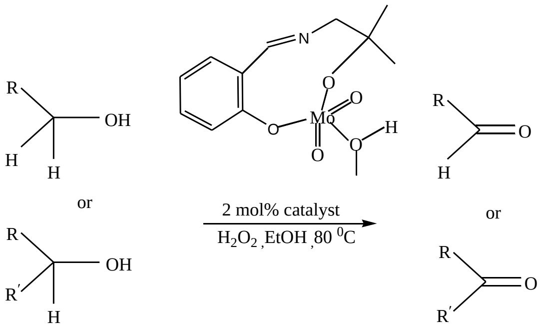
Oxidation of alcohols to aldehydes and ketones is one of the most important transformations in organic synthesis. In particular the oxidation of primary alcohols to aldehyde is important since they find wide applications as intermediates are fine chemicals particulary for perfume industry.[1] Many molybdenum species are known that catalyze the oxidation of alcohols to aldehydes/ ketones, and in all cases the active species is belived to be a Mo(VI) compound.[2] In addition, Molybdenum is found in a class of enzymes that catalyze oxygen atom transfer to and from an organic substrate. Therefor, very efficient and selective catalytic system employing a mild oxidant combined with molybdenum (VI) complex have been reported in recent years.[3] In this work the dioxo-molybdenum (VI) complex was synthesized under ultrasonic irradiation by using Schiff base ligand [2-[(2-Hydroxy-1,1-dimethyl-ethylimino)-methyl]-phenol] (H_2L) and dioxomolybdenylacetylacetonate. The complex was characterized by some spectroscopic method such as FT-IR, UV-Vis and CHN analysis. The size and morphology of the complex were investigated by SEM and XRD analysis. This complex was successfully applied as a new homogeneous catalyst for oxidation of various alcohols to the corresponding aldehydes or ketones. Use of hydrogen peroxide as green oxidant and ethanol as green solvent, high yields, short reaction times and no by-product formation make this method attractive and a useful contribution for oxidation of alcohols (Scheme 1)



Scheme 1. Oxidation of alcohols to corresponding carbonyl compounds

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Synthesis of nano copper oxide, a π-type semiconductor

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Copper oxide nanostructures have attracted significant attention because of their wide range of application such as high-Tc superconductor sensor, catalytic, optical, electrical, giant magnet resistance materials, gas sensors, solar energy transformation and preparation of organic-inorganic nanostructure composites.[1] CuO is a π-type semiconductor with the band gap~1.7 ev.[2] Further it can be used as an antimicrobial, antibiotics and antifungals agent when incorporated in coating, plastics, and textiles. Copper and copper-based compounds are efficient biocides properties, which are generally used in pesticide formulations and several health related applications.[3] Different methods available to prepare CuO nano particles namely sol-gel technique, sonochemical, alkoxide based route, electrochemical methods, precipitation-pyrolysis, microwave irradiations, solid-state reaction method, and thermal decomposition of precursor.[4]
A nano-sized Cu(II) complex (1), was synthesized by sonochemical irradiation. Compound 1 was characterized by some spectroscopic methods. To prepare the nanostructure of compound 1, two different concentrations of initial reagents, 0.01 and 0.05 M, were tested. Appropriate nano-sized compound 1 was obtained at both of concentrations. Particle sizes of the nanoparticles depend on the concentrations of initial reagents. Results show a decrease in the particles sizes the concentrations of initial reagents is decreased. Calcination of compound 1 at different sizes produced nanoparticles of CuO. The XRD pattern of the residue showed the obtained pattern matches with the standard pattern of CuO with the lattice parameter (a = 4.6883(4) Å, b = 3.4229(2) Å, c = 5.1319(3) Å, S.G. = C2/c and z = 4) which is the same as the reported values (JCPDS card number48-1548). SEM images show the complex with smaller size resulted residue with less size and better morphology.

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Synthesis and characterization of a new unsymmetrical Schiff base ligand and its Ni(II) complex

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The design and synthesis of suitable multi dentate ligands provide a significant contribution for the development of coordination chemistry, where a class of ligands having the azine fragment (C=N-N=C) appears to be of a very important type. Between the two nitrogen atoms of the C=N-N=C fragment only one (which comes from the condensation) takes part in complex formation in the majority of cases.[1] Hydrazones have wide applications in the field of analytical and medicinal chemistry and exhibit physiological activities in the treatment of several diseases such as tuberculosis. This activity is attributed to the formation of stable chelatecomplexes with transition metals which catalyze physiological processes.[2]

In view of the foregoing discussion and the continued interest in coordination chemistry, our present work manifests the preparation of a new unsymmetrical Schiff base ligand and its Ni(II) complex. In the first step, we have prepared the new unsymmetrical N_2O ligand functionalized with NH_2 groups by Schiff condensation of hydrazine with 2-hydroxy-1-naphtaldehyde. In the second step, the NH_2-functionalized compound was made to react with 5-(4-NO_2-phenyl)-azo-salicylaldehydefor producing the resultant ligand (Fig.1). The new ligand was characterized by IR, ^{1}H NMR, UV–Vis absorption and elemental analysis. Furthermore, a new complex of Ni (II) was also obtained by direct reaction of Schiff base ligand and Ni(II) ion in THF. The resultant complex was identified via IR and UV-Vis spectroscopy and C, H, N elemental analysis.

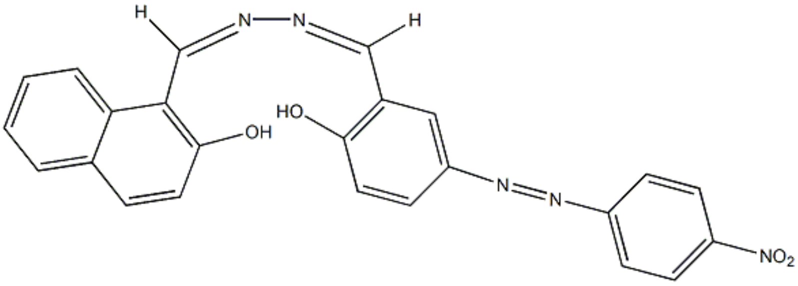

Fig.1. Structure of ligand

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Synthesis and characterization of thiosemicarbazone-based unsymmetric Schiff base ligand and its Fe(III) complex

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Thiosemicarbazonesare versatile ligands of considerablesignificance with respect to their variable coordination behavior, biological properties, physico-chemical properties of also catalytic activity of their transition metal complexes.[1,2] For instance, some iron(III) complexes of thiosemicarbazone-based ligands show antitumor activity by inhibiting ribonucleotide diphosphate reductase.[3] Moreover, to date a number of colorimetric and also fluorescent receptors based on thiosemicarbazone have been reported which are capable to detect transition metal ions in organic and aqueous media.[3]

We report here synthesis and characterization of a new unsymmetric thiosemicarbazone-based azo-azomethine ligand, H_2L, by condensation reaction of an ethyl derivative of azo coupled thiosemicarbazide with 4-chloro-2-amino phenol in ethanol. The prepared ligand was characterized using NMR, IR and UV-Vis spectroscopic methods as well as Mass spectroscopic data. Furthermore, a new Fe(III) complex was also prepared via direct reaction of H_2L with$FeCl_3$ in ethanol. The resultant complex was identified via IR and UV-Vis spectroscopy aswell as elemental analysis.

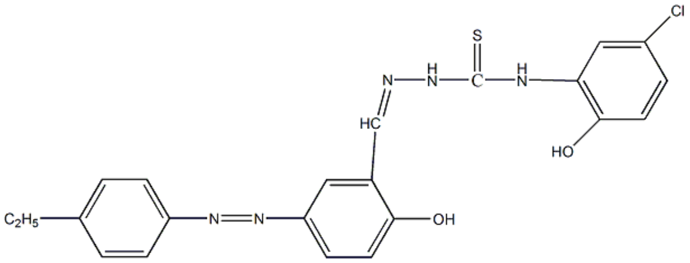

Fig.1. Structure of H_2L

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Synthesis and Characterization of a Series of Copper-Complexes with N, N′, N″ Schiff Base Ligands

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In this work, we present syntheses of some coordination polymers by employing of two flexible N-bridging ligands, (E)-N-(pyridin-2-ylmethylene)-1-(pyridin-3-yl)methanamine (L_1), and (E)-N-(pyridin-2-ylmethylene)-1-(pyridin-4-yl)methanamine (L_2). The use of unsymmetrical chelating and bridging ligands for the construction of discrete macrocycles and/or coordination polymers are less common.[1,2] Herein, we synthesized and used these ligands to construct discrete macrocycles and coordination polymers with Cu(I), Cu(II), namely, $[Cu_2(L_1)(PPh_3)_2I_2]_2$ (1), $[Cu_2(L_2)(PPh_3)_2I_2]_n$ (2) and $[CuL_1(NO_3)_2]_2$ (3). Compounds 1 and 2 were prepared by reaction of the ligands (L_1 and L_2) with PPh_3 and copper(I) iodide. $[CuL_1(NO_3)_2]_2$, (3) is prepared by reaction of L_1 with $Cu(NO_3)_2.3H_2O$.The compounds were characterized by elemental analysis, spectroscopic methods (IR, UV/Vis, TG/DTA) and X-ray crystallography. X-ray structural analysis of compound 1 reveals the formation of a centro symmetric tetra nuclear compound. The repeat unit of coordination polymer 2 comprises a Cu_2I_2 unit with a triphenylphosphane substituent on Cu1 and linked to an adjacent Cu_2I_2 unit by the ligand L_2 that acts as a bridge. 3 exhibits a common metallo-cyclophane$[M_2(L)_2(NO_3)_4]$ skeleton. Two Cu^{2+}cations linked by two L_1 ligands that chelate to each metal atom through the imine nitrogen (or amine nitrogen) atoms and the nitrogen atom of the 2-pyridyl ring and bind to the other metal atom of the pair via the nitrogen atoms of the 3-pyridyl ring for 3.

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Synthesis and Characterization of a New Zn(II) tetrazolate Framework and its Conversion to Nano/MicroZnO Structures by Hydrothermal Conditions

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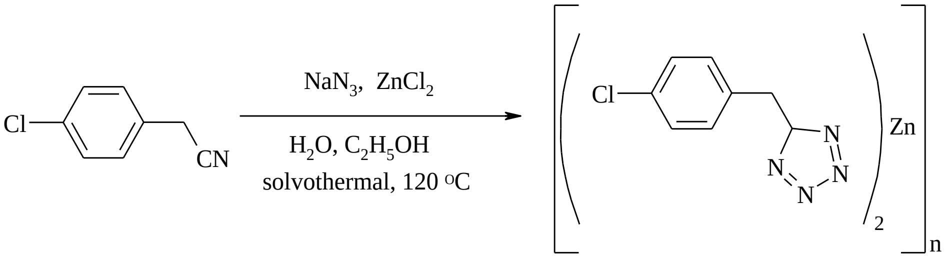
In this work we synthesized a tetrazole based Zn(II) metal organic framework, $[Zn(L)_2]n$ (1),(L=5-(4-Chlorobenzyl)tetrazolate) by in situ reaction of 4-chlorobenzeneacetonitrile, NaN_3 and $ZnCl_2$ under hydrothermal conditions. The compound was structurally characterized by elemental analysis, IR, and single crystal X-ray diffraction. Crystal structure of this compound reveals that this compound has a 2D network structure. Furthermore, thermal analysis and luminescence properties of this compound have been studied. Utilization of metal-organic frameworks to generate nanometal and metal oxides may be an affordable approach.[1-3] However, direct transformation of coordination polymers into metal nano and microstructures under hydrothermal conditions is an unexplored area. Thus, we used this coordination polymer to fabricate nano/micro ZnO crystals under some different hydrothermal conditions, which resulted in different morphologies (nanoplats, 3D flower-like ZnO microstructures composed of nanosheets, nanowires and nanorods) of ZnO Structures. The effects of reaction temperature and pH on the growth process and morphology of ZnO nano and microstructures were investigated. The obtained nano/micro structures have been characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy (EDX).



Scheme 1. Syntheses of coordination polymer

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Synthesis and characterization of dioxomolybdenum(VI) complex with an ONO Schiff base ligand and its application as a catalyst for epoxidation of olefins in water as a green solvent

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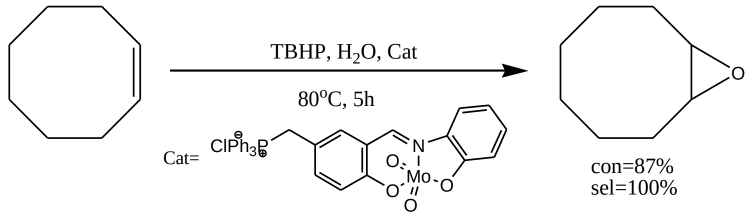
The search for broadly applicable metal catalysts operating in the aqueous phase is a research area of high interest.[1] Catalytic olefin epoxidation in the aqueous phase is an important topic for the synthesis of fine chemicals.[2] Among all kinds of epoxidation catalysts, metal-Schiff base complexes, especially molybdenum(VI) tridentate Schiff base complexes, have been proved to be efficient catalysts towards the substrate reactions.[3]

New dioxomolybdenum(VI) complex has been synthesized by reacting N-hydroxyphenyl-[5-(triphenylphosphonium)methyl] salicylidene amine chloride (PPh_3-H_2sap) as a water soluble ligand and $[MoO_2(acac)_2]$ in ethanolic solution. The water soluble ligand (PPh_3-H_2sap) was prepared by reaction of 2-aminophenol with (3-formyl-4-hydroxybenzyl) triphenylphosphonium chloride as a water soluble salicylaldehyde derivative. The resulting complex with the formula $[MoO_2(PPh_3$-$H_2sap)]$, was characterized by elemental analyses, ^{1}H NMR, ^{31}P NMR, IR, X-ray crystallography, UV-Vis spectroscopic studies. This complex was tested as a catalyst for the homogeneous epoxidation of olefins in water as a green solvent, using *tert*-butyl hydrogen peroxide (TBHP) as an oxidant. The catalytic system shows efficient reactivity in the olefins epoxidation reactions giving high yield and selectivity under atmospheric conditions, in most cases.



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Investigation of Hydrogen bond within some Fe and Ni complexes: A DFT study

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The formation of intramolecular hydrogen bond (H-bond) has very pronounced effects on the molecular structure and properties. Herein, the physicochemical properties of some Fe, and Ni complexes considering to the intramolecular hydrogen bonds investigated with the aid of DFT calculations.They are (**1**) [Ni(dmg)$_2$], (**2**) [Fe(dmg)$_2$], (**3**) FeCl$_2$ (hppH)$_2$, and (**4**) NiCl$_2$(hppH)$_2$]. Geometry optimization, vibrational frequency, and UV calculations for the mentioned complexes performed using Gaussian 09 at the DFT/B3LYP level with LANL2DZ and 6-311g(*d*,*p*) basis sets for metal and other atoms, respectively. The optimized structures have good agreement with the experimental ones. Because of more electronegativity and effective nuclear charge of Ni than Fe, its complexes should have intensity and lower energy of ligand to metal charge transfers (LMCTs) with higher wave lengths. The same notes could be derived from comparison of the H-bonds in **1** and **2**. More electronegativity of Ni in **1** makes the related H-bond (Ni–O–H···O, 1.20580 Å) shorter because of better donor (O) and acceptor (O) of H-bond and lower energy of LMCT than in **2**. wave lengths of the atoms involved in the mentioned H-bonds are 294.13 and 279.28 nm in **1** and **2**, respectively. The same conclusion could be extracted from the comparison of the electronic transitions and H-bond in **3** and **4**. The lower energy of LMCT in **3** (219.15 nm) than **4** (217.32 nm) with the shorter H-bond length in **3** (Fe–N–H···Cl, 2.22408 Å) than in **4** (Ni–N–H···Cl, 2.29832 Å) confirm the above discussion. So we can conclude that difference of ligand and/or donor atoms of ligand could affect on charge transfers and structural changings of compounds like H.bond lengths and power. As mentioned, more changing of LMCT wave lengths between **1** and **2** in comparison of **3** and **4** along with the more changing of H-bond lengths.

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Synthesis and characterization of tungsten (VI)-oxodiperoxocomplex with a oxazine ligand and its application as a catalyst for oxidation of sulfide to sulfoxide

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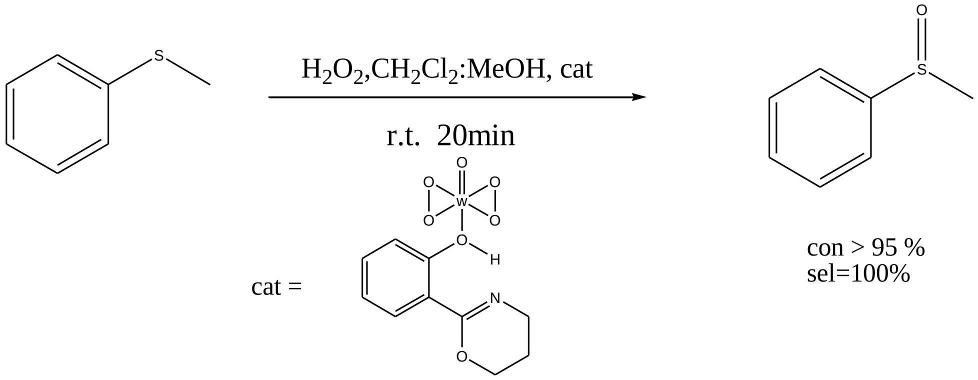
The application of transition metal complexes as catalysts in selective oxidation of sulfides to sulfoxides is important for producing sulfoxides as chemical intermediates to afford useful chemicals.[1] The chemistry of transition metal oxido–peroxido complexes has received special attention due to their importance in industrial, pharmaceutical, and biological processes.[2]



New tungsten(VI) complex has been synthesized by reaction of oxazine [3] as a ligand with tungsten(VI)oxodiperoxo in ethanolic solution. The oxazine ligand was prepared by reaction of 2-amino-1-propanol with methyl salicylate. The resulting complex with the formula of $[WO(O_2)_2(oxazine)]$, was characterized by elemental analyses, ^{1}H NMR, IR, UV-Vis spectroscopic studies. This complex was applied as an efficient catalyst for the homogeneous sulfide oxidation in solvent mixtureMeOH:CH_2Cl_2, using hydrogen peroxide as an oxidant in room temperature. Our catalytic system exhibits high catalytic activityin the sulfide oxidation reactions in terms ofhigh yield and selectivity.

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Design and synthesis of a novel colorimetric dipodal receptor for detection of Copper(II) ion in aqueous media

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Development of artificial receptors for colorimetric recognition of metal ions is a vibrant area of present day investigation due to the widespread applicability in the field of biochemistry and environmental science.[1] Among the various metal ions, copper(II) is the third most plentiful transition metal ion in human body and implicated in several physiological responses.[2] Thus for, numerous technologies have been developed for the detection of copper(II) ion at trace quantity levels including atomic absorption spectroscopy, inductively coupled plasma emission or mass spectrometry, X-ray photoelectron spectroscopy, surface-plasmon resonance detector and voltammetry. However, these methods are usually complicated, time-consuming and costly as a consequence of need for highly sophisticated instrumentation.[3] To overcome the previous drawbacks, we have developed a novel colorimetric azo-imine receptor (**1**), based on the combination of 2,6-pyridinedicarbohydrazide and azo-coupled salicylaldehyde scaffold. The devised receptor was found to exhibit a remarkable selectivity and sensitivity to Cu^{2+} as evidenced by an immediate color change in aqueous media. Importantly, the new copper(II) complex has been elucidated by spectroscopic methods (IR and UV-Vis) as well as elemental analysis and MALDI-TOF mass analysis. Successfully, the current receptor can detect Cu^{2+} ions even at 0.47 μM level, which is much lower than the World Health Organization (WHO) permissible level (30 μM) in drinking water.

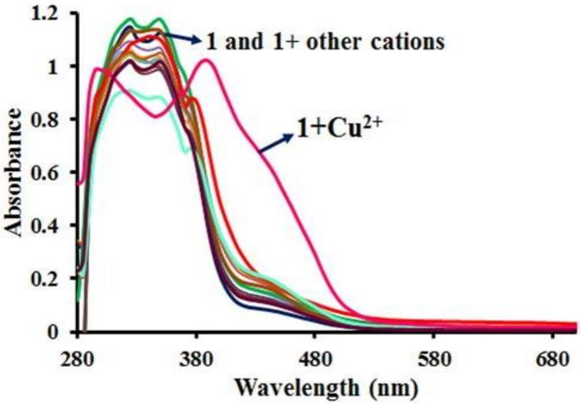

Fig. 1. UV-Vis absorption spectra of **1** in the presence of 3 equiv. of different cations.

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High dispersed platinum on layered manganese oxide as water-oxidizing catalysts

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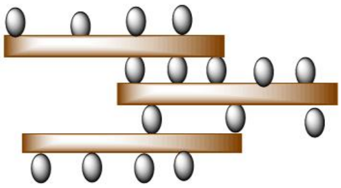
Mn oxides are environmentally friendly and cheap compounds for energy-issue concerns acting as super capacitors,[1] being catalysts in water oxidation[2] and finding applications in batteries.[3] Mn oxides can be prepared with different defects, morphology, porosity, textures which are flexible, with a wide diversity of crystal forms. In addition to bulk, Mn oxides can also be prepared as supported, colloidal and nano-sized forms with high surface areas, and also as composites with other materials. Mn oxide and platinum form interesting composites with promising applications. There are many strategies to increase efficiency of Mn oxide toward water oxidation. Among these strategies, some groups reported that platinum or gold significantly increases catalytic activity of Mn oxide toward water oxidation. Herein we report a new method to synthesize high dispersed platinum on layered manganese oxide. The nanocomposite was characterized by scanning electron microscopy, energy dispersive spectrometry, high-resolution transmission electron microscopy, X-ray diffraction, Fourier transform infrared spectroscopy, X-ray Photoelectron Spectroscopy, and atomic absorption spectroscopy. Then, we investigated the role of platinum nanoparticles on water-oxidizing activity of nanolayered manganese under the presence of cerium(IV) ammonium nitrate as a non-oxo transfer oxidant. The water-oxidizing activities of these composites with other previously reported Mn oxides are compared and also the important factors influencing the water-oxidizing activities of Mn oxides are discussed.



Scheme 1 The schematic structure of platinum/ manganese oxide.

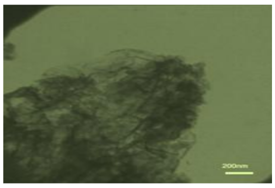


Fig. 1. TEM for platinum on layered manganese oxide.

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Synthesis of bis 2-(2-hydroxyphenyl)-2-oxazoline-Ni(II) complex and investigation of its catalytic activity in C-C coupling reaction

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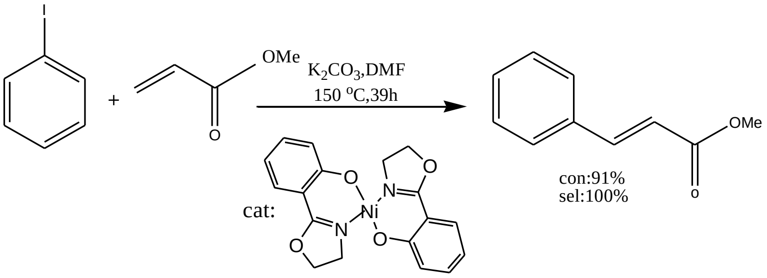
The Mizoroki–Heck reaction has become one of the most useful carbon–carbon bond-forming reactions in organic synthesis.[1, 2] The reaction has been applied to many areas, including bioactive compounds, natural products, drug intermediates, fine chemicals synthesis,UV absorbers, antioxidants and industrial applications.[3]



In this study a new oxazoline-nickle(II) complex has been synthesized by reaction of oxazoline ligand and [Ni($CH_3COO)_2.4H_2O$] in methanolic solution. The resulting complex [Ni(2-(2-hydroxyphenyl)-2-oxazoline)$_2$], was characterized by elemental analysis, ^{1}H NMR, X-ray crystallography, and UV-Vis spectroscopic studies. This complex was applied as an efficient catalyst for the homogeneous Heck reaction of arylhalides with olefins such as methylacrylate. This catalytic system exhibits high catalytic activity in the Heck reactions in terms of high yield and selectivity. For example in reaction between iodobenzene and methylacrylate; which is observed in present scheme, (E)-methyl cinnamate was produced in 91% yield after 39 hours.

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Rational design of a novel diaminomaleonitrile based chromogenic receptor for detection of Zinc(II) ion in aqueous solution

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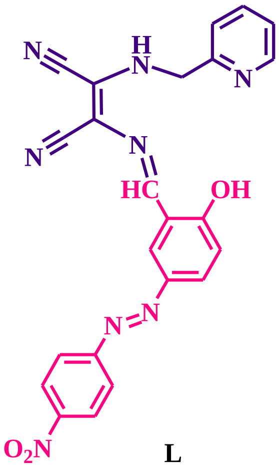
Design and also construction of artificial molecular receptors for selective recognition of metal ions has been an area of immense research interest over the past few decades due to wide spread applicability in the field of biology and environmental science.[1] Zinc(II), as one of the most abundant andessential trace element in the human body, plays pivotal roles invarious fundamental biological processes, such as cellular metabolism, energy generation, oxygen transport, gene expression, neurotransmission and regulation of metalloenzymes.[2] Here in, a novel azo-azomethine based chromogenic receptor (**L**) containing diaminomaleonitrile fragment and pyridine ring has been designed and synthesized. The designed receptor was found to show a remarkable sensitivity to Zn^{2+} as evidenced by an immediate color change from light green to orange in aqueous media. Importantly, the result ant zinc complex has been identified by spectroscopic methods (IR, ^{1}H NMR and UV-Vis) as well as elemental analysis. Successfully, the current receptor can recognize Zn^{2+} ions even at 0.43μM level, which is much lower than the World Health Organization permissible level.



L

Fig. 1. Structure of receptor **L**.

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In situ generation of highly active n-heterocyclic carbine complexes of palladium in Heck reactions

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Heck reactions, typically catalyzed by palladium complexes in solution, are of growing interest in organic and fine-chemical synthesis. Expensive and often sensitive ligands are necessary to activate palladium and to stabilize it against agglomeration (palladium-black formation).[1] The efficient activation of aryl chlorides, which are of particular interest for industrial applications remains a serious challenge that can only be overcome by some homogeneous system. Genuinely ligand-free, palladium/activated carbon catalysts convert bromo benzene with similarly high activity.[2] Herein we report 1,3-bis(3-methyl imidazolium-1-yl) benzene (Figure1) bromide/palladium catalytic system successfully catalyzes the Heck coupling reaction of aryl chlorides as well as aryl bromides with acrylates to give the corresponding olefins in reasonable yields. The results of Heck reaction exhibited a high selectivity (99/1) favoring the transproduct.It is clear that the natureof the ligand play an important role in determining the catalytic activity and selectivity. The use of multi functional ligands gives advantage as high capacity chelating molecules for the stabilization of catalytic active species during the catalytic process, which manipulate the activity of the catalyst. Also, increasing the rigidity of the supporting ligand decreases the number of the possible conformations of the metal–ligand assembly, thus leading to improved selectivity.

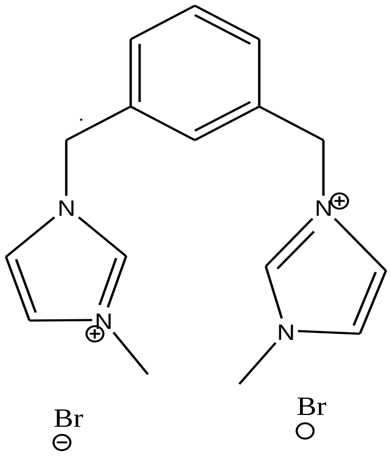

Figure1. 1, 3-bis(3-methyl imidazolium-1-yl)benzene

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Theoretical mechanistic study of reaction of a six-membered cycloplatinated(II) complex with MeI

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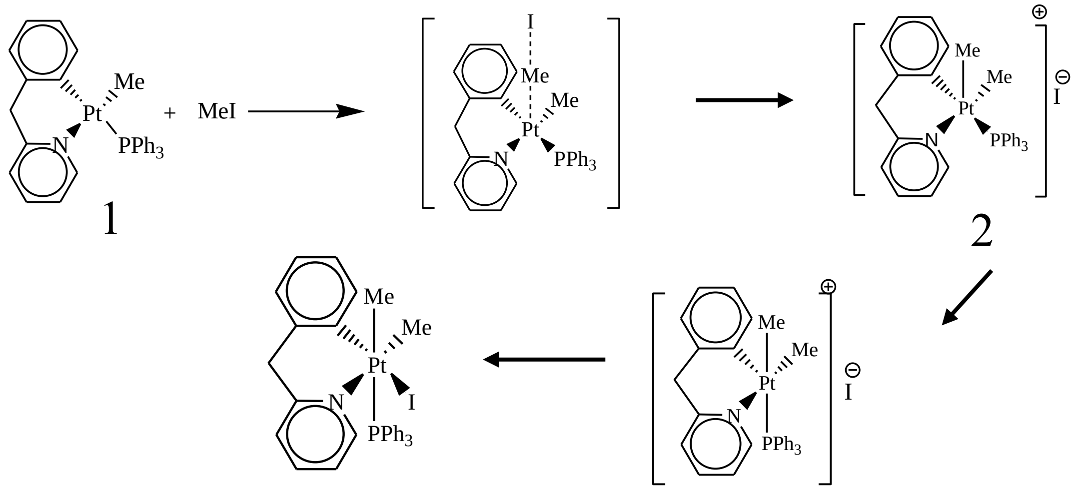
Cyclometalated platinum complexes, in particular those involving 2-phenylpyridinate and benzo[*h*]quinolate, are interest due to their potential applications in optoelectronic devices and catalytic processes such as oxidative addition reactions. [1-3] The oxidative addition reaction of MeI to the $[PtMe(bzpy)(PPh_3)]$, **1,** complex (bzpy = 2-benzylpyridine) was theoretically investigated using density functional theory calculations to gain more insight into the mechanism of the reaction, as well as to try and determine the geometry of the transition states and energy barriers (see scheme). The DFT study suggested the formation of transition states including Pt…C(MeI)…I fragment, followed by the formation of the ionic five-coordinate $[PtMe_2(bzpy)(PPh_3)]^+I^-$, **2,** intermediate with the incoming CH_3 group in the apical position and with the iodide ion out of coordination sphere of Pt center. The DFT studies were in agreement with the experimental finding.



Scheme

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Synthesis, Characterization and Spectral Study of Diaminomaleonitrile-based Unsymmetric Ligand and its Ni(II) Complex

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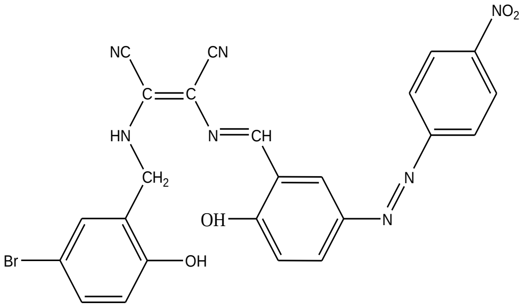
Ever since, diaminomaleonitrile (DAMN) and its derivatives, as intermediates, have been extensively utilized in the synthesis of various type of heterocyclic compounds. [1] In the other hand, unsymmetric DAMN-based Schiff-base ligands and their transition metal complexes have been extensively studied for their interesting physico-chemical properties as well as their potentially catalectic activities. [2]

In the present work, new unsymmetric diaminomaleonitrile-based azo-azomethine ligand **(H_3L)** has been synthesized via condensation reaction of 2-amino-3-((5-bromo-2-hydroxybenzyl) amino) maleonitrile with 2-hydroxy-5-((4-nitrophenyl)diazenyl)benzaldehyde in methanol solution. The prepared azo ligand has been characterized by elemental analysis, IR, UV-Vis and ^{1}H NMR spectroscopic methods. Furthermore, the solvatochromic behavior of the ligand was studied by UV-Vis spectroscopy. Also, a new Ni(II) complex was also prepared by reaction of **(H_3L)** and $Ni(ClO_4)_2$. $6H_2O$ in $CHCl_3$/ MeOH. The prepared complex was characterized by elemental analysis, IR, UV-Vis spectroscopy. The thermal properties and also antimicrobial activities of the prepared ligand and its corresponding complex were studied.



Scheme1. Structure of the ligand **(H_3L)**

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Synthesis and characterization of a new unsymmetric Diaminomaleonitrile-based Azoimine ligand and its Copper(II) complex

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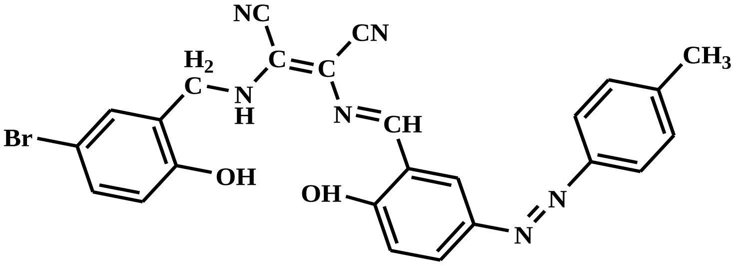
During the past decades, considerable attention has been drawn to wards the synthesis of azo-azo methine ligands. These compounds can be advanced into materials for nonlinear optics, optical storage media, chemosensors, liquid crystals, photochemical molecular switches, nanotubes andin manufacture of protective eye glasses and filters[1]. Moreover, transition metal complexes of azoimine compounds have been targeted because of their impressive chemical and physical properties.[2] Also, the reduced Schiff base ligands provide suitable conformational and coordination environments for the metal ions.[3] In this regard, we have developed a new unsymmetric azoimine ligand (**H_3L**) via condensation reaction of 2-amino-3-((5-bromo-2-hydroxybenzyl)amino) maleonitrile with 2-hydroxy-5-(p-tolyldiazenyl) benzaldehyde in methanol solution. The target ligand was proposed in accordance with the elemental analysis, ^1H NMR, IR, UV-Vis spectral data.Also, the solvatochromism behavior of this ligand was studied by UV-Vis spectroscopy. Furthermore, a new complex of Copper(II) was also obtained by direct reaction of (**H_3L**) and Copper(II) perchlorate in chloroform. The Cu(II) complex was characterized by elemental analysis, IR, UV-Vis and MALDI-TOF mass analysis. The thermal properties and also antimicrobial activities of the prepared ligand and its corresponding complex were studied.



Scheme1. Structure of the ligand **H_3L**

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Crystal structure and spectroscopic properties of trinuclear manganese complex

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The investigation of high-nuclearity metal clusters continues to be of considerable interest because they represent nice systems that span both quantum and classic phenomena[1]. The chemistry of transition metal complexes of hydroxy (aryl-OH and alkyl-OH) rich molecules containing imine/amine groups is important in the biomimetic studies of metalloproteins. Coordination and biomimetic chemistry of these molecules have taken lead position in the recent literature at least in case of a few metal ions, such as, vanadium, manganese, iron and molybdenum[2,3]. Up to now, a great number of mixed-valence manganese clusters have been synthesized and their magnetic properties have been widely studied, mainly because they often exhibit large and sometimes abnormally large spin values in the ground state (S) and a negative uniaxial anisotropy (D) arises from the presence of Jahn–Teller distorted Mn(III) ions[4]. In this research we report synthesis, characterization and spectroscopic properties of a New trinuclear manganese complex with Schiff baseligand, $[Mn_3(L)_2(\mu\text{-OAc})_4]{\cdot}CH_3OH$ (**1**), where H_4L is 2-(hydroxymethyl)-2-{[(1E)-(2-hydroxy-1-naphthyl)methylene]amino}propane-1,3-diol. H_4L was synthesized by the reaction of 2-hydroxy-1-naphthaldehyde and Tris(hydroxymethyl) aminomethanein methanol. The reaction was reflux at 70°C for 4 hours and the resulted white precipitates were filtered off and washed with cold methanol. This ligand was characterized by elemental analysis and spectroscopic methods (IR, NMR, UV-Vis). Trinuclear Mn complex (**1**) has been synthesized by the reaction of $Mn(OAC)_2{\cdot}6H_2O$ with H_4Lin methanol. The spectroscopic properties of complex **1** were studied by IR, NMRand UV-Vis methods. X-ray analysis indicated that compound **1** is a trinuclear manganese complex that containing Mn(II)–Mn(III) cores. The central Mn(II) ion and two outer Mn(III) ions connected by acetate and alkoxide bridging groups and the Mn(III)–Mn(II)–Mn(III) angle is close to linear arrangement (~160°). The Mn(II)/Mn(III) separation is about 3.21° A. The central and external Mn ions have distorted six coordinated octahedral coordination environments.

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Synthesis and X-ray structure of trinuclear Co(II) complex with polyamines

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Polyamines form an important class of compounds due to the roles in biological systems and their applications for the detection of metal ions and metal ion complexation.[1] Metal complexes of polyamine ligands have been used in many areas of inorganic to bioinorganic chemistry[2-3]. Transition metal complexes of polyamines ligands have been used as model for metalloenzymes, as luminescence materials, as catalyst, in molecular electronics, and in coordination polymer chemistry [4].

In this research we report synthesis, characterization, crystal structure and spectroscopic properties of a new trinuclearcobalt(II) complex with polyaminesligand (H_4L), $[Co_3(L)(\mu\text{-}N_3)_2(N_3)]$ (**1**), where H_4L is 2,2'-{ethane-1,2-diylbis[[2-(2-hydroxyphenyl) imidazolidine-3,1-diyl]ethane-2,1-diylnitrilo (E)methylylidene]}diphenol. H_4L was synthesized by the reaction of pentaethylene hexamine with salicylaldehyde in methanol. The reaction mixture was refluxed for 48 hours and the resulted white precipitates were filtered off and washed with cold methanol. This product was characterized by elemental analysis and spectroscopic methods (IR, NMR, UV-Vis). Trinuclear Co(II) complex (**1**) has been synthesized by the reaction of $CoCl_2 \cdot 6H_2O$, H_4L and NaN_3in methanol. Dark brown crystal of complex 1 was obtained by slove evaporating of methanolic solution during one week. The spectroscopic properties of complex **1**were studied by IR, NMR and UV-Vis spectroscopic methods. In the IR spectrum of complex the strong peak at about 2090 cm^{-1} is due to the presence of N_3 and indicates the azide is coordinated to the metal core. The UV-Vis spectrum of complex shows intraligand and LMCT transitions. The structure of complex **1** was determined by X-ray analyze and showed that this compound is a trinuclear complex of Co(II) which the azide ligands act as bridging groups and connect the cobalt ions in end-to-on (EO) mode. The coordination environment around cobalt atom is distorted octahedral.

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Synthesis and characterization of new compounds of ferrocenylboronic ester

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Boronic esters with general structure $RB(OR)_2$ are derivatives of boronic acids $RB(OH)_2$, containing carbon-boron bond, belonging to the class of organoborane compounds. They are conveniently prepared by condensation reaction of boronic acid and alcohol.[1]

Boronic esters have various applications[2,3] such as: using as antibacterial agent, as catalyst in classical reactions, e.g., Suzuki coupling, addition und cyclo addition reactions, using as sensor and etc. We report here on the synthesis of new derivatives of ferrocenylboronic ester **3** and**6**. At first, we synthesized the parent compounds: acetylferrocene **1**/α-hydroxyethylferrocene **2** and1,1′-diacetylferrocene**4**/1,1′-bis(α-hydroxyethyl)ferrocene**5** and also dibromoborylferrocene ($FcBBr_2$, Fc=ferrocene). By the deprotonation of the compounds **2** and **5** with n-butyllithium (n-BuLi) under argon atmosphere and further reaction with $FcBBr_2$ were obtained the new compounds of bis(1-ferrocenylethoxy)ferrocenylborane**3** and 1,1′-bis(ferrocenylethoxy)-ferrocenylborane**6**. All compounds are characterized by ^{1}H, ^{13}C- and ^{11}B-NMR-spectroscopy. The ^{11}B-chemical shift of **3** and **6** showed a broad signal at $\delta = 29$ and 32 ppm repectively, as expected for such compounds.

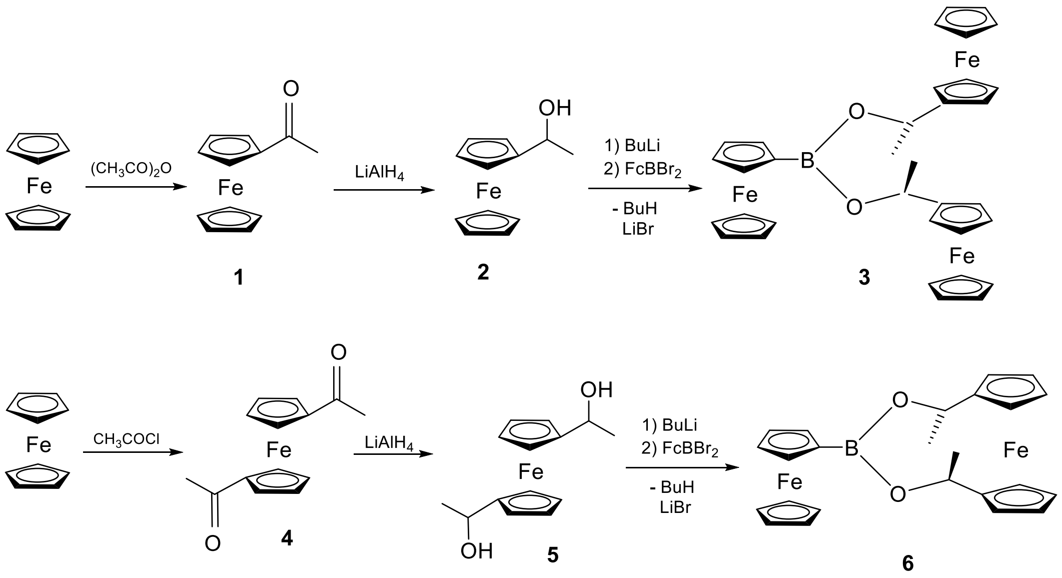

Fig. 1. Synthesis of new organoborane compounds based on sandwich complex of iron (Fe^{II}).

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New *cis*-dioxomolybdenum(VI) complex of tridentate Schiff base ligand derived from nicotinic acid hydrazide:Synthesis, spectral characterization and crystal structure studies

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The expanded research in molybdenum complexes is mainly due to its biochemical role in metalloenzymes and its rich chemistry. Molybdenum is the only element of the second transition metal series that is essential for life. It is the only element from second transition series which occurs in the biologicalsystem.[1] Molybdenum biochemical role is based on its ability to facilitate electron exchanges and to form stable complexes with oxygen-, nitrogen- and sulfur-containing ligands. In combination with oxo and imido ligands, molybdenum plays a very important role in catalytic chemistry[2] and biochemistry of molybdenum.[3]

A new hydrazone Schiff base has been prepared and characterized by elemental analyses, spectroscopic methods, and single crystal X-ray diffraction. The corresponding *cis*-dioxomolybdenum(VI) complex was synthesized with tridentate Schiff base ligand derived from 5-bromosalicylaldehyde and nicotinic acid hydrazide. This complex was characterized by ^{1}H NMR, ^{13}C NMR, IR and its solid state structure was determined using single crystal X-ray diffraction. The hydrazone ligand coordinates to Mo through the phenolate O, imine N, and enolic O (Fig 1).

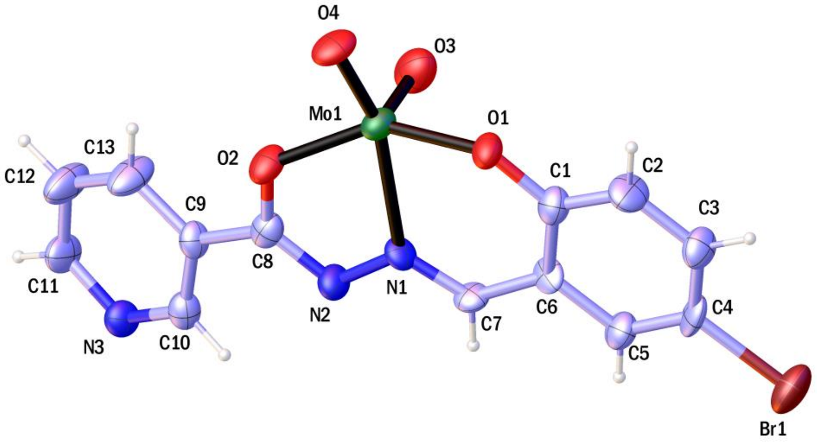

Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

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Optimization of effective parameters to the synthesis of tetraacetyldibenzylhexa-azaisowurtzitane (TADB) from hexabenzylhexaazaisowurtzitane (HBIW) over Pd supported on MWCNTs using design of experiment

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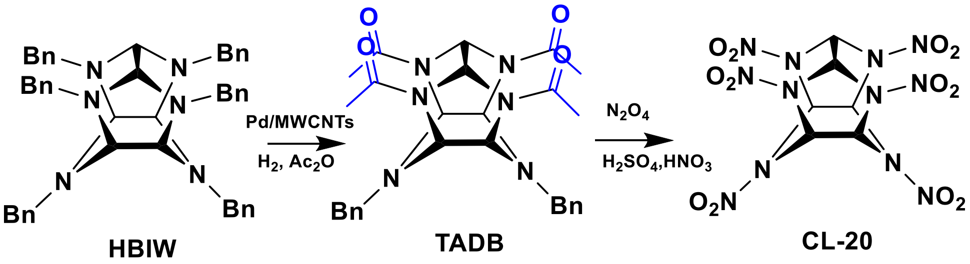
Recent investigation of the design and synthesis of explosive have focused on the nitramine with significantly higher energy and density. Hexanitrohexaazaisowurtzitane (CL-20) is the outstanding caged nitramine applicable in both explosive and propellant. Tetraacetyldibenzylhexaazaisowurtzitane (TADB) is one of the intermediates in the preparation of CL-20 (scheme 1). TADB is synthesized via reductive N-debenzylation of hexabenzylhexaazaisowurtzitane (HBIW) over palladium supported on activated carbon catalyst[1]. Herein, we optimized parameters affecting on hydrogenolysis N-denenzylation reaction over Pd supported on functionalized multi-walled carbon nanotubes (MWCNTs)[2] by using design of experiment (fractional factorial design method in the first step to screen important factors and response surface methodology using a central composite design in the last step). Among the MWCNTs without any functions, carboxylated-MWCNTs and hydroxylated-MWCNTs, the hydroxylated ones have been shown the best results. The reaction yield was promoted to 76% in the optimized reaction condition.



Scheme1. Synthesis of CL-20.

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Synthesis and Characterization of Mn(II) and Pd(II) Complexes of Bis(picolyl amine) and Bis(phenol) amine Ligands Supportedon Ordered Mesoporous Silica (SBA-15)

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In coordination chemistry, various ligands are used to modulate the electronic and steric properties of the metalion and consequently the reactivity of metal species.[1]As homogeneous catalysts are mostly often difficult to separate forreuse after reactions, the immobilization of a homogeneous catalyst onto a solid surface is one of the major challenges in catalysis chemistry. By loading these complexes onto mesoporous materials, one can achieve fixed homogeneous catalysts, which facilitates the separation and reuse of valuable catalysts, able to reduce both environmental pollutions and material costs. Covalent bond grafting is one of the most important strategies which have been developed for loading of such molecular catalysts.[2,3] In our work, new Mn(II) complex of bis(phenol)amine ligand and Pd(II) complex of bis(picolyl amine) ligand supported on functionalized SBA-15 were synthesized.The precursor and supported complexes were characterized by different techniques such as: FT-IR, TGA, SEM, TEM, EDX, XRD, ICP, CHN and porosimetry. All results confirmed the successful anchoring of complexes onto the functionalized SBA-15 by covalent bonding.

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Study of Hydrogen bond in some Fe and Ni complexes with NMR and NBO calculations

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In the present work we study geometry optimization, NMR, and NBO calculations for the (**1**) [Ni(dmg)$_2$], (**2**) [Fe(dmg)$_2$], (**3**) $NiCl_2(hppH)_2$, and (**4**) $FeCl_2(hppH)_2$ complexes performed using Gaussian 09 at the DFT/B3LYP level with LANL2DZ and 6-311g(*d*,*p*) basis sets for metal and other atoms, respectively. Structural changing (e.g. H. bond length) could discussed by NMR data such as nuclear chemical shift. Because of more electronegativity and effective nuclear charge of Ni than Fe, it pulls more electronic charge through H. bond (M–O–H···O and M–N–H···Cl) resulted to more shielding of metal center in **1** (-3076.84 ppm) and **3** (-7557.61 ppm) comparison to **2** (2473 ppm) and **4** (-20682.1 ppm), respectively. The inverse data within chemical shifts of H. bond donor atoms (O and N) obtained that confirm this trend. Also, as expected H. bond acceptor atoms (O and Cl) show more shielding in **1** (-343.372 ppm) and **3** (102.93 ppm) comparison to **2** (-494.471 ppm) and **4** (416.8 ppm), respectively. Therefore, the related H. bond is shorter in **1** (1.20580 Å) and **3** (2.29832 Å) comparison to **2** (1.63488 Å) and **4** (2.22408 Å), respectively. Moreover, the calculated NBO metal center charges show less electronic density on more shielded centers in **1** (0.766 e) and **3** (0.454 e) than to **2** (0.65 e) and **4** (0.583 e), respectively. These obtained results show good consistency with NMR results.

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Synthesis and Characterization of Bis(phenol) amineLigand Supported on SBA-15 and Investigation of the Catalytic Activity of its Mo Complex in Sulfide Oxidation Reaction

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Supported metal complexes have received a great deal of attention in recent years due to their catalyst enhancement and recyclability.[1] One of the most important ways of heterogenization of metal complexesis their immobilization on insoluble ordered mesoporous silica which provides an elegant solution to the separation and recovery of catalysts.[2] Among this group, complexes supported on SBA-15 have a unique place in catalyst chemistry.[3] In the recent work, a novel molybdenum based catalyst, MoL^{GDC} -AP@SBA-15 has been synthesized by covalent grafting of bis(phenol) amine ligand with chlorine substituent[4] on to functionalized ordered mesoporous silica (SBA-15) followed by complexation with molybdenumsalt. The catalyst was characterized by FT-IR, TGA, SEM, TEM, EDX, XRD, ICP, CHN. Oxidation of sulfides to corresponding sulfones or sulfoxides, in solvent-free conditionor ethanol as a solvent was carried out respectively. The interesting features of this catalytic system include high selectivity, low reaction time, high yield and the efficient use of hydrogen peroxide as a cheap, environmental friendly and readily available oxidant under mild condition (room temperature). The recycling experiment results showed that MoL^{GDC} -AP@SBA-15 could be easily recovered and recycled for four times without loss of the activity and selectivity.

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Melamine Nitrate salt: A new nitration Reagent for the synthesis of HNIW from TADNOIW

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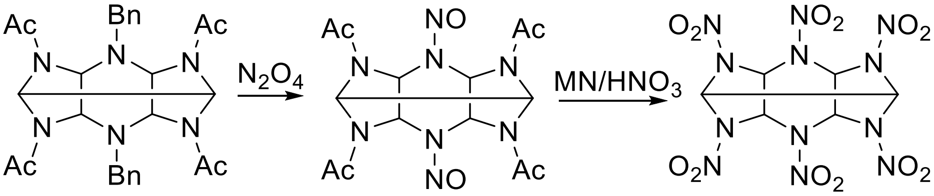
One of the most important new energetic compounds for ordnance applications is 2,4,6,8,10,12-hexanitro hexaaza isowurtzitane (HNIW/ CL-20). The preparation of HNIW is a multistep process which usually consists of condensation reaction of glyoxal with benzylamine to form HBIW (hexabenzylhexaazaisowurtzitane) follows by catalytic debenzylation/ acetylation reactions to generate tetra acetyl dibenzyl hexaazaisowurtzitane (TADB) precursor .[8] Subsequently, HNIW synthesizes by nitrolysis of TADB in the different nitrolysis systems includes: nitrosation (to form tetraacetyldinitrosohexaazaisowurtzitane (TADNOIW)) or formylation (to form tetraacetyl diformyl hexaazaisowurtzitane (TADNOIW)). However, the preparation of HNIW in the final step requires the use of non environmentally friendly mixture of $HNO_3/H_2SO_4$with its drawbacks especially to the industrial scales (scheme 1). In this study, we introduced acid catalyzed nitrolysis of TADNOIW using MN/HNO3 (98%) as new nitrolysis system to the synthesis of HNIW. Melamine nitric acid complex (melaminume nitrate) as a novel and economic nitration reagent was easily prepared by the direct reaction of melamine with nitric acid at room temperature and identified by IR spectroscopy as well as nitrate test (figure 1). This nitrolysis protocol is an environmentally cleaner method, since no emission of mixed acidic disposal occurs.



Scheme 1. Synthesis of HNIW from TADB intermediate.

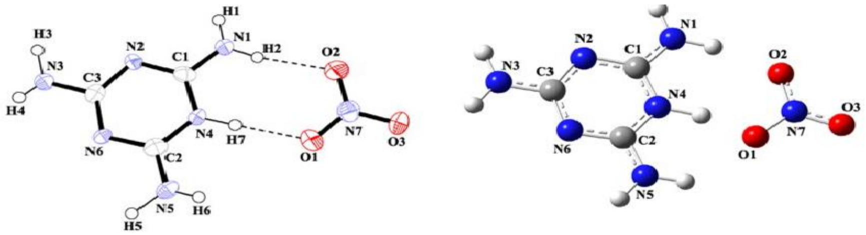


Figure 1. Melamine nitrate complexe.

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Synthesis and characterization of new Schiff Base complexes containing trans-cinnamaldehyde using Gd and La

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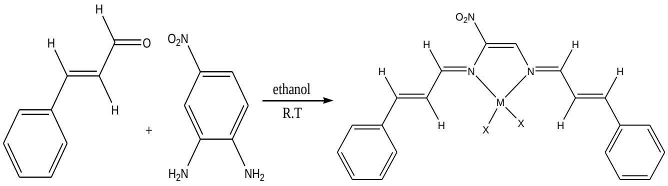
Schiff bases, named after Hugo Schiff [1], and were reported in the 19th century by Schiff (1864). Schiff base ligands with aldehydes are formed more readily than with ketones. [2] Schiff bases generally are bi-, tri-, or tetra- dentate chelate and easily react with almost all transition metals ions and form very stable complexes with them.[3,4] Over the past few years macroacyclic Schiff base ligands have received vital attention not only because of their pharmacological properties, soft-hard donor character and coordination behavior, but also for their capacity for chemical recognition of anions and metals of biochemical and environmental importance. Metal ions have enormous importance in many biological processes, but the increased concentration of metal ions especially heavy metal ions exerts toxic effects on living system. Therefore, separation and determination of metal ions in environmental sources and living organisms play an important role.

Cinnamaldehyde is an aromatic aldehyde and main component of bark extract of cinnamon. The main advantage of cinnamaldehyde is that direct contact is not required for being active as antimicrobial. Cinnamaldehyde has been shown to be active against a range of forborne pathogens bacteria. Nontoxic doses of cinnamaldehyde and cinnamaldehyde derivatives have previously been reported to potentiate the cell-inactivating effect of cis-diamminedichloroplatinum (II) in human NHIK 3025 cells in culture.

In this work new Schiff Base complexes containing cinnamaldehyde unit using Gd and La as template agent were synthesized and then characterized by various methods such as IR, CHN (elemental analysis), and mass spectroscopy.



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Synthesis and characterization of new Schiff base ligands containing 2-cloro and 3-cloro benzene and their complexes with Cu, Mn, Zn, Cd, and Ni metal ions

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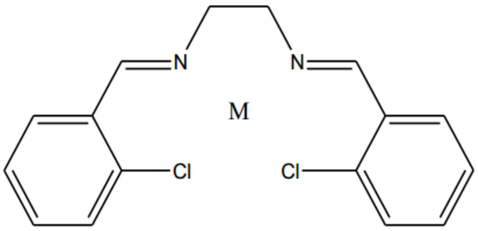
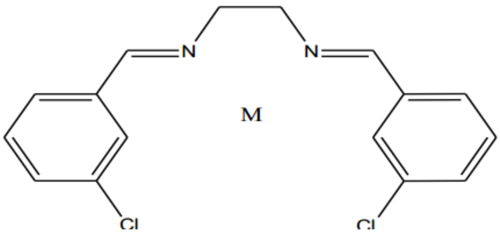
Schiff base are an important class of ligands due to not only their useful physical and chemical properties but also for the biological importance. [1,2]

Over the past few years macrocyclic Schiff base ligands have received vital attention not only because of their pharmacological properties, soft-hard donor character and coordination behavior, but also for their capacity for chemical recognition of anions and metals of biochemical and environmental importance. Metal ions have enormous importance in many biological processes, but the increased concentration of metal ions especially heavy metal ions exerts toxic effects on living system. Therefore, separation and determination of metal ions in environmental sources and living organisms play an important role. Macrocyclic Schiff base ligands showed good extraction abilities for the removal of different metal ions. [3]

In this work two new Schiff base ligands were synthesized in mild condition and then their properties for coordination to Cu^{2+}, Mn^{2+}, Zn^{2+}, Cd^{2+}, and Ni^{2+} were studied. Finally they were characterized by various methods such as IR, NMR, CHN (elemental analysis), and melting point.



Scheme 1.



Scheme 2.

Scheme 1: {3-[(2-Chloro-benzylidene)-amino]-propylidene}- (2-chloro-phenyl)-amine.
Scheme 2: {3-[(3-Chloro-benzylidene)-amino]-propylidene}- (3-chloro-phenyl)-amine.

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Cycloplatinated complex containing 1-phenylpyrazole; kinetic and DFT investigation of the reaction with MeI

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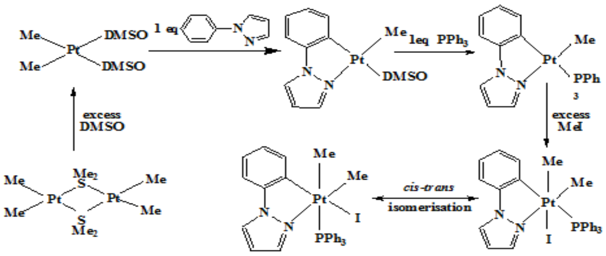
The Chemistry of cycloplatinated compounds is one of great current interest because of the wide range of potential applications they may have in many areas, such as organic synthesis, homogeneous catalysis, photochemistry and design of advanced materials and biologically active agents. The most widely studied examples are with nitrogen donors in which C-H activation takes place at phenyl ortho positions to produce five-membered metallocycles. In recent years interest in C^N cyclometallates ligands has mostly been addressed to platinum(II) derivatives due to their potential applications as chemosensors, luminescent devices, etc.

In the present work we have synthesized a new series of organoplatinum complexes [PtMe(ppz)(L)] (L = DMSO, PPh_3 and ppz is deprotonated 1-phenylpyrazole) (Scheme 1). These compounds were fully identified by using NMR (^{1}H, ^{31}P) spectroscopy and elemental analysis. Besides, kinetic of the oxidative addition reaction of new complex [PtMe(ppz)(PPh_3)] with MeI was studied using UV-Vis spectroscopy. It was suggested that the latter oxidative addition reaction was proceed by an S_N2 mechanism. The rates of the reactions at different temperatures were measured and consistent with the proposed mechanism, large negative $\Delta S^{\neq}$ value was found. Also, this mechanism was theoretically investigated using DFT calculations and the geometry of transition states and energy barriers were determined.



Scheme 1

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2D Silver(I) coordination polymer with hcb topology: synthesis and structure

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Coordination polymers (CPs) and Metal-Organic Frameworks (MOFs) with novel structures have attracted much attention in the past two decades not only because of their realistic and potential applications as functional materials, but also for their fascinating networks and structural topologies.[1,2] Structure of the CPs and MOFs depends on various factors such as the coordination behavior of the metal ions, geometry of the organic ligands, solvent systems and reaction condition.

The Ag(I) ion with d^{10} electronic configuration show a range of coordination geometries including linearity, triangle, tetrahedron and trigonal-pyramid with occasional instances of square and octahedron. This feature makes this ion an excellent candidate for the modeling of infinite coordination polymeric frameworks. In this work, we report synthesis, characterization and crystal structure of a new Ag(I) coordination polymer containing triangle Ag(I) nodes and bifunctional imidazolyl-based ligand as linkers. Single crystal X-ray diffraction reveals 2D sheet structure with **hcp** topology and unusual ABCDEFABCDEF packing mode. In addition, the structure has been characterized by PXRD, FT-IR spectroscopy and elemental analysis.

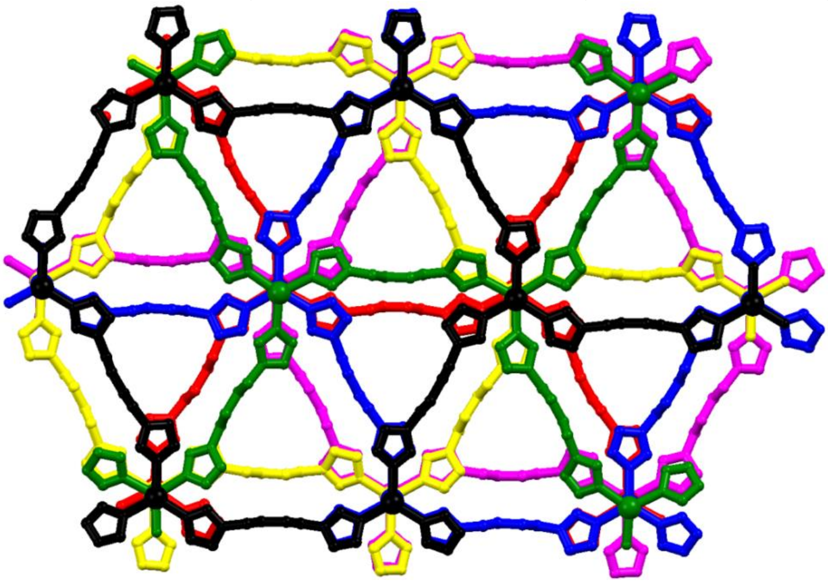

Figure 1: 2D structure of the Ag(I) CP with hcb topology and ABCDEFABCDEF packing.

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Synthesis and structure of a cationic double-stranded helical silver(I) coordination polymer

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Since the discovery of DNA as the first double-stranded helices, formation of helical coordination polymers is a fascinating challenge for chemists. Selection of liker ligand is a key factor in obtaining helical structures in coordination compounds[1,2] Herein, from the reaction of silver(I) tetrafluoroborate and a flexible bifunctional imidazolyl-based ligand in acetone/water mixed solvents a new 1D silver (I) coordination polymer were isolated which have been characterized by elemental analysis, PXRD, FT-IR spectroscopy and single crystal X-ray diffraction. In the polymeric structure, each Ag (I) ion coordinated by two discrete linker ligands and form 1D helical arrangement. Two adjacent 1D chains held together via Ag···Ag (2.985Å) interactions and form a double-helix DNA shaped structure. Linker ligands show *gag* conformation for the saturated NCCCCN chain with (Ag)N-to-N(Ag) distance of 8.694 Å. Part of the 1D helical structure is shown in figure 1.

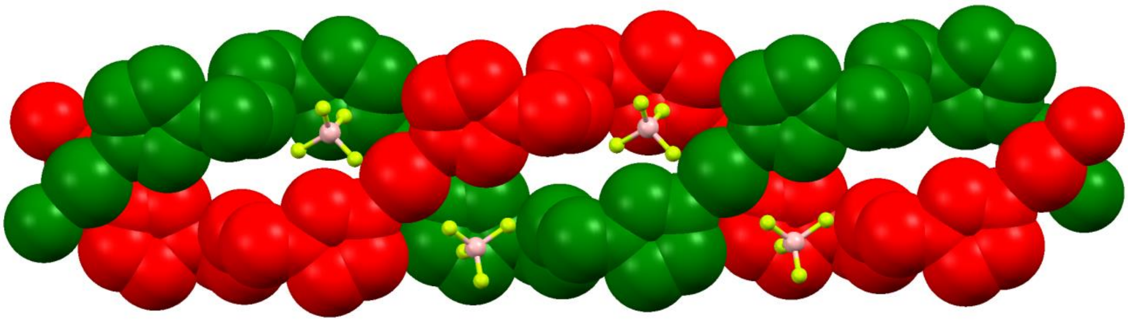

Figure 1: Space-filling representation of infinite double helical structure of Ag(I) coordination polymer. BF_4^- anions neutralize positive charge of the structure.

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Synthesis and characterization of boron oxide doped alumina

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Mesoporous materials are those possessing pore dimensions between 2 and 50 nm. Recently, mesoporous materials are gaining research interest because of their desirable characteristics such as high surface area, large pore volume, tunable mesoporous channels with well defined pore-size distribution, controllable wall thickness as well as modifiable surface properties. Mesoporous materials have extremely high surface areas and large pore volumes which provide the sufficient capacity for the adsorption of analytes. They possess the performances in thermal stability, chemical stability, compositional controllability, and as well as the flexibility in post-functionalization to enable the further introductionof hydrophilic, hydrophobic, polar as well as positive or negative charged functional moieties on surface. They are used in catalysis (as catalysts or supports), adsorption, pollutant remediation, sensors, drug delivery systems andphotocatalysis, solar cells, fuel cells and batteries.

In this report new silica mesoporous species has been synthesized via hydrothermal method. Boron oxide was doped into the framework and was characterized by N2- sorption, XRD, SEM and FT- IR Results showed that the pore size are about 3.28 nm. SEM image revealed a homogenous morphology. XRD analysis showed a amorphous phase, without showing a separate phase from Al or B source.[1,2]

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Synthesis, characterization and antibacterial activity of cadmium selenide quantum dots doped by dyspersium and europium

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Recently, nanoparticles (NPs) of different compositions and dimensions have become used as versatile and sensitive tracers.[1] The creation of dsigner NPs for enhanced sensitivity in sensing applications greatly benefits from their small size, where their properties are strongly influenced by increasing their surface area.[2] Indeed, metal-NPs have many interesting and unique properties potentially useful in a variety of biological and biomedical systems and devices.[3] Such as using water-soluble CdS quantum dots (QDs) as sensitizers is proposed for the chemiluminometric determination of epinephrine. The method is based on the quenching effect of epineph.[4] In the present article, our attention is focused on the synthesis, characterization and the antibacterial activity of cadmium selenide quantum dots doped by dysprosium. We confirm their characterization with SEM analysis (Fig. 1.) The antibacterial activityof the QDs has been tested against Staphylococcus Aureus and Bacillus Subtitles which are Gram (+) bacteria and some Gram (-) bacteria like *Escherichia Coli* and *PseudomonaAeruginosa*. The result of test showed that the QDs haveantibacterial effect.

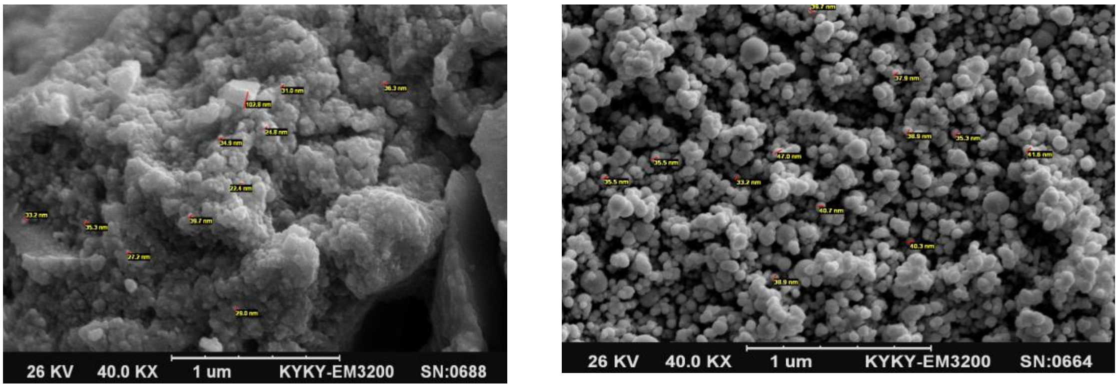

Fig. 1. Right fig is QD without doping and the left one is doped by dysprosium.

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Investigation of chemiluminescence properties of cadmium selenide quantum dots doped by dysprosium and europium

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Quantum dots (QDs), or colloidal semiconductor nanocrystals (NCs), are extremely interested for their remarkable size-dependent optical and electronic properties in the past two decades.[1] Also this semiconductor nanocrystals because of their particular light emission properties are in high rate of attention in chemiluminescence reactions.[2] Such as fluorescence (FL) method using water-soluble CdSe quantum dots (QDs) is proposed for the fluorometric determination of hydrogen peroxide and glucose.[3] Semiconductor nanoparticles like quantum dots (QDs) have the potential that can overcome to some problems, encountered by organic dye molecules. These QDs are one of the best choices for the detection of heavy metal ions in aqueous media. Unlike organic fluorophores, QDs exhibit high photochemical stability, excellent resistant to chemical degradation and photo- degradation.[4] In the present article, our attention is focused on the synthesis of cadmium selenide quantum dots doped by dysprosium and europium and investigation of their chemiluminescence properties.The result of chemiluminescence test showed that quantum dots doped by dysprosium are enhancer with Mn catalyst and quencher with Cr catalyst.

Fig. 1. Chemiluminescence of QDs.

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Synthesis, characterization and photocatalytic activity of coupled Dye/TiO_2/Nb_2O_5 as a visible-light-active nanocatalyst

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Semiconductor photocatalysts can be modified to expand their photoresponse to the visible region for pollutant degradation in several ways, including doping with cations/anions or coupling with another small-band-gap semiconductor. All of them are expensive and time-consuming; however, dye-sensitization, is a new and simpler method that can extend TiO_2 photoresponse.[1,2] In this study, we applied the dye-sensitization technique to prepare visible-light-active nanocatalyst Dye/TiO_2/Nb_2O_5(DTN). In common practice the semiconductor material (powder) is dipped into the dye solution for specified time interval under dark.[3] The prepared nanophotocatalyst (DTN) was characterized by X-ray diffraction studies (XRD) that depicted the formation of anatas and rutil phases and showed the particle sizes of about 67 nm. Fourier transform infrared spectroscopy (FT-IR) proves adsorption of dye on the catalyst surface. Scanning electron microscopy (SEM) shows the morphology of the synthesized particles that are spherical shapes. Energy dispersive X-ray analysis (EDAX) shows the purity of the prepared compound. We employed nanophotocatalyst (DTN) for the degradation of pollutant under visible light. Parametric studies were performed for the catalyst loading, initial pollutant concentration, solution pH, and visible light intensity. As a result, the simultaneous presence of both semiconductor and dye led to attracting a wider range of light and improving photocatalytic properties.

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Synthesis and characterization of biological active orthopalladated complexes of stabilizedylide with natural amino acids

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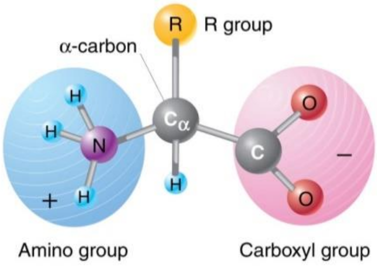
Bioinorganic chemistry describes the mutual relationship between inorganic and biochemistry, dealing with synthesis and biological investigation of inorganic complexes. Medicinal inorganic chemistry as an important integral part of bioinorganic chemistry, with focus upon the design of novel metal-based anticancer drugs is a thriving area which has shown significant advancements.[1,2] In continuation of our interest in the synthesis of new biological active palladium complexes[3,4] and according to the design of new antitumor agents, we design new organometallic structures of Pd (II) using a number of different natural amino acids as bio-potential ligands. The cyclopalladation of stabilizedylide and subsequent reactions with natural amino acids were investigated to yield a new series of chiral orthopalladated complexes potentially have biological activities. The new complexes were fully characterized by ^{1}H, ^{13}C-{^{1}H} and ^{31}P-{^{1}H} NMR spectroscopy, elemental analysis and FT-IR technique. Spectroscopic data surely revealed the existence of stereoisomers for mononuclear products due to the presence of chiral carbons.



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Removal of fluoride from aqueous solution by adsorption on Hydroxyapatite/zeolite Nano composite

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Adsorption is one important technique in fluoride removal from aqueous solutions. The viability of adsorption techniques is greatly dependent on the development of adsorptive materials. This study investigated the sorption of fluoride on to hydroxyapatite/Zeolite Nano composite from aqueous solution. Synthesis of Nano composite has been characterized by XRD, FT-IR, SEM and TGA and the effects of contact time, initial concentration, initial pH, adsorbent dosage and temperature on removal efficiency were also investigated. The adsorption equilibrium and kinetics of fluoride ion on this adsorbent were then examined at room temperature. Kinetic data were analyzed by pseudo first and second order models. The sorption data were then correlated with the Langmuir, Freundlich and Tempkin isotherm. According to the correlation coefficient, the adsorption of fluoride on the hydroxyapatite/Zeolite Nano composite was correlated well with the Langmuir and freundlichmodels.The results indicate that the HAp/zeolite can be used as an efficient adsorbent for the removal of fluoride ions from aqueous solution.

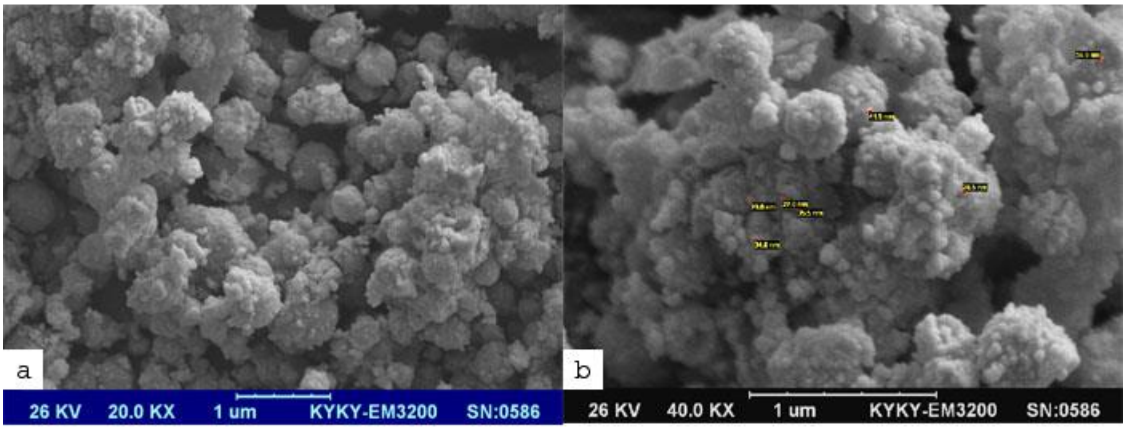

Fig. 1. SEM microghraph of HAp/Zeolite nano composite.

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Schiff-base assisted synthesis of lead selenide nanostructures

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In this work, nanostructured PbSe materials have been prepared via a solvothermal method at 180 ˚C with the aid of new lead precursors like Schiff-base compounds; Pb(salpn) and Pb(salophen) complexes. Besides lead complexes as lead precursor, $SeCl_4$, and $N_2H_4.H_2O$ (Hydrazine) as starting materials were used and propylene glycol (PG) as solvent was applied in this work. On the other hand, the effect of preparation factors such as type of reducing and capping agent on the morphology of PbSe nanostructures was investigated. The as-prepared PbSe nanostructures were characterized by XRD, SEM, TEM, EDS, and FT-IR. The SEM micrographs of the products indicated that PbSe nanostructures with lower particle size were obtained after solvothermal treatment for 3 h at 180 ˚C in the presence of hydrazine hydrate as reducing agent. Mechanism of synthesized PbSe was studied. The as-obtained results indicated that pure and homogeneous PbSe nanostructures have been form by using Pb(salpn) as precursor.

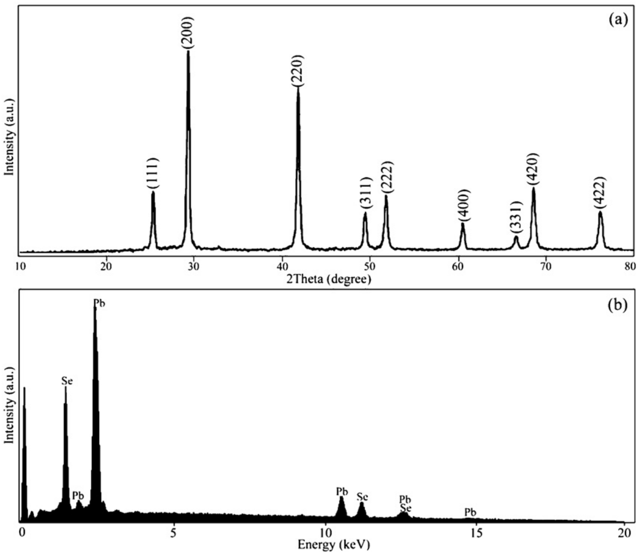

Fig. 1.(a) XRD pattern and (b) EDS spectrum of sample PbSe.

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DFT investigation of structure and stability of some organoplatinum complexes with phosphorus-donor ligands

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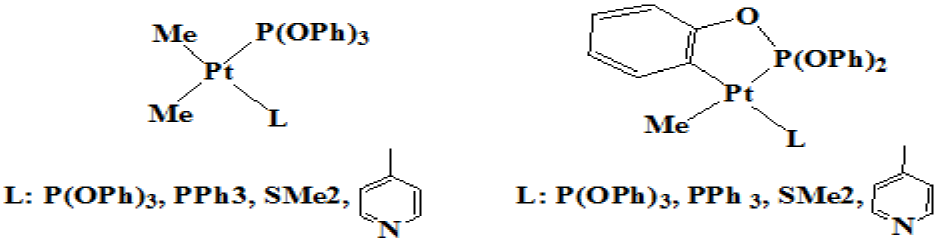
Phosphorus(III) ligands, especially phosphines and phosphites, have extensively been used as auxiliary ligands in forming transition metal complexes. These ligands are very useful as they present wide varieties of steric effects and electronic properties when coordinate to transition metals. Thus, by changing the substituents at the phosphorus atom, it is possible to greatly manipulate the chemical behavior of their complexes. Organoplatinum complexes with phosphines, PR3, as ligands are widely studied and the complexes have been involved in many chemical transformations. [1] Phosphine ligands are usually strong σ-donor ligands and only weak π-acceptors, this effect can be increased with electron-donating groups in the rest R, while electron with-drawing groups in R favor the π-acceptor backbonding. [2] We are intersted to investigate the cycloplatinated(II) complexes shown in scheme 1.



Scheme 1

Gaussian 03 is used to fully optimize all the structures in different solvents at the B3LYP level of density functional theory without imposing any symmetry. The LANL2DZ basis set is chosen to describe Pt and the 6-31G (d) basis set is used for other atoms. To evaluate and ensure the optimized structures of the molecules, frequency calculations are carried out using analytical second derivatives. The HOMO and LUMO orbitals of all structures calculated. NBO analysis was also carried out with the internal module GAUSSIAN 03. The structural parameters, quantum properties involving: bond length, bond angle, HOMO-LUMO orbital, gap energy, electron affinity, electronegativity, chemical potential, finally, the results will be compared with experimental data.

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Synthesis of palladium(II) complexes of arsoniumylideas a recyclable catalyst in the Suzuki coupling reactions

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A homogeneous solution of triphenylarsine (prepared by reacting trichloroarsine with chlorobenzene in benzene) and phenacyl bromide (prepared by reacting cetophenone with bromidein glacial acetic acid) in 30 mL of benzene was heated under reflux for 4hr. The resulting precipitate of phenacyl triphenyl arsonium bromide was removed by filtration and a sample was recrystallized fromchloroform-benzene. Further treatment with an aqueous solution of NaH (50%in mineral oil) led to elimination of HBr, giving the free ligand. To a magnetically stirred solution of $PdCl_2$ in acetonitrile, was added a methanolic solution (5 mL) of the ylide BPAsY (0.106 g 0.25 mmol). After 8 h the solvent was removed under reduced pressure to 3 mL. After addition of diethyl ether (30 mL) a white solid product was separated by filtration. Yield: (85.0%),IR (KBr, cm^{-1}): ^1H NMR ($CDCl_3$): The immobilized palladium catalyst was an efficient catalyst for the Suzuki cross-coupling reaction of several aryl halides with phenyl boronic acid in aqueous phase at room temperature. The yields of the products were in the range from 60% to 95%. The prepared heterogeneouscatalyst was characterized by XRD, FT-IR and TEM.

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Antibacterial activity of Moxifloxacin-zinc hydroxide nitrate nanohybride composite

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Fluoroquinolones are a domestic of synthetic antibacterial agents by an increasing admiration. The whole use of quinolones along with that of second and third group quinolones is growing for greatest countries. One of those third generation fluoroquinolones is moxifloxacin (MOX). [1-3] MOX is more effective than another similar drugs for example ciprofloxacin or levofloxacin in experimental keratitis in rabbits [4]. Penetration of MOX into the inflamed ocular tissue of rabbits has been found to be better than ciprofloxacin, lomefloxacin, ofloxacin, or levofloxacin.[5] In this work, MOX was intercalated in zinc hydroxide nitrate (ZHN) nanoparticles by ion exchange. XRPD analyses confirmed that MOX molecules were intercalated between the interlayer spaces of ZHN. FT-IR spectroscopy study shows that the intercalation takes place without change in the structure of the MOX. The thermal analysis results show that the MOX is stabilized in the interlayers by electrostatic interaction. The antibacterial activities of nanocomposite tested against microorganisms. The results show that the synthesized nanocomposites have good inhibition against two gram-positive and gram-negative species. MOX-ZHN can prevent the growth of harmful bacteria's more effectively than the MOX drug.[6]

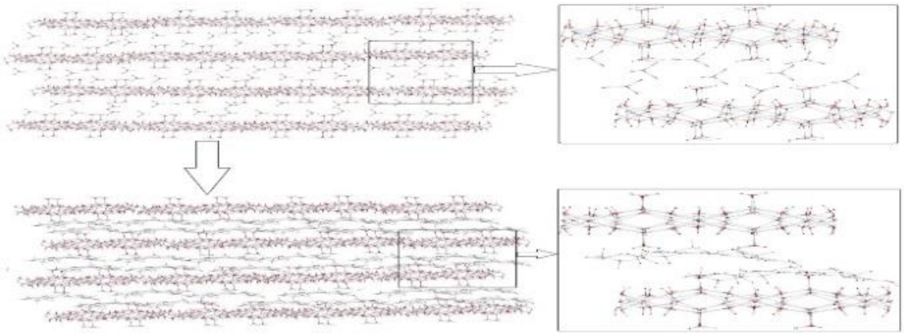

Fig. 1. Schematic structure of the ZHN and MOX-ZHN layers.

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Hydrothermal Synthesis Of Antimony OxideNanocrystals

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A simple hydrothermal method has been developed for synthesizing of $Pr_xSb_{6-x}O_{13}$ nanocrystals at a high yield at 180°C that is a new method for preparing these nanocrystals. Antimony oxide often promotes the activating catalysts used for selective partial oxidations and for related reactions such as oxidative coupling. Antimony oxide can be used as a catalyst, retardant, dielectric, fining agent and optical material. XRD patterns indicate that the $Pr_xSb_{6-x}O_{13}$ nanocrystals with 0-2 % mol are isostructural with Sb_6O_{13}. SEM shows the size of particle changes with doping Pr^{+3} ions into Antimony sites and the size of particles decrease. Floresance specta also shows this result. FT-IR, XRD, UV, Flouresance and SEM , TEM were used to analysis the structure characteristics of $Pr_xSb_{6-x}O_{13}$ nanocrystals.

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A Theoretical Study of Chemical Modification of Single-walled carbon nanotubes SWNTs (5,5) By siloxanederivatives

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Carbon nanotubes(CNTs) are frequently reported as being discovered in 1991 by Iijima, who was studying the soot produced after vaporizing graphite and subsequently published an influential paper on his discovery. [1] Since their discovery, [2] carbon nanotubes have stimulated intense experimental and theoretical interest in their physics, chemistry, and materials science. Their unique structure and properties make them suitable for a variety of potential applications .[3] There are two different categories of CNTs, multi-walled (MWCNTs) which consist of two or more layers of concentric graphite cylinders having outer diameters typically ~ 2.5-30nm and single-walled (SWCNTs) made of only one cylinder of graphite. [4] Single-walled CNTs have diameters as low as ~1nm and in general are the ones which have been used for creating carbon nanotube based electronic devices. Single-wall nanotubes _SWNTs_ are multifunctional materials that have potential for use as efficient gas storage elements and in battery devices, as sensors and electromechanical systems in nanoelectronics, and as biocompatible agents and sensors in medicine. [5] In this research, (SWNTs) were incorporated into siloxane-derivatives. The effect of incorporate of siloxane compound such as $Si(OH)_3$ (in perpendicular directions) upon total energy of structure have been studied. Theoretical study on the structural properties and reactivity of (5,5) Walled Carbon Nanotube and CNT-$Si(OH)_3$, CNT(-$Si(OH)_3)_2$in the ground state have done by using the Hartree-Fock method with 6-31G* basis set. Delocalization of charge density between the bonding or lone pair and antibonding orbitals calculated by NBO analysis.

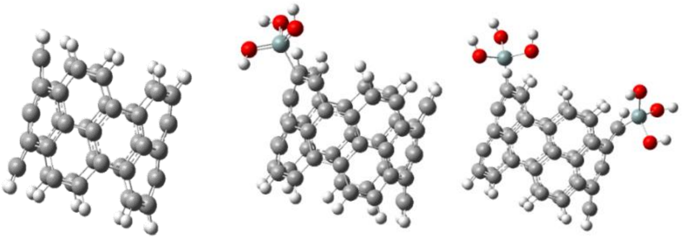

Fig.1. Optimized structure of CNT (5,5) and Complexes between CNT (5,5) and siloxane in perpendicular situations.

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A New VanadiumComplex of Redox-Active *O*-Aminophenol Ligand as Model Complex of Vanado-Enzymes

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Metalloenzymes often featurered ox-active ligandsdue to their easily redox processes by one or more electrons. These ligands usually convert to the radical species upon binding to transition metals .[1, 2]

In the present work, a new vanadium complex of tridentate *o*-aminophenolligandHL^{BAP} was synthesized and characterized by IR, UV-vis, ^{1}H NMR spectroscopic and single crystal X-ray diffraction techniques. X-ray diffraction studies exhibited a distorted octahedral geometry in which vanadium(IV) ion has been coordinated by four phenolic oxygens and two amine nitrogens of two L^{BAP} ligands (L^{BAP} represents the deprotonated from of HL^{BAP}). ^{1}H NMR and X-ray analysis results show that one of ligands is iminosemiquinone form while another one has been coordinated to vanadium centre in itsiminoquinone form. The UV-vis spectroscopy of this complex shows both intra-ligand and ligand to metal charge transfers.

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Synthesis and Characterization of Vanadyl Complex of a Noninnocent *O*-Amino Phenol-Based Ligand and It'sApplication in Oxidation of Sulfides

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Catalytic oxidations, especially sulfoxidation reactions, are among the most useful reactions in biological, industrial and academic processes .[1,2] The oxidovanadium compounds as functional and structural models for the native form of the vanadium haloperoxidase enzyme (VHPO).[3,4]A new vanadyl complex of tridentate *o*-aminophenol benzoxazole based ligand HL^{BAIC} was synthesized and characterized by IR, UV-vis, ^1H NMR elemental analysis, atomic absorption, single crystal X-ray diffraction, and cyclic voltammetry and mass spectroscopy techniques. X-ray crystallography analysis revealed an O_h mononuclear complex in which vanadium(IV) ion has been surrounded by iminosemiquinone L^{BAIC} ligand (L^{BAIC} represents the deprotonated form of HL^{BAIC}) and 3,5-Di-*tert*-butyl semiquinonate (SQ) ligand. It is evident from X-ray crystallography studies and broadening of ^1H NMR peaks that $VOL^{BAIC}(SQ)$ complex is paramagnetic. Electrochemical studies were conducted to evaluate the redox-active behavior of the complex, and the results demonstrated quasi-reversible metal-centered reduction and ligand-centered oxidation process for this complex. Finaly, the catalytic activity of this vanadyl complex in efficient and selective oxidation of sulfides to corresponding sulfonesunder mild conditions was investigated.

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Synthesis, Characterization and Single Crystal structures of anovel Zinc(II)nitrate Comple

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In recent years metal compounds, which have a stable d^{10} electronic configuration, have received a lot of attention in the fields of inorganic chemistry, biochemistry and environmental chemistry. About twenty zinc enzymes are known in which zinc is generally tetrahedrally four coordinate and bonded to hard donor atoms such as nitrogen. [1] Previously, it has been reported that zinc(II) and cadmium(II) complexes with Schiff bases type chelating ligand canbe used as an effective emitting layer and showed photo physical properties. [2] Zinc complexes have been shown to be active as antitumor, anti-HIV and antimicrobial agents . [3]

In the present study, we report the structure of one new zinc(II) complex. The metal complex has been synthesized and characterized by elemental analysis, ^{1}H NMR, ^{13}CNMR, IR and UV–Vis spectroscopy. Structural determination by X-ray crystallography.

The structure of the title compound, consists of discrete $[Zn(C_{14}H_{14}N_2)_2NO_3]^+$cation and NO_3^- anion. The zinc(II) cationcentre has a six-coordinated environment (unusual coordination number for zinc^{2+}). The zinc^{2+} coordinated by two molecules of 2,6-dimethyl phenyl) pyridine-2yl methylene amine and one molecule of nitrate. The imino pyridines and nitrate coordinated as bidentate ligands.

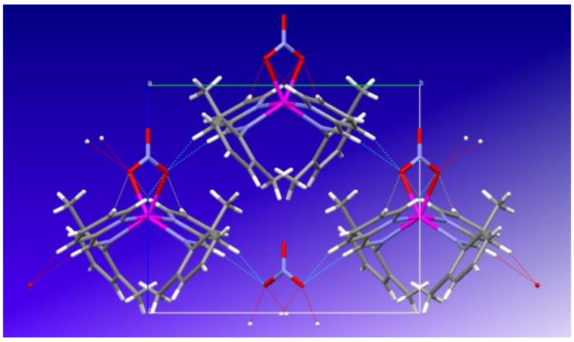

Fig. 1. The packing diagram of the title compound. Intermolecular C—H···O hydrogen bonds are shown as blue dashed lines.

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Synthesis, Characterization, X-ray Diffraction and DFT Calculation of a Bidentate [N, N] ligand

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Recently, the bidentate [N, N] ligand such as pyridineimine have drawn much attention owing to their valu able applications in the fields of catalysis, conjugated organic devices. These bidentate ligands can be modified by tuning thesubstituents. Therefore, different steric and electronic properties are achieved easily[1] Schiff base ligands are considered "privileged ligands" because they are easily prepared by the condensation between aldehydes and amines. Schiff base ligand played central role in transition metal coordination chemistry .[2]

In this paper the iminopyridine ligand, $C_{14}H_{14}N_2$, was synthesized and characterized by elemental analysis, ^{1}H NMR, ^{13}CNMR, IR and UV–Vis spectroscopy. Structural determination by X-ray crystallography. Then, we report the results of an experimental spectroscopic study with density functional theory (DFT) modeling. Thegeometry optimizations at the B3LYP/6-311G**level. A good agreement was obtained between calculated and measured X-ray diffraction patterns.

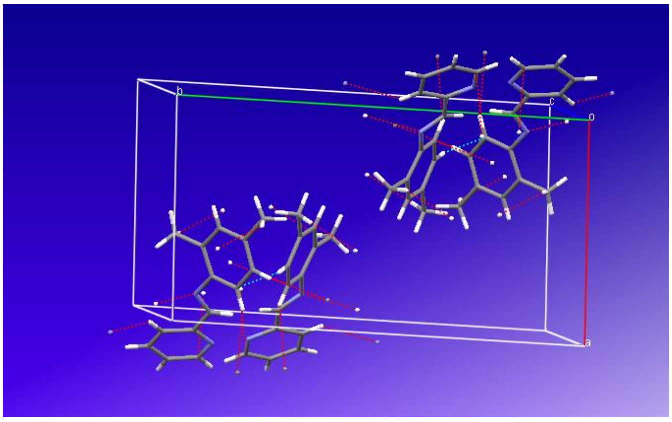

Fig. 1.A view of the unit cell packing for[(2,4-dimethylphenyl)-iminomethyl]-pyridine.

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DFT analysis of fullerene interaction with an osteoporosis drug for drug delivery: NBO and NQR computations

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Fullerene (C_{60}), the third allotrope of carbon after diamond and graphite, is a nanoscale carbon material with unique photo-, electro-, chemical, and physical properties, however, its inherent hydrophobicity limit its use in biology and thus leads to the research in searching water-soluble fullerene derivatives [1,2]. Bisphosphonates (BPs) have become well established as front-line agents for the treatment of tumor-associated bone disease and, more recently, for the treatment of cancer treatment-induced bone loss. By virtue of their ability to chelate calcium ions and rapidly target bone mineral, BPs selectively affect bone-destroying osteoclasts that have ingested BPs from the bone surface [3]. The aim of this study is evaluation of the interactions of the fullerene C_{60} nanocage (**1**) with a BP compound, risedronate, with formula $C_5H_4N(CH_2)C(OH)(PO_3H_2)_2$ (**2**). We first determined the total energy of the system as a function of distance of this drug to the exterior surface of the fullerene C_{60}. DFT computation was performed at B3LYP level of theory using 6-31G(d,p) basis set by Gaussian 09 software. The binding energies of isolated drug and its complex were calculated from the equation $\Delta E_{\text{binding}} = E(\text{molecule}) - \Sigma\ E(\text{atom})$ and $\Delta E_{\text{binding}} = E(\text{complex}) - \Sigma\ E(\text{drug})$, respectively. The optimum physisorption distances do not exceed 3.2 Å in this complex. Furthermore, log P value which corresponds to log ($1/IC_{50}$) that is the lipophilicity of this molecule and is used to predict its toxicity is 4.18. The band gap (Eg) of compound **3** is 2.82 eV. We used q_{zz} from the results of the Gaussian program and then calculated χ using the equation $\chi = e^2Qq_{zz}/h$. Selected calculated nuclear quadrupole coupling constants (NQCCs, χs) for the quadrupole nuclei ^{2}H (I=1), ^{17}O (I=5/2) and ^{14}N (I=1) of compound **3** are 23.88 kHz, 2.21, -0.58, 2.87 MHz, respectively.

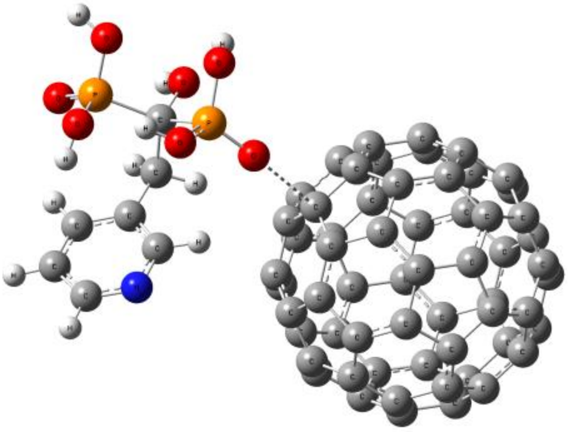

Fig 1. Optimized geometry of the fullerene-risedronate complex.

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A study on the interaction of fullerene (C_{60}) with alendronate drug: NBO and QTAIM analyses

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Bisphosphonates (BPs) are analogs of inorganic pyrophosphate, containing two phosphonate groups linked by stable phosphoether bonds to a central (geminal) carbon atom. The ability of BPs to selectively affect osteoclasts, and there by inhibit bone resorption, is based on their three-dimensional structure that allows the chelation of divalent metal ions1, especially Ca^{2+}.[1] Because of their unique physicochemical properties, fullerenes (C_{60}) are potential candidates for many biomedical applications, including anticancer therapy.[1] It was found that fullerenes and their derivatives possess diverse medical applications and are promising as HIV inhibitor, gene or drug delivery carriers.[2,3] In order to investigate the electronic and structural properties of isolated fullerene C_{60}.[1] and one of the derivatives of bisphosphonates, alendronate drug, with formula $H_2N(CH_2)_3C(OH)(PO_3H_2)_2$ (**2**) as well as that of its related complex **3**, DFT computation was performed at B3LYP level of theory using 6-31G(d,p) basis set by Gaussian 09 software. Also, log *P* value which corresponds to log ($1/IC_{50}$) to evaluate the lipophilicity of this molecule and to predict its toxicity was 4.97. The band gap (E_g) of compounds **3** between the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) as a measure of electron conductivity is 2.74 eV. The QTAIM theory deals with charge density, ρ(r), and Laplacian of the charge density, $\nabla^2\rho(r)$, at bond critical points (bcps). The $\nabla^2\rho(r)$ at the bcps takes positive values for ionic bonds, hydrogen bonds, and van der Waals interactions called closed-shell interactions. By contrast, covalent bonds exhibit large, negative $\nabla^2\rho(r)$ values. The P=O, P-O, N–H, N-C bonds in the **3** compound are clearly covalent, while the P(O)…C(fullerene) bond represents the typical electrostatic interaction.

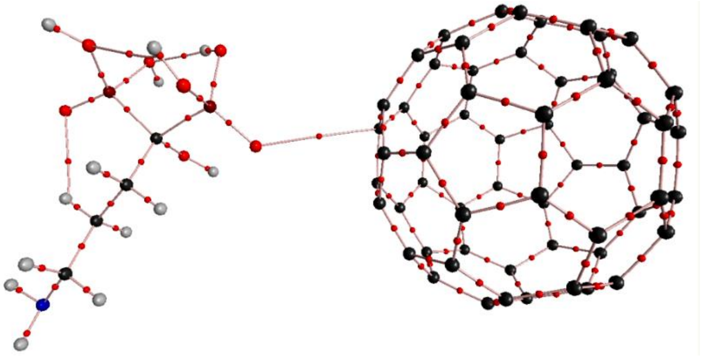

Fig 1. The molecular graph of compound **3** obtained by QTAIM analysis at B3LYP/6-31G(d,p) level of theory.

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Comparative characterization of a Ni-Salen Complex: DFT Calculations

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A nickle(II) complex using a salen-type ligand, *N*,*N*'-ethylene bis(4-hydroxysalicylideneim-ine), abbreviated with H_2L, has been synthesized and characterized by spectroscopic techniques (UV–Vis and FTIR), TGA, CHN analysis, molar conductance, and confirmed with Density Functional Theory (DFT) calculations using the ADF 2009.01 package. Electronic spectrum of the Ni(II) complex is dominated by charge transfer and intraligand bands at $\lambda < 436$ nm. DFT calculations showed that the HOMO with -4.824 eV energy is metal-dominated, with the $H \rightarrow L_{+1}$ (85%) transfer.

The magnitude of bond lengths and angles predicted by DFT calculations are comparable to those determined by X-ray crystallography for similar complex which has the same as bonds as mentioned Ni(II) complex.

The experimental vibration frequencies of the Ni(II) complex was correlated with the values estimated by DFT calculations. The good agreement between the experimental and theoretical vibration data allowed the assignment of relevant IR bands to molecular vibration modes.

Ultraviolet–visible (UV–Vis) spectrum of the mentioned molecule in the gas phase and ground state was evaluated using DFT with the standard PW91 method and compared with experimental.

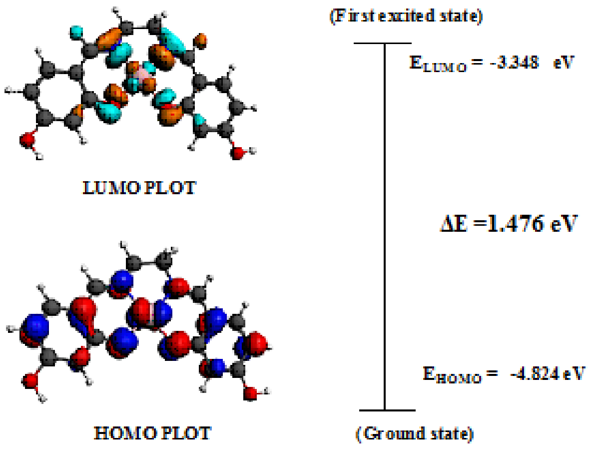

Fig. 1. Atomic orbital compositions of the frontier molecular orbitals for NiL.

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Comparative characterization of a Zn Complex: DFT Calculations

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The N,N'-1,2-cyclohexylenebis(2-hydroxyacetophenonylideneimine) Ligand, H_2L, was synthesized by condensing 1,2-diaminocyclohexane with 2-hydroxyacetophenone in ethanol as solvent. Synthesis of the complex was carried out using the mentioned ligand and $ZnCl_2$ in the methanol. The composition and properties of the ligand and it complex were established by elemental analysis, FTIR, ^{1}HNMR and UV/Vis spectra. Spectroscopy data reveal that the complex is in five coordination mode in which the Zn(II) was attached to two nitrogen and two oxygen atoms of the ligand and oxygen atom of the methanol.The fully optimized geometries have been calculated using density functional theory (PW91/DZP) by ADF 2009.01 package. A combined experimental and theoretical studies were conducted on the molecular structure and vibrational spectra of H_2L and related Zn(II) complex. The optimized geometric bond lengths and bond angles shows the best agreement with the reported experimental values of H_2L. The calculated HOMO and LUMO energies in both ligand and complex show that the electronic transition occurs within the molecules. The UV absorption spectrum was examined in methanol solvent and compared with the calculated in gas phase as well using PW91/DZP method.

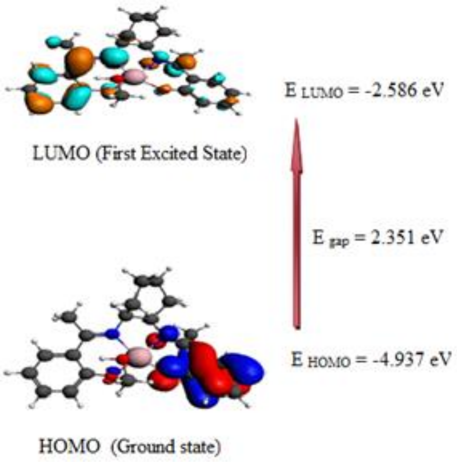

Fig. 1. Atomic orbital compositions of the frontier molecular orbitals for ZnL.

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Hydrothermal synthesis of tin dioxide nanostructures and its application in dye sensitized solar cells

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Pure SnO_2 nanoparticles with tetragonal structure were successfully synthesized by using a hydrothermal method and then were employed as a photoanode in dye-sensitized solar cells (DSSCs). (DSSCs) based on metal oxide semiconductor photoanodes and redox electrolytes are of great interest for application in solar energy conversion. SnO_2, an important n-type wide band gap semiconductor (3.6 eV) with high chemical stability and special electrical and optical properties, has been widely used for various applications, such as transistors, catalysts, gas sensors, transparent conducting electrodes, secondary lithium batteries and dye-sensitized solar cells.[1-4]

A Schiff base ligand was applied to prepare uniform SnO_2 nanoparticles. The morphology and crystalline size of nanoparticles have been characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier Transform Infrared (FT-IR) spectrum, Electron Dispersive X-ray spectroscopy (EDX) and ultraviolet-visible (UV-Vis) spectroscopy. The optical band gap of the SnO_2 nanoparticles was estimated to be 3.8 eV. The photovoltaic properties of SnO_2 electrodes have been investigated and it was shown that using uniform SnO_2 nanoparticles as an active electrode are more beneficial than agglomerated nanoparticles

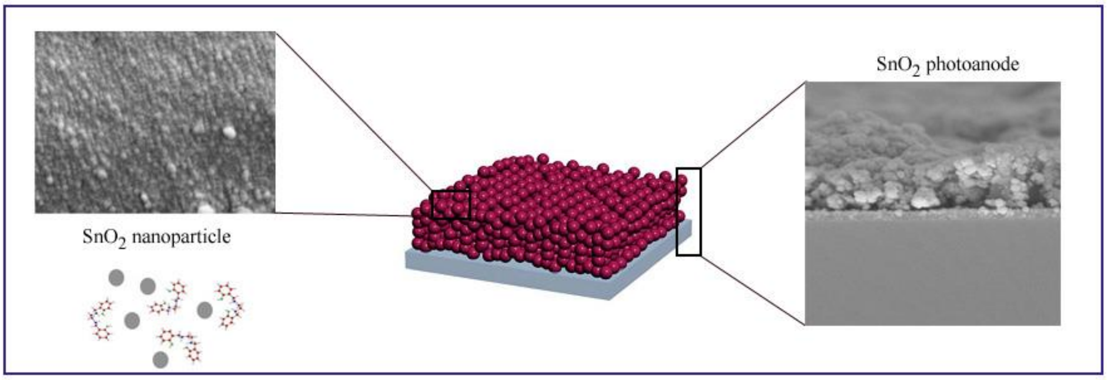

Fig. 1. Employing as-synthesized SnO_2nanoparticles via hydrothermal method in DSSCs as working electrode

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Investigation of photocatalytic performance of ZnO nanorods decorated calcined Mg–Al LDH in dye removal from wastewater

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The nanocomposites of magnesium–aluminum–carbonate–layered double hydroxides (Mg–Al–CO_3 LDHs) and ZnO nanorods were prepared via a homogeneous precipitation process. The presence of ZnO nanorods made the calcined Mg–Al–CO_3–LDHs, the strong adsorptive adsorbents for anions, have a photo catalytic activity. Both Mg–Al–CO3–LDHs and the nanocomposites with various ZnO/Mg–Al–CO3–LDHs mass ratios from 0.5:1 to 3:1 were synthesized and tested. Nanostructure of the composite was approved by scanning electron microscopy (SEM). The photo catalytic behavior of the nanocomposite was evaluated in removal of methyl orange (MO), an anionic dye, in a photo catalytic reactor. The adsorption ability of the nanocomposites and their photo catalytic activities for the removal of MO were evaluated by UV–Vis extinction spectra. The optimization of the photo catalytic process was carried out by considering of four factors which are: nanocomposite amount, dye concentration, irradiation time andcalcination temperature. All experiments designed by Minitab17 software.

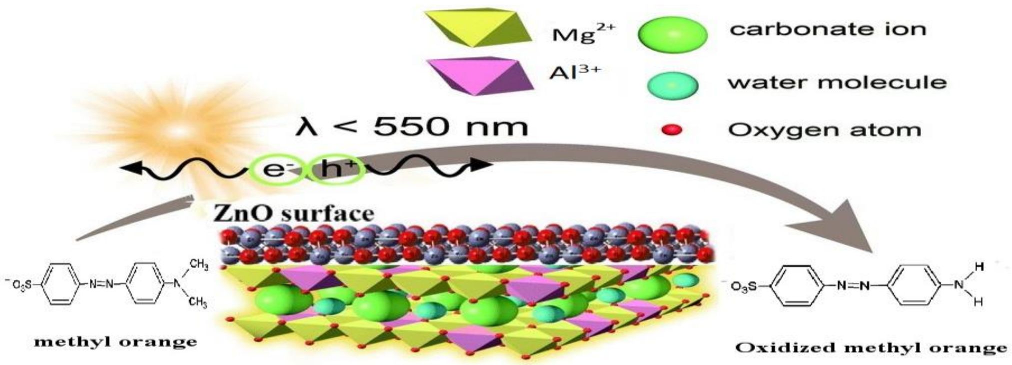

Fig. 1. ZnO nanorods decorated calcined Mg–Al LDH

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Investigation of performance of nanostructure Mg-Al LDH in desulfurization of gas oil

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The nanostructure Mg-Al layered double hydroxide (LDH) was synthesized by co-precipitation method and investigated to remove the sulfur-containing compounds fromgas oil. The LDH was investigated by X-ray diffraction (XRD), scanning electron microscopy (SEM), and Fourier Transmission Infrared (FTIR). The double layered structure of the sample was approved by XRD. SEM indicated the nanostructure of the sample. The modeling and optimization of the desulfurization process was carried by Minitab 17. LDH dosage, sulfur concentration, and calcination temperaturewere considered as effective factors on the efficiency of sulfur removal. The results revealed that the calcination temperature is the main factor which affects on the performance of the LDH in desulfurization process.

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Prediction of Electron Affinity Energy of the Phenacenes family

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Topological indices are real numbers that are presented as graph parameters (e.g., the degree of vertices, distances, etc.) during studies conducted on the molecular graphs in chemistry and can describe some physical and chemical properties of molecules.[1] In this article, the first Zagreb index was calculated in the family phenacenes and a suitable model was provided to predict the Electron Affinity Energy property through first Zagreb index while considering some elements of this family. Therefore, we first proveded the first Zagreb index for the family of phenacenes given by:

$$M_1(G) = 26n - 2$$

Where n is number of rings. Electron Affinity Energy of the phenacenes family ($C_{4n+2}H_{2n+4}$), were calculated using Gaussian 09 software and the experimental data of references were compared with those mentioned in valid papers. Fig 1 shows the changes in Electron Affinity Energy of phenacenes family according to the first Zagreb index (M_1). Therefore, Electron Affinity Energy ($E_{affinity}$) of molecules $C_{4n+2}H_{2n+4}$ could be well predicted by the following relations:

$$E_{affinity} = -(8 \times 10^{-8})M_1{}^4 + (4 \times 10^{-5})M_1{}^3 - 0.009M_1{}^2 + 0.8015M_1 - 26.2111$$

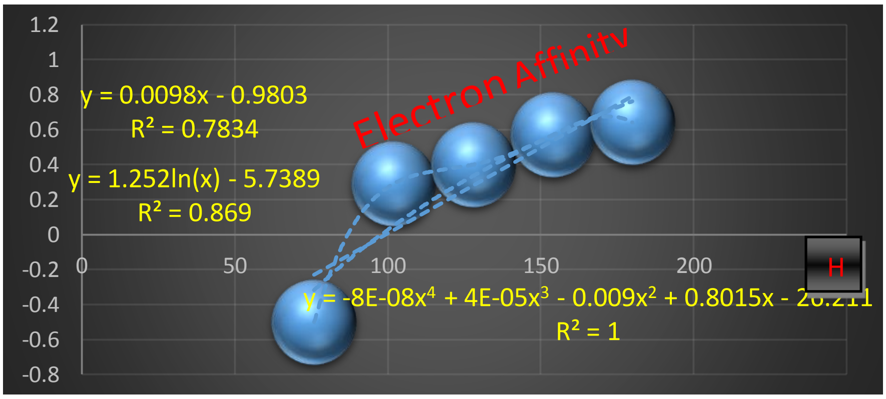

Fig.1: The Electron Affinity Energy ($E_{affinity}$) versus first Zagreb index

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Synthesis, characterization and electrochemical behavior of new binuclear Cu(II) and Ag(I) complexes.

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A large number of Schiff bases and their complexes have been studied for their interesting and important properties, e.g.coordination polymers[1], their ability to reversibly bind oxygen[2] andcatalytic activity.[3] High affinity for the chelation of the Schiff bases towards the transition metal ions is utilized in preparing their solid complexes. Hence, significant contemporary interests have grown gradually in this field to explore their physical, magnetic, optical and electronic properties through the variation of transition metal ions like nickel(II), copper(II), iron(II/III) and manganese(II/III) in different coordinationenvironments with organic co-ligands with suitable bridging units.[4]

In this study Schiff base derived from the reaction of 4-pyridine carboxaldehyde and ethylenediamine. This compound reacted as a neutral ligand with Cu(II) and Ag(I). $[(H_2O)_3(NO_3)_2Cu(L)Cu(NO_3)_2(H_2O)_3]$ and $[(NO_3)\ Ag(L)Ag(NO_3)]$ were synthesized and characterized by the elemental analysis, IR, UV-Vis, CV and ^{1}H-NMR spectroscopies. The cyclicvoltammetry study in DMSO solution gave all the expected waves for the redox processes of the Cu(II), Ag(I) and the ligands. Electronic spectra of the title complex show the Charge Transfer and intra ligand $\pi \rightarrow \pi^*$ transitions.

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Gas Phase Oxidation of Toluene and Ethyl Acetate and Isopropanol over mono and bi-metal Nano Catalysts

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Volatile organic compounds (VOC) are an important group of air pollutants. They are organic compounds that may undergo photochemical reactions with nitrogen oxides in the presence of sunlight, yielding even more hazardous compounds, such as troposphere ozone or organic peroxides (the so-called photochemical smog). [1] Increasing environmental awareness promotes the stricter regulation of industrial action. 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. In this process, high elimination efficiency can be achieved at relatively low temperature, which resulted in considerable environmental and economic benefits in comparison to the case of the thermal incineration.[2]

In this study activities of nanostructure AgZSM-5 and Fe-Ag-ZSM-5 catalysts for catalytic conversion of ethyl acetate, Isopropanol and toluene were studied. The catalysts were prepared by wet impregnation method and were characterized by XRD, BET, SEM, TEM, DRS and ICP-AES techniques. Toluene showed lower reactivity than others for conversion on Ag-ZSM-5 catalysts. In a binary mixture of organic compounds, the compunds showed an inhibition and promotional behaviors respectively, in which the conversion of toluene was decreased at temperatures above 250 °C. This study revealed the promotion role of iron and silver in increasing the catalytic activities of bimetallic catalyst were confirmed.

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Preparation of stabilized oil based nanofluid and study of thermal and electrical properties

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In the present work, stabilized graphene, copper oxide, alumina, nanofluids were prepared by two step method. In the first step graphene, copper oxide and alumina nanoparticles were synthesised through methods that is reported in the literatures. The size and structure of synthesized nanoparticles were characterized by standards technique such as X-ray diffraction (XRD), Fourier Transmission Infrared (FTIR) and Scanning electron microscopy (SEM) images. The surface of nanoparticles was modified with different methods and suitable surfactants to disperse in the oil without agglomeration. In the second step surface modified nanoparticles were dispersed in base oil by sonication. Finally thermal conductivity of synthesized nanofliuds was measured with different concentration. Also electrical conductivity and breakdown voltage of nanofluids was measured with respect to concentration of synthesized nanoparticles.

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Synthesis and characterization of palladium-cupper binary nanoalloy thin film as an efficient catalyst for Suzuki-Miyaura reaction

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A toluene-water planar interface has been used as an ideal template for self-assembly of Pd-Cu nanoalloy into nanofilm. The morphology and structure of the prepared thin film was characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive analysis of X-ray (EDAX). Suzuki cross-coupling reaction of aryl halides with arylboronic acids is one of the most widely used methods for the formation of carbon–carbon bonds.[1] Many palladium complexes have been used as homogeneous and heterogeneous catalysts for these reactions in organic solvents and, more recently, in aqueous media as well. However, the interest in palladium catalyst has shifted from Pd complexes to Pdnanoparticles(NPs). Their high surface-to-volume ratio and their highly active surface atoms compared to those of the bulk catalysts make Pd NPs as a promising alternative in the search for milder reaction conditions.[2] In this study, the catalytic activity of PdCunanoalloy thin film was evaluated by Suzuki-Miyaura cross-coupling reaction. Mild reaction conditions, absence of inert atmosphere and high yields of desired products are the notable features of using this catalyst.

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Synthesis and characterization of platinum-cupper nanoparticles thin film at liquid/liquid interface, a suitable catalyst for *p*-nitrophenol reduction

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Toluene–water interface has traditionally been employed to prepare particle assemblies and films of metals and semiconductors. The interface between water and an organic liquid, however, has not been investigated sufficiently for possible use in preparing nanocrystals and thin films of alloys.[1,2] In this study, we demonstrate the use of liquid–liquid interface as a medium for preparing ultrathin films of Pt-Cu nano catalyst for *p*-nitrophenol reduction reaction. An organometallic complex and $NaBH_4$ were choosen as platinum precursor and reducing agent, respectively. The obtained film was characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive analysis of X-ray (EDAX) analysis. Catalytic activity of Pt-Cu nanoalloy thin film was investigated in reduction of *p*-nitrophenol to *p*-aminophenol. Therefore, pseudo-first-order kinetics with respect to *p*-nitrophenol could be used in this case to evaluate the catalytic rate. The results reported in this study demonstrate the versatility and potential of the liquid–liquid interface for preparing nanomaterials and ultrathin films and encourage further research in this area.[3]

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Synthesis and study of photocatalytic activity of water-dispersible TiO_2 nanoparticles

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Nanocrystalline TiO_2 is one of the most studied oxides, owing to its widespread applications in pigmentation, catalysis, photocatalysis, gas sensing, and so on.[1] In TiO_2-based photocatalysts, the photogenerated charge carriers (e^- and h^+) migrate to the nanoparticles surface, where they act as redox sources. Eventually, this process leads to destruction of pollutants.[2] Nevertheless, TiO_2 nanoparticles (NPs) tend to aggregation when dispersed in aqueous solution, which is troublesome in investigation of their optical and catalytic properties under solution-like conditions. Therefore, it is desirable to prepare highly water-soluble TiO_2 NPs for photocatalytic and other applications. [3]

In this study, TiO_2 NPs were surface-modified with several surfactants such as sodium oleate and glycolic acid, in order to make them water-soluble. The prepared ligand-capped TiO_2 nanoparticles were characterized by several techniques. The X-ray diffraction (XRD) pattern of the TiO_2 NPs displayed highly crystalline anatase structure. The morphology of coated TiO_2 NPs were examined by transmission electron microscope (TEM) and illustrated spherical particles with good monodispersity. The photocatalytic properties of these NPs were evaluated by photocatalytic degradation of methylene blue (MB) and showed a higher photocatalytic activity than commercial anatase TiO_2 NPs. Finally, the resultant TiO_2 NPs were easily dispersed in water without any considerable aggregation.

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Solid-state anion-replacement of three new isostructure of lead(II) coordination polymers via mechanochemical approach

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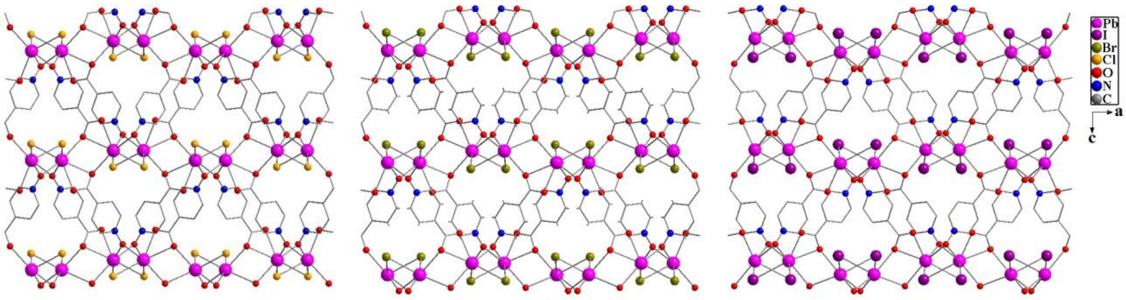
Mechanochemical synthesis is experiencing a dynamic re-discovery in the areas of organic and metal-organic materials. Typical mechanochemical reactions are those activated by co-grinding or milling of powder materials. These reactions are usually carried out either manually, in an agate mortar, or electro-mechanically, as in ball milling. Grinding, milling and relatedtechniques can lead to the formation of covalent, coordinationor hydrogen bonds in materials ranging from discreteorganometallic and inorganic complexes to coordinationpolymers.[1-3]

A series of new isostructural three-dimensional (3D) lead (II) coordination polymers $[Pb(INO)X]_n$ [X= Cl (**1**) , Br (**2**), I (**3**); INO = Isonicotinic acid n-oxid] have been synthesized and determined by single-crystal X-ray diffraction.Reversible solid-state structural transformations under mechanochemical reactions have been studied. Powder X-ray diffraction (PXRD), Scanning electron microscope (SEM) and IR spectroscopy have been used to fully characterize the solid products. The thermal stability of compound **1**, **2** and **3** has been studied by thermal gravimetric (TG) and compared each other. All three of them crystallize in the orthorhombic space group*Pbcn.*



a **b** **c**

Fig. 1. A fragment of the 3D framework of isostructural compounds a) **1**, b) **2** and c) **3** viewed along c direction.

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Preparation of drug intercalated Mg-Al Layered Double Hydroxide nanoparticles

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Among many different nanoparticles that have been shown to facilitate drug delivery, LDH nanoparticles have attracted particular attention owing to their many desirable properties. In this way, many kinds of LDHs of less toxicity are used. Mg-Al-LDH is one of the less toxic layered double hydroxides, which was used in the present work. First layered double hydroxide was prepared using thermal and hydrothermal methods. The synthesis condition was optimized for Mg-Al-LDH ratio of 6:1(i.e. water was used as the solvent, the pH value was 10, the aging time was 22h, and the crystallization temperature was 70˚C). Then Baclofen was intercalated into Mg-Al-NO_3-LDH. Once more, the synthesis condition was optimized (i.e. water was used as the solvent, the pH value was 10, the aging time was 72h, and the crystallization temperature was 120˚C). Different functional groups in LDH, Baclofen, and LDH-Baclofen were studied using FT-IR spectra. X-Ray diffraction pattern (XRD) was used to examine the particle size and crystallinity of LDH and LDH-Baclofen at nano-size. The number of the water molecules and the molecular formula of LDH and LDH-Baclofen were found using Thermal Gravimetric Analysis (TGA), Elemental Analysis, and Atomic Absorption methods.

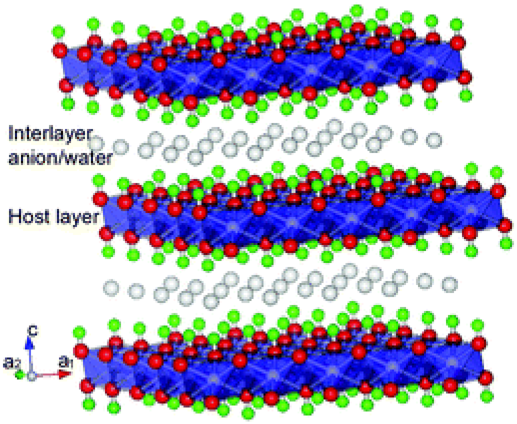

Fig. 1. Schematic model of LDH structure.

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Synthesis and characterization of coordination complexes of chrome and mercury metal ionscontaining pyridine-2,5-dicarboxylic acid N-oxide

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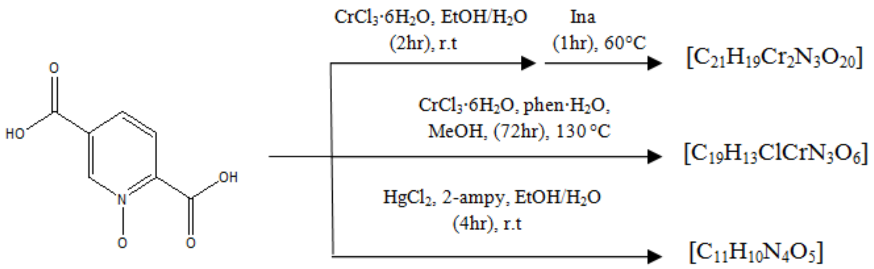
According to research conducted in our research group on the pyridinedicarboxylate family due to their various applications in the fields of pharmaceuticals, non-linear optics, magnetism, electrical conductivity, catalyticactivity,*etc*, we decided tooxygenate nitrogen of pyridine ring of pyridine-2,5-dicarboxylic acid as N-oxide to investigate synthesis, coordination modes, and structure types of these compounds in view of crystal engineering concepts. In this work we report the synthesis of two novel coordination complexes with Cr^{III} and one coordination complex based on the proton transfer mechanism with three heterocyclic bases such as 1,10-phenanthroline (phen), 2-aminopyrimidine (2-apym), and isonicotinamide (Ina). The ligands and complexes were characterized by physico-chemical approaches including elemental analysis (CHN), solid infrared (IR), mass spectrometry and conductometry techniques. Based on the conductivity analysis, high conductivity indicated the ionic nature of compounds, while low conductivity indicated molecular compounds. According to observed chemical shifts of related bands of carboxylate and N-O functional groups one can confirm that these groups are coordinated to chrome metal for two compounds.



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Facile Chemical Synthesis of Cobalt Tungstates Nanoparticles

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Cobalt tungstate nanoparticles were synthesized by a chemical precipitation reaction in aqueous ambient involving direct addition of cobalt ion solution to the solution of tungstate reagent. Optimization of the synthesis procedure was carried out using Taguchi robust design as statistical method. In order to controllable, simple and fast synthesis of cobalt tungstate nanoparticles, effects of some synthesis conditions such as reagents concentrations (i.e., cobalt and tungstate ions), flow rate of cobalt feeding and temperature of the reactor on the particle size of synthesized cobalt tungstate were investigated by the aid of an orthogonal array (OA9).[1,2,3] The results of optimization process showed that cobalt tungstate nanoparticles could be prepared by controlling the effective parameters and at optimum conditions of synthesis procedure, the size of prepared cobalt tungstate particles was about 55 nm. Chemical composition and microstructure of the prepared cobalt tungstate nanoparticles were characterized by means of X-ray diffraction, scanning electron microscopy, FT-IR spectroscopy and Fluorescence.

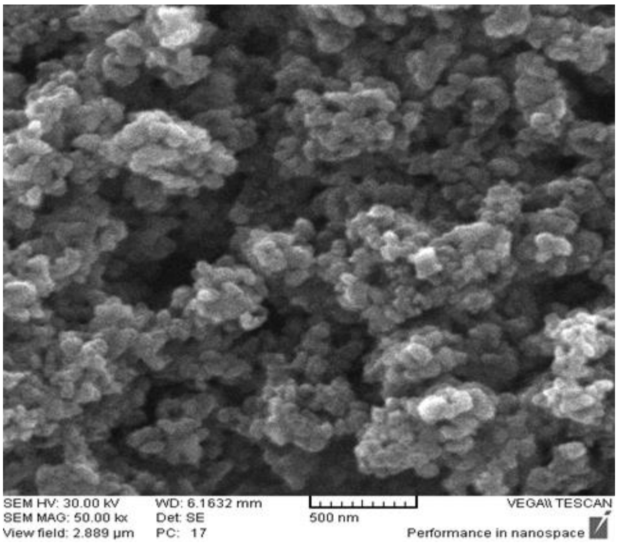

Fig. 1. SEM image of CoWO4 nanoparticles prepared via precipitation under optimum conditions.

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Facile Synthesis Optimization and Structure Characterization of chromium Tungstate Nanoparticles

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The study involves a direct precipitation method developed for the facile and efficient synthesis of Cr_2WO_6 nanoparticles. Effects of various parameters such as chromium and tungstate ion solution concentrations, flow rate of reagent addition, and reactor temperature on diameter of synthesized chromium tungstate nanoparticles were investigated experimentally by the aid of orthogonal array design.[1,2,3] The findings of the study revealed that the diameter of the produced Cr_2WO_6 nanoparticles can be fine-tuned through the adjustment of the reaction parameters, including chromium and tungstate ion solution concentrations and the reaction temperature, and at optimum conditions of synthesis procedure, the size of the produced chromium tungstate particles was about 50 nm. Finally, scanning electron microscopy, X-ray diffraction, FTIR, and photoluminescence techniques were used for structural and morphological characterization of the product, so as to monitor the role of the mentioned parameters on the targeted properties in the product.

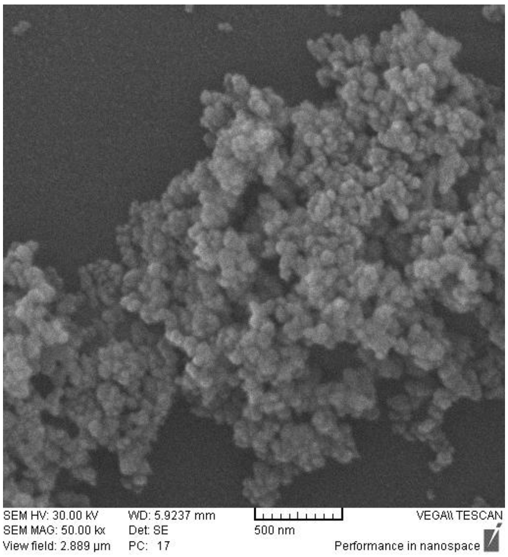

Fig. 1. SEM image of Cr_2WO_6 nanoparticles prepared via precipitation under optimum conditions.

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Coordination complexes of copper and cobalt metal ions containing pyridine-2,5-dicarboxylic acid N-oxide: Synthesis and characterization

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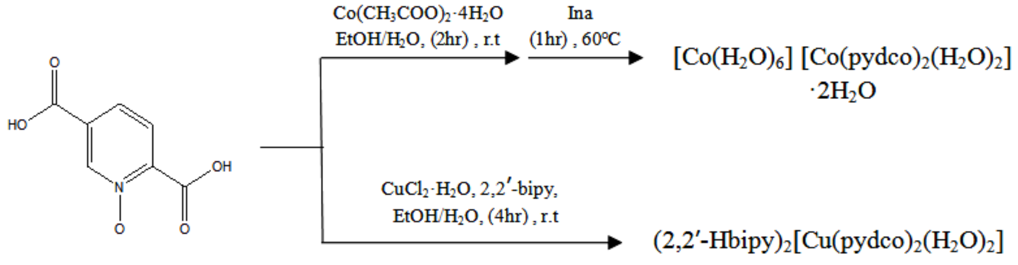
Recently, the subject of main chemical researchesis some how related to the field of noncovalent intermolecular interactions that leading to the formation of unique coordination compounds and gave rise to two new branches of chemical research, that is supramolecular chemistry and crystal engineering. Where as pyridinedicarboxylates have particularly importance in pharmaceutical industry and food chemistry, they have attracted attention of many researchers in synthesis of proton transfer and related coordination compounds. Many studies were carried out on proton transfer between a carboxylic acid and a heterocyclic amine. Therefore we synthesized pyridine-2,5-dicarboxylic acid N-oxide(pydco) hoping to change of coordination modes and geometry of desired complexes of Co^{II} and Cu^{II}metal ions in the presence of heterocyclic amines. The synthesized compounds formulated as (2,2′-Hbipy)$_2$[Cu(pydco)$_2$(H$_2$O)$_2$] (**1**), [Co(H$_2$O)$_6$][Co(pydco)$_2$(H$_2$O)$_2$]·2H$_2$O (**2**) (2,2′-bipy =2,2′-bipyridine, Ina = Isonicotinamide) are characterized by some physico-chemical methods such as elemental analysis, infrared spectra (IR), conductometry, and thermal gravimetric analyses (TGA). Based on the conductivity analysis, high conductivity showed the ionic nature of compounds. According to observed chemical shifts of related bands of carboxylate and N-O functional groups one can confirm that these groups are coordinated to copper and cobaltmetal ions in two compounds.



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Mass Spectrometry Investigation of Some New Phosphoramide and Thiophosphoramide Compounds

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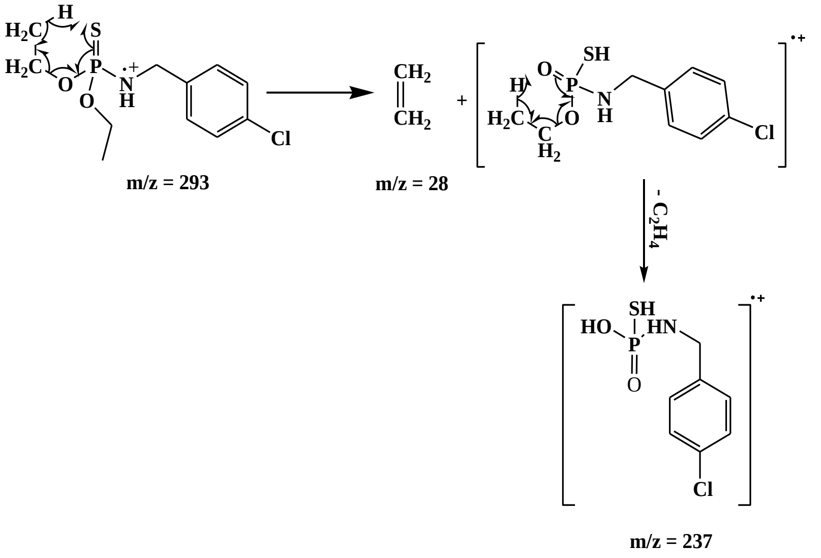
In this research, some new phosphoramide and thiophosphoramide compounds were prepared from the reaction of amines with $P(O)Cl_3$ and $(C_2H_5O)_2P(S)Cl$ (commercial substances), $4–CH_3-C_6H_4NHP(S)Cl_2$ (1), $((C_6H_5CH_2)(CH_3)N)P(S)Cl_2$ (2) and $CHCl_2C(O)NHP(O)Cl_2$ (3) (synthesized initial phosphorous-chlorine compounds). The compounds were studied by IR spectroscopy and mass spectrometry. In mass spectra, the fragmentation pathways and re-arrangements are discussed. The formula of new compounds are as follows: $(4-CH_3-C_6H_4NH)P(S)(NHC_6H_4-3-Cl)_2$ (4), $(4-CH_3-C_6H_4NH)P(S)(NHC_6H_4-4-Cl)_2$ (5), $((C_6H_5CH_2)(CH_3)N)P(S)(NHC_6H_4-4-CH_3)_2$ (6), $(4-Cl-C_6H_4CH_2NH)P(S)(OCH_2CH_3)_2$ (7), $P(O)(NHCH_2C_6H_4-4-CH_3)_3$ (8), $(CHCl_2C(O)NH)P(O)(NHCH_2C_6H_4-4-CH_3)_2$ (9) and $(CHCl_2C(O)NH)P(O)(NHCH_2CH_2CH_3)_2$ (10). Mass spectra of all compounds 4, 5, 6, 7, 8, 9 and 10 show the ion molecule fragments, at m/z (intensity) = 421 (61), 421 (5), 395 (14), 293 (2), 407 (51), 413 (8) and 289 (11), respectively. The base peaks are as follows: for 4, 7 and 8 at m/z = 28, for 6 and 9 at m/z = 120 and for 5 and 10 at m/z = 126 and 150, respectively. The interesting rearrangement in mass spectrum of compound 7 is involved two McLafferty re-arrangement pathways (Scheme).



Scheme. The rearrangement in mass spectrum of compound 7 is represented.

Synthesis, Spectroscopic Study, X-Ray Crystallography Investigation and Hirshfeld Surface Analysis of Three New Phosphorous-Nitrogen Compounds

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New phosphorous-nitrogen compounds 2,3-F_2—$C_6H_3C(O)NHP(O)[N(CH_3)CH_2C_6H_5]_2$ (I), $C_6H_5OP(O)[NHCH(CH_3)_2]_2$ (II) and $(CH_3O)_2P(S)[NHC_6H_4NH]P(S)(OCH_3)_2$ (III) were synthesized and characterized by ^{19}F NMR for (I) and ^{1}H, ^{13}C, ^{31}P NMR and IR and mass spectroscopy and single crystal X-ray determination for all three compounds. In the ^{31}P NMR spectra, the $^{31}P\{^1H\}$ signals of (I), (II) and (III) are revealed at 12.95, 10.49 and 69.55 ppm, respectively. The chemical shits observed are within the expected values for analogous phsophoramide and thiophosphoramide compounds.[1,2] In the crystal structure of (I), centrosymmetric dimers are built from pairs of N—H…O═P hydrogen bonds. In the structure (II), the molecules are aggregated in a one-dimensional arrangement *via* N—H…O═P hydrogen bonds along the *b* axis. In the structure (III), the two-dimensional array is generated from the N—H…O hydrogen bonds along the *ab* plane. In structure (II), the oxygen atom of P═O group is a better H-atom acceptor than the oxygen atom of the C_6H_5O group, as the latter oxygen atom doesn't take part in hydrogen bonding interaction. The better hydrogen-bond acceptor capability of P═O group with respect to the oxygen atom of RO group in structures with an $[RO]P(O)[N]_2$ segment were analyzed through the analysis of the structures deposited in the Cambridge Structural Database. In contrast with the structure (II), in the structure (III), the O atom of CH_3O group is involved in N—H….O hydrogen bonding, whereas, the P═S group doesn't take part in the hydrogen bonding interaction (Fig. 1). The Hirshfeld surfaces and fingerprint plots[3] were also employed for analysis of intermolecular interactions.

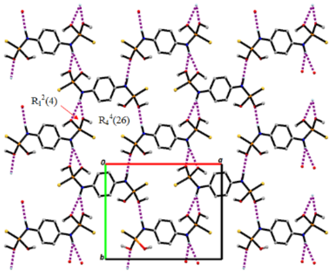

Fig. 1. A crystal packing diagram for structure (III) is represented, showing a 2D network that formed by N-H…O hydrogen bonds.

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Synthesis, crystal structure and spectral studies of a novel Zn(II) complex With 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine ligand

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One of the best potential polydentate nitrogen ligands are 1,2,4,5-terazine and its derivetives.[1] They have been applied as bridging ligands for the construction of di– and polynuclear species, and as coordinative π-acceptor moietiesin the study of photophysical and redox proprties of transition metal complexes. In particular 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine (bptz) can bridge metal ion to form bis-chelating complexes in the cis/trans (syn/anti) coordination modesor as a building block for supramolecular assemblies.[2,3] The reaction of $Zncl_2$ with 3,6-bis(2-pyridyl)-1,2,4,5-tetrazine (bptz) in the presence of chloroform / acetonitrile with 1:1 ratio and temprature (55 ^{0}C) by branched tube method produce a new binuclear complex $[Zn(bptz)_2(Cl)_2]$. The new complex characterized by IR, ^{1}H NMR spectroscopy and single crystal X-ray diffraction. The single crystal X-ray analyses for Zn(II) complex revealed that coordination number is six and Zn(II) atom has a distorted octahedral geometry and bptz acts as a bis-bidentate chelating ligand. IR (cm^{-1}): 1595 (m, C=N), 1392 (s, C=C).^{1}H NMR (300 MHZ, CD_3OD, 25^{0}C) : δ=8.94(d, H^3), δ=8.61(d, H^6), δ=8.15(t, H^4), δ=7.73(t,H^5) ppm for 4,5-H_2bptz.

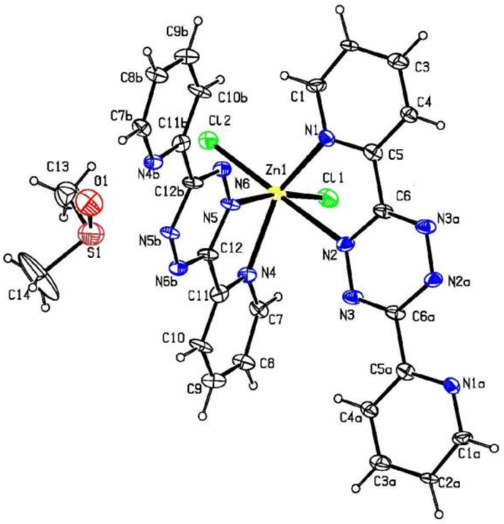

Fig. 1. The ortepwiew of the $[Zn(bptz)_2(Cl)_2]$ complex.

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Synthesis and characterization of Cd(ll) complex on the basis of 3,6- bis (2-pyridyl)-1,2,4,5-tetrazine

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Compound 3,6- bis(2-pyridyl)-1,2,4,5-tetrazin (bptz) has a peculiar electronic structure: Due to the presence of four nitrogen atoms in the tetrazine ring, the lowest unoccupied molecular orbital (LUMO) in bptz has a very low energy. Furthermore, the two pyridyl substituents allow bidentate coordination of one or more metal centers of a widely varied nature.[1,2] In the present work, reaction of the potentially bis-bidentate bridging ligand bptz with $Cd(OAC)_2$ and KSCN in aqueous methanol/wather with 3:1 ratio afforded dinuclear complex in which two Cd(SCN)(OAC) units are bound to the N,N-bidentate compartments of bptz. The synthesized complex characterized by FT-IR, ^1H NMR spectroscopy, element analysis and electronic absorption. IR(cm^{-1}) 1352 (ν_s COO), 1403 (ν_a COO), 2059 (s, SCN^-), 1677 (m, C=N). ^1H NMR (300 MHZ, CD_3OD, 25 °c): δ=8.94 (d, H^3), 8.61 (d, H^6), 8.16 (t, H^4), 7.73 (t, H^5) ppm fpr 4,5 – H_2 bptz; 0.75, 1.22 ppm for (H_3-OAC). Yield 0.29 gr (64٪). Anal. Calc. for $C_{19}H_{18}N_8Cd_2S_2O_5$: C, 31.37; H, 2.4; N, 15.40. Found: C, 31.28; H, 2.31; N, 15.27 ٪. In the electronic spectra of complex (1):[$Cd(bptz)(OAC)_2(SCN)_2$]tow strong absorption were observed at about 229 and 355 nm. On the basis of the intensity and position of the lowest energy absorption, it has been assigned to intra ligand and CT transitions.[3] The electronic spectra and suggested structure of complex is shown in Figs. (1-2).

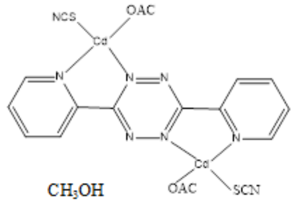

Fig.2. Complex structure

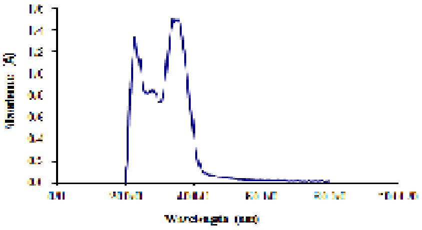

Fig .1. Electronic spectra of the complex (1) 10^{-3} in DMSO

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Sonochemical synthesis of new Zn(II) complexes of a bidentate Schiff base ligand: biological active and precursor for preparation of zinc(II) oxide nanoparticles

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Schiff base ligands have been known to be used in the preparation of many potential drugs, and are known to possess a broad spectrum of biological activities.[1,2] Zn(II) complexes of these ligands have been widely investigated in various areas of bioinorganic chemistry such as anticancer, antioxidant activities and DNA binding and cleavage studies.[3-5] On the other hand, although many methods have been developed to synthesize zinc oxide nanoparticles but the use of coordination compounds as precursors for the preparation of zinc(II) oxide has not yet been investigated thoroughly.[6,7] In this work, we report the synthesis and characterization of some new nano-structure zinc(II) complexes of a new Schiff base ligand entitled as bis((E)-3-(4-(dimethylamino)phenyl)allylidene)-2,2-dimethylpropane-1,3-diamine. Synthesized compounds were characterized by FT-IR, ^{1}H, ^{13}C NMR, UV–visible spectra and molar conductance. The nano-structure compounds were synthesized by sonochemical method and then characterized by FT-IR, XRD and SEM. Also, the ZnO nanoparticles were synthesized by calcination of zinc iodide complex at 600 ˚C under air and confirmed by XRD and SEM (Fig. 1). The antimicrobial activity of the ligand and its zinc complexes against four bacteria of *Staphylococcus aureus* and *Bacillus subtilis* as Gram-positive, and *Escherichia coli* and *Pseudomonsaeruginosa* as Gram-negative and two fungi of *Candida albicans* and *Aspergillusorayzea* was screened. Also, the DNA cleavage ability of all the complexes was studied by electrophoresis method. Finally, thermal behavior of all complexes was investigated based on TG/DTG/DTA curves. Some activation parameters of thermal decomposition processes were derived by coats-redfern relationship.

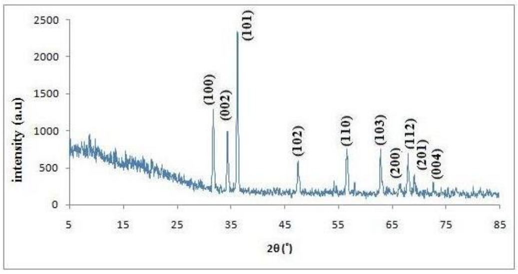

Fig. 1. XRD pattern of zinc oxide.

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An Amide-Functionalized Microporous Zn-Metal-Organic Framework for CO_2 Capture

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Porous metal−organic frameworks (MOFs), constructed from metal-based nodes and multitopic organic ligands as linkers,[1] have recently begun to be explored as a potential new class of CO_2 captures and separators, owing to their very high surface areas, tunable pore sizes and shapes, adjustable pore surface functionality, and flexible structures.[2]

Here we report that the control of the pore size of MOFs functionalized with amide groups enables greater interactions between the host framework and guest CO_2 molecules. Our strategy relies on pillaring two-dimensional (2D) layers comprising Zn(II) ions and the V-shaped dicarboxylate ligand with linear multipyridylamide-based ligands, see Figure 1. We have found that the resulting porous MOF present high affinity for CO_2 (195 K), a tendency that could be explained due to the presence of amide groups decorating the pores, which may establish strong interactions with the CO_2 molecules. In this context, this framework can be considered as potential CO_2 adsorbent.

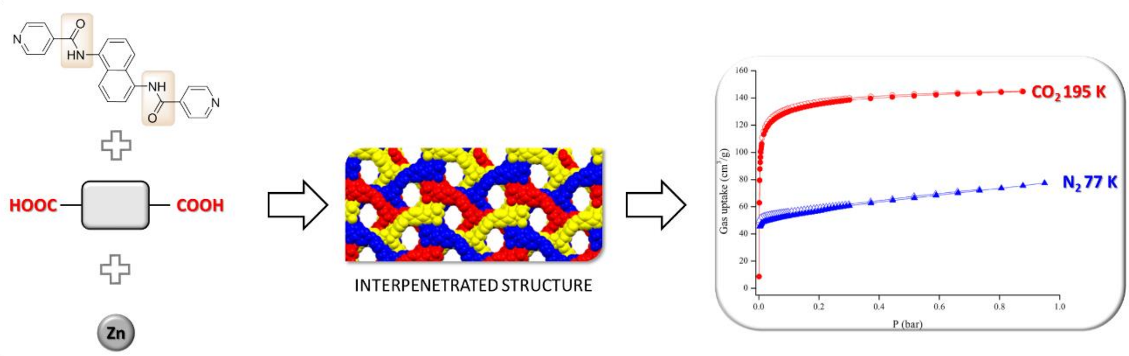

Fig. 1. The packing of the structure leads to a three-fold interpenetration Zn-metal-organic framework (in yellow, red and blue) possessing 1D pores; and type I CO_2 and N_2 isotherms at 195 K and 77 K, respectively.

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Microporous amine decorated metal-organic framework for highly efficient reversible adsorption of iodine

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Metal–organic frameworks (MOFs) are highly porous materials generally consisting of two building elements: inorganic coupling units and organic linkers.[1] These frameworks offer an enormous porosity, which can be used to store large amounts of gases and, as demonstrated in more recent applications, makes these compounds suitable for adsorptive removal of hazardous materials.[2] A guest-filled phase of twofold interpenetrated 3D metal–organic framework, (**TMU-16-NH$_2$**), was synthesized by the solvothermal reaction of NH$_2$-BDC (NH$_2$-BDC = 2-amino-1,4-benzenedicarboxylic acid), 4-bpdh (2,5-bis(4-pyridyl)-3,4-diaza-2,4-hexadiene), and $Zn(NO_3)_2\cdot 6H_2O$ in DMF at 80 °C for 48 h, and isolated as red color block-shaped crystals. The formula of the compound was determined to be $[Zn_2(NH_2\text{-}BDC)_2(4\text{-}bpdh)].3DMF$ (**TMU-16-NH$_2$**) by single-crystal X-ray diffraction studies, and the phase purity of the bulk material was independently confirmed by powder X-ray diffraction (PXRD). In this way, 1D channels are formed with a width of 13.4 × 17.6 Å^2, permitting a double interpenetration that results in four much smaller 1D channels each of 4.6 × 7.1 Å^2 in cross-section. In this compound, we successfully loaded the porous crystals with I_2 by suspending them in a solution of I_2 in cyclohexane. The delivery of I_2 from **TMU-16-NH$_2$**-I_2 performed in ethanol, a nonaromatic solvent, at room temperature.

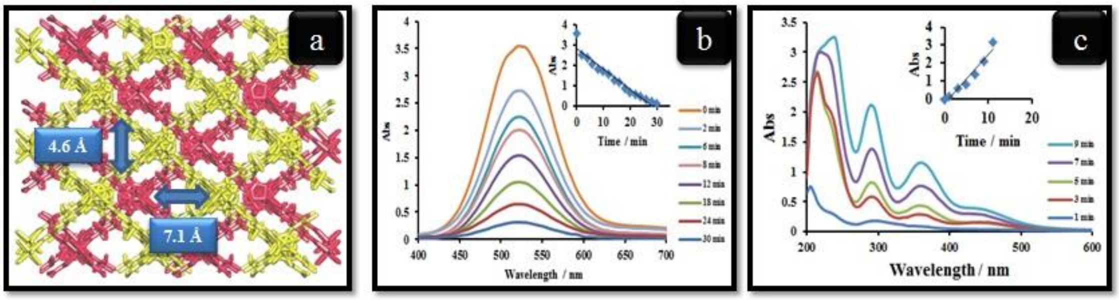

Fig. 1.a) Cylinder model representations of the structures of the open phase **TMU-16-NH$_2$**. The two interpenetrating frameworks are shown in red and yellow. The disordered guest molecules in **TMU-16-NH$_2$** are omitted for clarity, b) UV/vis absorption spectra for the I_2 sorption by single crystal **TMU-16-NH$_2$**,c) Temporal evolution of UV/vis absorption spectra for the I_2 delivery from a single crystal of **TMU-16-NH$_2$** in 3 mL of MeOH. Inset: The controlled delivery of I_2 ($[I_2] = Kt$) in the first 30 and 10 min, respectively.

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Synthesis and structural characterization of some novel mono and binuclear complexes of first row transition metals based on the substituted terpyridyl ligands

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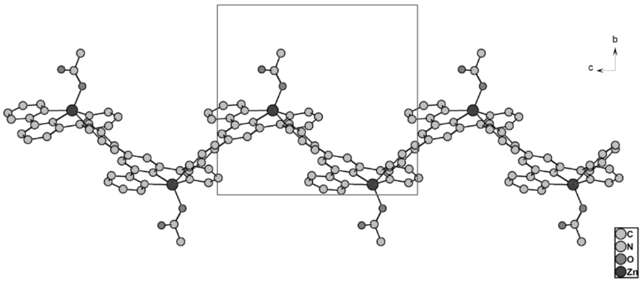
2,2':6',2"-Terpyridine ligand (tpy) has been studied for many years as a strong chelating ligand to a variety of metal ions including main group elements, early and late transition metals. [1,2] These complexes have been studied for their applications including photo-sensitizers, DNA metallo-intercalators, medicinal chemistry and molecular self-assembly for decades. [3] We have recently reported that for the formation of chalcogeno-acetylene by copper -(I)-terpyridine catalyst, a mixture of copper(I) iodide and atpy (atpy = 4'-(4-anisyl)-2,2':6',2"-terpyridine) results in the best performance among a series of copper(I) salts. [4] In this context, we report an approach to the formation of coordination polymers using the reaction of a series of terpyridine ligand containing potential oxo (tpyOH) or nitrogen atom donor (pytpy). Therefore, the reactions of some 4'-substituted terpyridine ligands with a series of first row-transition metals have been investigated. The results reported here in are important in design of crystal engineeing by a controllable fashion. The thermal behaviors of these complexes have also been investigated.



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Zinc ferrite nano-composite catalyzed photodegradation of Disperse Yellow 3 at various buffer pHs: A kinetic study

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Wastewaters from industries cause a large amount of chemically unpleasant materials such as organic or inorganic compounds into the echosystem that are harmful for life of human. Nearby 10-15% of all the dyes used in the industry are lost inside wastewater pending synthesis and processing.[1] Various techniques have been used for removal of pollutant wastes,[2,3] but the most of these methods are useless and there is a need to expand more effective methods in destroy dyes from the wastewater.[4,5] A proper method for elimination of pollutants from water is utilization of non-poisonous photocatalyst like nano-metal oxide semiconductors for mineralization of organic pollutants to carbon dioxide, water and mineral acids.[6,7]

In this research, the photocatalytic activity of zinc ferrite nano-composite was tested for degradation of Disperse Yellow 3 dye under 400 W high pressure mercury lamp under aerobic conditions at room temperatureat in buffer pHs. Decolorization process was monitored by spectrophotometrical method. The effects of UV light, buffer pHs, radiancy time and nano-photocatalyst amounts were studied. The photocatalytic degradation of dye was found to obey from a first order reaction. Kinetic as certainment of photodegradation of Disperse Yellow 3 dye, showed that the photoprocess is in agreement with improved Langmuir-Hinshelwood (L-H) model. Based on L-H model, rate constant and L-H adsorbtion constants at all media were calculated.

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Nanostructures mercury(II) coordination compounds: Spectral, thermal, DNA cleavage and antimicrobial activities

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During the past two decades, considerable attention has been paid to the chemistry of the metal complexes of Schiff bases containing nitrogen and other donors.1,2 This may be attributed to their stability, biological activity and potential applications as catalyst.3 Also, it is well known that some drugs have higher activity when administered as metal complexes than as free ligands.4 In this work, synthesis of a new series of mercury(II) complexes with a N2-Schiff base ligand entitled as 2-methyl-N1,N5-bis((E)-3-phenylallylidene)pentane-1,5-diamine (L) is described. The compounds were characterized by various techniques such as elemental analysis, FT-IR, UV–visible, NMR spectra and conductometry. Accordingly, HgLX2 (X = Cl−, Br−, I−, SCN− and N3−) was suggested as molecular formula of the complexes. Furthermore, the ligand and its mercury halide/pseudohalide complexes have been screened in vitro both for antibacterial activity against some gram-positive and gram-negative bacteria and also for antifungal activity (Fig. 1). The metal complexes were found to be more active than the free Schiff base ligand. The results indicated that all compounds are antibacterial and antifungal active. The DNA cleavage ability of the ligand and its complexes were monitored by electrophoresis technique. Thermal behaviors of ligand and its mercury complexes were studied from room temperature to 900 °C under argon atmosphere. Some activation parameters such as enthalpy, entropy, activation energy and Gibbs-free energy of the thermal decomposition steps were calculated by graphical methods. Moreover, nanostructures form of these new mercury(II) complexes have been also prepared through sonochemical process confirmed by XRD and SEM.

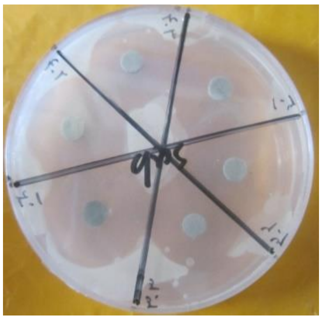

Fig. 1. Image of inhibition zones around constructed disks ($HgLI_2$ and $HgL(N_3)_2$ against Bacillus subtilis).

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Synthesis and characterization of platinum-cobalt nanosheet thin film at liquid/liquid interface, a suitable catalyst for *p*-nitrophenol reduction

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Toluene–water interface has been employed to prepare metal nanocrystals by the reduction of the metal salts. The liquid–liquid interface itself has been exploited to form nanocrystals and their assemblies to a limited extent, such as Au, Ag, Pt, Pd and Cu NPs, chalcogenides such as CdS, CdSe, ZnS, CoS, NiS, CuS, PbS, oxides such as ZnO, CuO and nanostructured peptide fibrils.1 Thin films are of great importance for many chemical and electrochemical applications such as electronic devices, sensors, catalysts and electrodes. The method involves dissolving an organic precursor of the relevant metal in the organic layer and the appropriate reducing reagent in the aqueous layer. The product formed by the reaction at the interface contains ultrathin nanocrystalline films of the relevant material formed by closely packed nanocrystals.2 This study discusses synthesis of platinum-cobalt nanosheet thin film via a simple reduction of organometallic precursor including [PtCl2(cod)], (cod=cis, cis-1,5-cyclooctadiene), in the presence of [Co(acac)2] at toluene-water interface. The structure and morphology of the thin film was characterized with X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive analysis of X-ray(EDAX) techniques. TEM measurements revealed that the PtCo bimetallic thin film contains nanosheets. The catalytic activity of the nanosheets was investigated in the reduction of p-nitrophenol to p-aminophenol.

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Photodegradation kinetics of Disperse Flor Pink BG in the presence of Zinc Oxide nanoparticlesat various pHs

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The industrial colors are one of the most contaminant compounds. Some of the industrial dyes are poisonous that may be a reason for their carcinogenic effects.1,2 However, these dyes have widely been used in cloth, cosmetics and health, food colorants, edition, and medicinal industries. So dyes especially azo dyes have been found to be very damaging from the environment points of sight. In last years, environmentally chemists have presented a intermezzo of manners for removal of unpleasant chemicals included physical adsorption,3 progress oxidation processes, 4-6 biosorption7 and finally photocatalytic processes. One of the effective methods for contaminant removal is photocatalytic degradation that uses ultera violet light and semiconductor as effective factors. The goal of semiconductor photocatalysis is to efficiently eliminate organic contaminants.

In this research, photocatalytic degradation of Disperse Flor Pink BG dye was examined in the presence of zinc oxidenanoparticles at non-buffer pHs under 400 W high pressure mercury lamp under aerobic conditions at room temperature. The effects of UV light, non-buffer pHs, irradiation time and nano-powder zinc oxide amounts were investigated. The photochemical degradation of dye was found to be have as a first order reaction. Kinetic investigation of photodegradation of Disperse Flor Pink BG dye, showed that the reaction obey from improved Langmuir-Hinshelwood (L-H) model. Based on the L-H model,observed rate constant, half time of degradation process and adsorbtion constant were graphically calculated.

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Sonochemical synthesis of some nanostructure cadmium(II) complexes: thermal behavior, antimicrobial activity and precursor for the synthesis of cadmium(II) oxide

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However, cadmium is one of the most toxic metallic elements but it seems that complexation of this metal ion by coordination with ligands is a way for decreasing of its toxicity and also using of these compounds as materials with potential medicinal properties[1] so that coordination compounds of cadmium with Schiff base ligands have been also investigated in the various fields of medicinal chemistry.[2-4] Among the different approaches used for synthesis of nanomaterials, sonochemistry has been extensively examined over many years.[5] Synthesis and characterization of a new Schiff base ligand titled as N^1,N^2-bis((E)-3-(2-nitrophenyl)allylidene)butane-1,4-diamine and its cadmium(II) complexes is the purpose of this work. Compounds were synthesized in alcohol solution and then characterized by FT-IR, NMR, UV–visible spectra and molar conductance. Based on spectral data, the general formula of $CdLX_2$ (X = halide and/or pseudo-halide) was proposed for the cadmium complexes. The nanostructure cadmium complexes were prepared by sonochemical method. The new nano-structures compounds were again characterized by XRD and SEM. Moreover, CdO nanoparticles were prepared by calcination of cadmium chloride complex at 500 ˚C and characterized by XRD and SEM. Furthermore, the antimicrobial activities of compounds against some Gram-positive and Gram-negative bacteria and two fungi of *Candida albicans* and *Aspergillusorayzea* were screened. All compounds showed antimicrobial effects and the complexes had the higher activity with respect to free ligand. The DNA cleavage ability of the complexes was studied by agarose gel electrophoresis method (Fig. 1). Finally, thermal behaviors of all compounds were studied by TG/DTG analysis data.

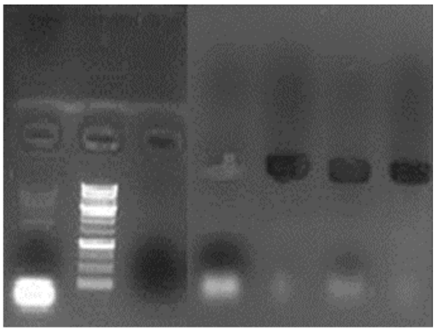

Fig. 1. Gel electrophoresis picture for DNA cleavage abilities of cadmium complexes.

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Some new nanostructure cadmium(II) complexes: thermal analysis data, biological activity, DNA cleavage and precursor for synthesizing CdO nanoparticles

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Modern chemists still prepare Schiff bases, and nowadays active and well-designed Schiff base ligands are considered ‘‘privileged ligands’’. A great deal of Schiff bases have been reported to possess biological activities.[1,2] On the other hand, it has been found that in general the complexation of Schiff bases with most transition metal atoms reinforces their biological activities.[3,4] In continuation of our previous studies on new Schiff base complexes,[5] herein, we report synthesis, spectroscopic, thermal characterization and antimicrobial investigation of some new cadmium halide and pseudo-halide complexes with bis((E)-3-(4-(dimethylamino)phenyl)allylidene)butane-1,4-diamine as a N_2-donorSchiff base. The newly synthesized ligand and its complexes have been characterized on the basis of the results of the molar conductance and spectroscopic studies viz. FT-IR, ^{1}H and ^{13}C NMR and UV–visible. Antibacterial/antifungal activities of the compounds were screened by the disc diffusion method against the Gram-negative bacteria *Escherichia coli* and *Pseudomonasaeruginosa*, the Gram-positive bacteria *Staphylococcus aureus* and *Bacillus subtilis* and the fungi strain *Aspergillus niger* and *Candida albicans*. The antimicrobial activities were determined for all compounds and the complexation was found to enhance the inhibitory activity. Moreover, the DNA cleavage potential of the compounds was investigated by electrophoresis method. Thermal behaviors of all compounds were studied by TG/DTG analysis data. Finally, nanostructure forms of the cadmium complexes were prepared under sonochemical conditions. The nano-structure character was confirmed by FT-IR, XRD and SEM techniques. Also, the cadmium complexes were used as precursors for preparing of CdO nanoparticles under calcination method at 500 ˚C that confirmed by XRD and SEM analyses.

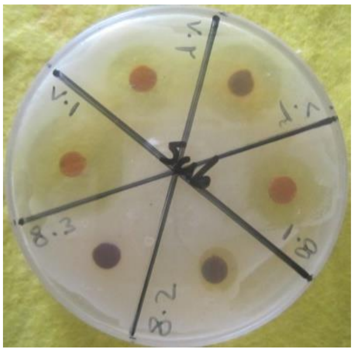

Fig. 1. Image of inhibition zones around constructed disks ($CdLCl_2$ and $HgLBr_2$ against Bacillus subtilis).

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Synthesis, spectral characterization, in vitro antibacterial/antifungal activities and DNA cleavage of some nanostructure Zn(II) compounds

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Among different metal elements, zinc is one of the essential chemical elements for living organisms and the second most abundant transition metal in the human body, and has the important structural, catalytic and enzymatic roles.[1,2] Also, the role of zinc in nucleic acid chemistry is noteworthy because Zn(II) ions are integral constituents of zinc finger proteins, which recognize DNA and bind to DNA.[3] On the other hand, the use of coordination compounds as precursors for the preparation of zinc(II) oxide is an operative approach to synthesize metal oxides with controlled sizes and morphologies.[4] Herein we want to report synthesis and characterization of some new zinc(II) complexes with a new Schiff base ligand obtained by condensation of (2*E*)-3-phenylprop-2-enal and butane-1,4-diamine. Synthesized compounds were identified by various techniques including FT-IR, UV–visible, ^{1}H and ^{13}C NMR spectra, and conductometry. The nano-structure zinc complexes were prepared under sonochemical conditions confirmed by XRD and SEM analyses (Fig.1). Also, ZnO nanoparticles were synthesized by direct thermolysis of zinc iodide complex suggested based on XRD and SEM images. The antimicrobial activity of the ligand and its zinc complexes were studied against four bacteria *(Staphylococcus aureus, Bacillus subtilis, Escherichia coli* and *Pseudomonsaeruginosa)* and two fungi (*Candida albicans* and *Aspergillusorayzea)* by disc diffusion and minimum inhibitory concentration (MIC) methods. Moreover, cleavage of DNA by all the synthesized compounds was examined using electrophoresis technique.

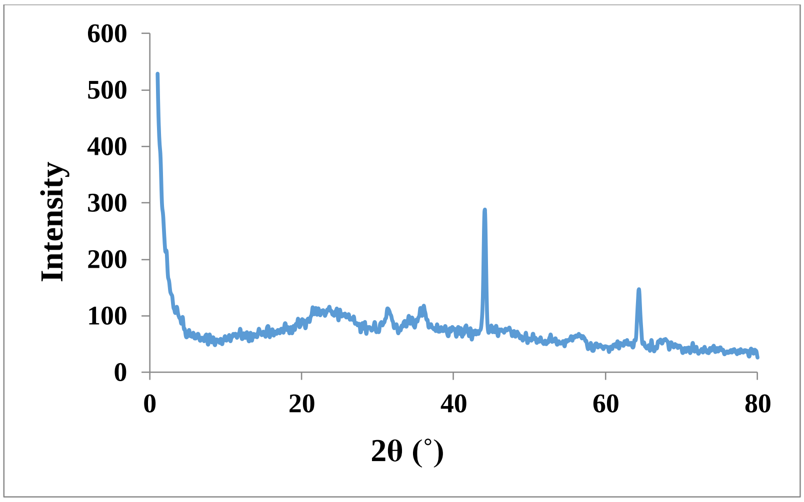

Fig. 1. XRD pattern of zinc bromide complex.

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Synthesis and characterization of Ni(II)-Sca complex

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Saccharin (or o-sulphobenzoimide) is widely used as an artificial sweetener. The chemistry of saccharin has attracted attention because of its suspected carcinogenous nature and the potential use of saccharin as an antidote for metal poisoning. Metal complexes of saccharin may also have relevance to the understanding of its human metabolism. [1]

The Ni(II) complex, $[\mathrm{Ni}\,(\mathrm{phen})_2\,(\mathrm{Sac})_2]$, where phen is 1,10-phenanthroline and Sac is saccarinato, has been prepared and characterized by elemental analysis and spectroscopy methods. The infrared spectra of the complex show a group of bands due to saccarinato ligandes. The sulphonyl stretching vibrations are observed at 1250 and 1153 cm^{-1} for $\upsilon_{as}(SO_2)$ and $\upsilon_s\,(SO_2)$, respectively and band for $\upsilon(CO)$ is observed at 1658 cm^{-1} [2]. The absorption bands seen in λ= 400-900 nm are typically characterized by d–d transitions. The intense absorption bands seen in the UV region are assigned to ligand-centered ($\pi \rightarrow \pi^*$and $n \rightarrow \pi^*$) transitions.[3]

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Synthesis and characterization of platinum-palladium-nickel-zinc nanoparticles thin film at liquid/liquid interface, a suitable catalyst for methanol oxidation

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Fuel cells technology is widely believed to play a key role in the next generation of environmentally friendly energy solutions. The poor performance of the traditional catalysts limits the widespread commercialization of fuel cells. One of the major challenges in the successful commercialization of fuel cells is the development of cost-effective highly durable catalysts. Alloying is a strategy that has been used to find non-Ptelectrocatalysts that are effective and less expensive for the MOR. Mixing two or more metals can result in a catalyst that has distinct properties from its monometallic components.[1] Toluene–water interface has traditionally been employed to prepare particle assemblies and films of metals and semiconductors.[2] The interface between water and an organic liquid, however, has not been investigated sufficiently for possible use in preparing nanocrystals and thin films of alloys.[3] In this study, we demonstrate the use of liquid–liquid interface as a medium for preparing ultrathin film of Pt-Pd-Ni-Znnano catalyst for methanol oxidation reaction. An organometallic complex and $NaBH_4$ were choosen as platinum precursor and reducing agent, respectively. The obtained film was characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and energy dispersive analysis of X-ray (EDAX) analysis.Catalytic activity of Pt-Pd-Ni-Znnanoalloy thin film was investigated in methanol oxidation reaction.

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Synthesis of magnetic hollow silica nano composites for targeted drug delivery

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Magnetite particles (microspheres, nanospheres and ferrofluids) are widely studied for their applications in biology and medicine such as enzyme and protein immobilization, magnetic resonance imaging (MRI), RNA and DNA purification, magnetic cell separation and purification and magnetically controlled transport of anti-cancer drugs, as well as hyperthermia generation.[1–3] In this work, we report a synthesis of multifunctional core/shell silica nanocomposites in mixed water–ethanol solvents at room temperature. Water-soluble CTAB-stabilized nanoparticles (Fe_3O_4) are used as templates and tetraethoxysilane (TEOS) is used as a precursor to fabricate multifunctional hollow silica nanocomposites. Owing to the high abundance of folate receptors in many cancer cells, folic acid is used as the targeting ligand. By coupling with folic acids, the multifunctional silica nanocomposites conjugates are successfully used for tumor cell imaging. The structural, morphological and magnetic properties of as-prepared sample were characterization by X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectra, scanning electron microscopy/energy dispersive x-ray analysis (SEM-EDAX) and magnetic measurements were investigated using vibrating sample magnetometer (VSM). Our results demonstrate a robust hydrophobic nanoparticles-based approach for preparing multifunctional and biocompatible hollow silica composites, which could be also suitable for silica coating of other kinds of nanoparticles.

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Synthesis and structural characterization of a novel dichloridotetrakis (1-H-indazole-κN^2) copper(II) complex

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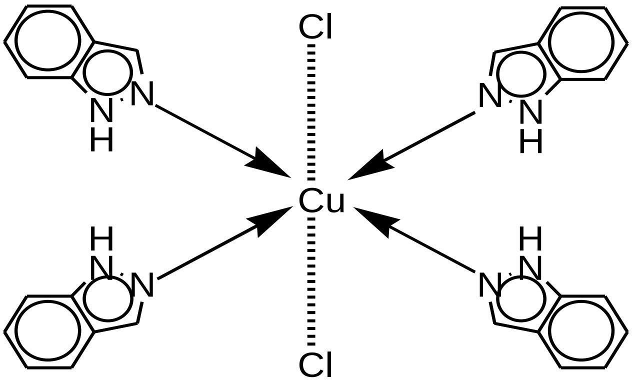
The Cu atom in the title compound, $[CuCl_2(C_7H_6N_2)_4]$, is surrounded by four N-heterocycles that define an N_4 squareplanar geometry. The coordination geometry is distorted towards an elongated octahedron owing to the presence of the two Cl^- anions that this prolongation tally the Jahn-Teller distortion, which are located at about 2.01 Å above and below the square plane.[1,2,3] There are two independent molecules in the asymmetric unit, each with their the copper(II) cations are located on centres of inversion, whereas the two crystallographically independent 1H-indazole ligands and the chloride anion occupy general positions. The crystal structure of the title compound, $[CuCl_2(C_7H_6N_2)_4]$, has been characterized by X-ray crystallography. The complex crystallizes in the triclinic space group $P\bar{1}$ with a = 10.338 (1) Å, b = 10.923 (1) Å, c = 13.730 (1) Å, α = 72.545 (3)°, β = 77.329 (3)°, γ = 73.890 (3)° lattice specification.



Scheme. The structure of $[CuCl_2(C_7H_6N_2)_4]$.

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New nano-structured Zn(II) compound: synthesis, structure, DFT and Hirshfeld surface analysis

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In the last few years the analysis of crystal structures using tools based on Hirshfeld surfaces has rapidly gained in popularity. Hirshfeld surfaces in the crystal structure were constructed on the basis of the electron distribution calculated as the sum of spherical atom electron densities.[1,2] In this work, we report synthesis and structure of a four-coordinated Zn(II) complex with a N_2-schiff base ligand and azide anions. The nano-structure Zn(II) complex was Synthesized by sonochemical method and characterized by FT-IR, XRD and SEM. Complex structure was determined by single crystal X-ray crystallography. This compound crystallizes in a monoclinic system with space group C2/c. The molecular structure shows distorted tetrahedral geometry. The geometry of the compound was optimized using DFT method with the B3LYP function. There is a good agreement between structural parameters from DFT calculation and X-ray crystallography result. We also used the Crystal Explorer software to calculate and display the Hirshfeld surface and 2D fingerprint plot (Fig. 1). The N···H/H···N interactions can be seen in the Hirshfeld surface as the bright red areas. The other visible spots on the surface correspond to C···H/H···C contacts. The 2D fingerprint plot reveal that H···H contact is the main intermolecular interaction (49.2%). The N···H/H···N interactions comprise 28.3% of Hirshfeld surface and are represented by two spikes in the 2D fingerprint plot. Also, the proportion of C···H/H···C interactions is 19.5% and these interactions are observed as wings on the top left (H···C interaction) and bottom right (C···H) of the 2D fingerprint plot.

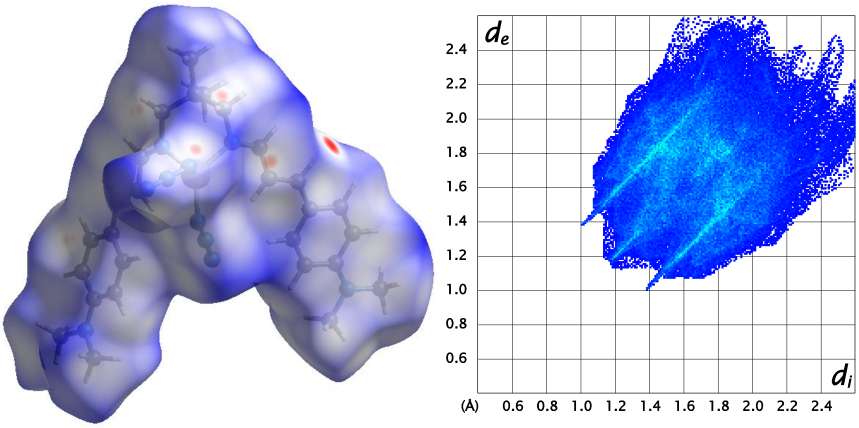

Fig. 1. (left) 3D Hirshfeld surface mapped with d_{norm}, (right) 2D fingerprint plot.

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Green synthesis of silver nanoparticles:Surface plasmons resonance (SPR) spectroscopy

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From visual inspection, change in color of Persian oak (Querusbrantii)a corns bark extract from yellow to cloudy grayish brown (figure 1b) by adding silver nitrate solution is due to the nanoparticle surface plasmons. The UV-Vis experiment confirms the formation of silver nanoparticles. In figure 1a, we show the spectra for a reaction time of 1440 h. The curves display a pronounced peak at 420-470 nm, as expected from the plasmon resonance of silver nanoparticles. During the reaction period, an increase in absorbance was observed in this wavelength, which can be due to the increase in production of colloidal silver nanoparticles.

Quercusbrantii a corns were collected from a population growing in Chalabeh (34˚21´ N 47˚15´ E, altitude 1443m) from Kermanshah. Quercusbrantii, the Persian oak (covering more than 50% of the Zagros forest area) is the most important tree species of the Zagros in Iran. Barks of these acorns, i.e. fruit wall (Pericarp), were dried at room temperature, ground by using mortar and pestle and stored at refrigerator (4°C). In general, oak barks depending on different plant parts contain types of tannins, specially gallotannic and quercitannic acids, in different levels.It may be noted that all tannins are phenolics,whichplay both roles as reducing and stabilizing agent.

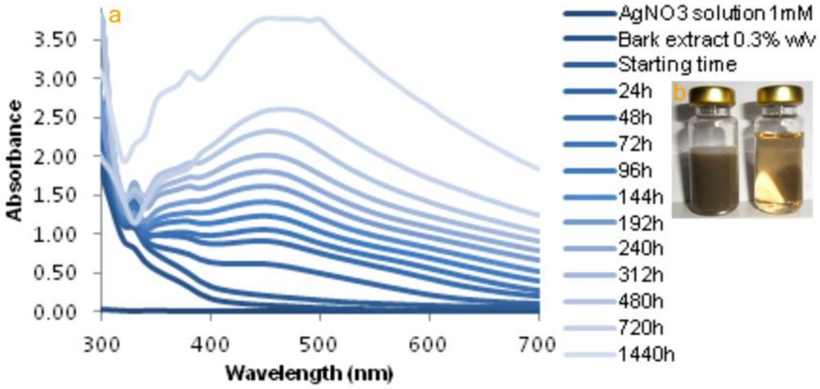

Fig. 1.a) UV-Vis absorption spectrum of the produced colloidal silver for VR of 1:1 b) Color changing due to the formation of silver nanoparticles.

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Folin-Ciocalteu reagent:A molybdotungstophosphoricheteropolyanion reagent for quantifying phenolic and polyphenolic antioxidants

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Folin-Ciocalteau (F-C) reagent consists of a mixture of the heteropolyacids, phosphomolybdic and phosphotungstic acids in which the molybdenum and the tungsten are in the 6+ oxidation state. It was first introduced by O. Folin and D.Ciocalteu in 1927. On reaction with a reductant, the molybdenum blue and the tungsten blue are formed, which may be having either blue (or) green colour with a λ_{max} of 620–780 nm, and the mean oxidation state of the metals is between 5 and 6. The following reaction is slow at acidic pH and faster when basic. It is very sensitive, precise but lack specificity. Singleton and Rossi further improved the method with a molybdotungstophosphoricheteropolyanion reagent that reduced polyphenols more specifically with the λ_{max} for the product at 765 nm.They also imposed mandatory steps and conditions to obtain reliable and predictable data: (1) proper volume ratioof alkali and F-C reagent; (2) optimal reaction time and temperature for color development; (3) monitoring of optical density at 765 nm; and (4) use of gallic acid as the referencestandardphenol.

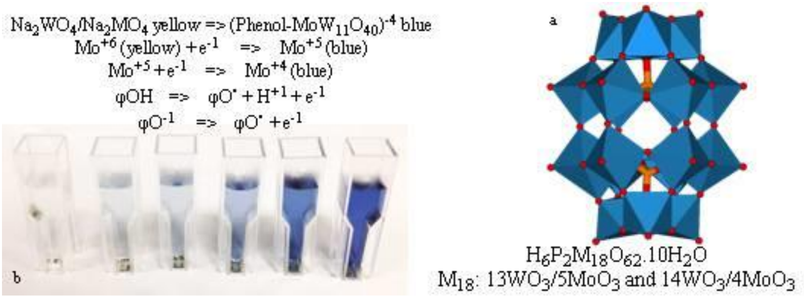

Fig. 1. Dawson structure of F-C reagent (a) and oxidation of phenols by F-C reagent (b).

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Synthesis, characterization and topological analysis of coordination polymers containing d^{10} metal ions

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Over the past few decades, extensive endeavors have been focused on the rational design and controllable synthesis of coordination polymers due to their fascinating structures/topologies, gas storage, catalysis, separation, drug delivery and potential application in different areas of science such as materials and nanotechnology. [1-2] From the viewpoint of the synthetic strategy of crystal engineering, the suitable selection of organic ligand and metal ions play a structure directing role on the construction of coordination polymers.[3-4] In fact, the topology of coordination polymer can be controlled by metal centers, structure/conformational flexibility and coordination mode of the bridging ligands. Also the influence of molar-ratio of organic and metal tecton[5] and solvent system on the structure of resulted coordination polymer have been investigated.[6]

In this regard, we consider self-assembly of bridging ligands as an organic tecton and d^{10} metal ions as a metallic tecton. In this work, several coordination polymers have been synthesized from related metal salts and selected bridging ligands. These compounds have been characterized by several spectroscopic methods as well as x-ray structural analysis. Crystal structure analysis shows that, topology of resulted d^{10}-metal ion containing coordination polymers depend on metal center, anions and reaction conditions.

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Synthesis and Surface modification magnetite nanoparticles with poly (ethylene glycol) and folic acide for improved intracellular uptake

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Magnetite particles (microspheres, nanospheres and ferrofluids) are widely studied for their applications in biology and medicine such as enzyme and protein immobilization, magnetic resonance imaging (MRI), RNA and DNA purification, magnetic cell separation and purification and magnetically controlled transport of anti-cancer drugs, as well as hyperthermia generation.[1–3] In this work, Magnetite nanoparticles (NPs) were synthesized by co-precipitating Fe^{2+} and Fe^{3+} in an ammonia solution. Then, Super paramagnetic magnetite nanoparticles were surface-modified with poly (ethylene glycol) (PEG) and folic acid, respectively, to improve their intracellular uptake and ability to target specific cells. The structural, morphological and magnetic properties of as-prepared sample were characterization by X-ray diffraction (XRD), Fourier transform infrared (FT-IR) spectra, scanning electron microscopy/energy dispersive x-ray analysis (SEM-EDAX) and magnetic measurements were investigated using vibrating sample magnetometer (VSM). PEG and folic acid were successfully immobilized on the surfaces of magnetite nanoparticles and characterized using fourier transform infrared spectra. The present finding show that surface modification protocols can also be used to modify the surfaces of other nanoparticles for targeting intracellular delivery.

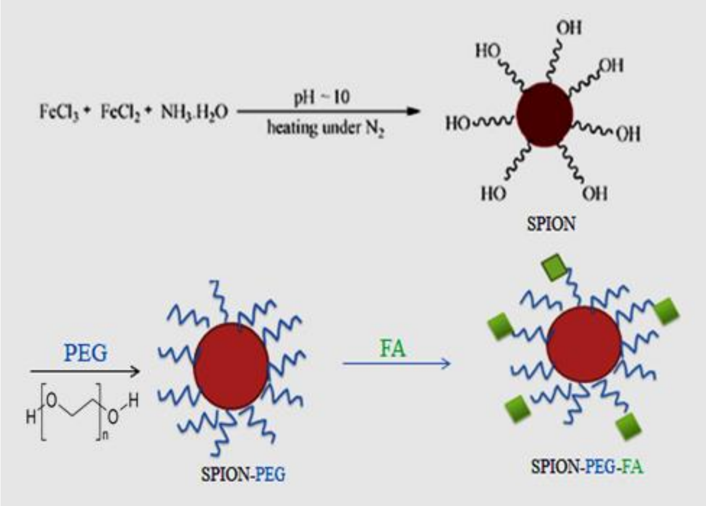

Fig. 1. Chemical reaction schemes for immobilizing of PEG and FA.

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Magnetically separable nanocatalyst for selective oxidation of sulfides to sulfoxides

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A molybdenum complex, $[MoO_2Cl_2(DMSO)_2]$, was immobilized on Schiff base magnetic $Fe_3O_4@SiO_2$nanoparticles by covalent linkage. First, superpara magnetic Fe_3O_4 nanoparticles were prepared by the co-precipitation method.[1] Secondly, the surface of Fe_3O_4 was encapsulated with silica in order to increase the functionality and stability of nanoparticles. Then, the Fe_3O_4 nanoparticles were surface-modified with 3-aminopropyltriethoxysilane (APTS) which introduced $-NH_2$ on to the surface of support.[2] After functionalization by APTS, free amino groups on the surface can react with many different carbonyl compounds to form Schiff base ligand. For preparation of $Fe_3O_4@SiO_2$/Schiff base, $Fe_3O_4@SiO_2-NH_2$ nanoparticles were reacted with dialdehyde and then reacted with the $MoO_2Cl_2(DMSO)_2$ complex to synthesize Mo(VI) nanocatalyst.

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

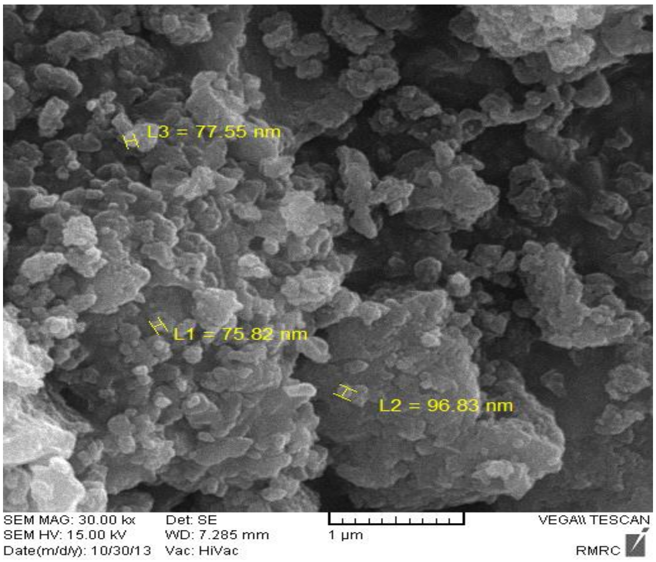

Fig. 1.SEM images of Mo (VI) nanocatalyst

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Electrochemical Behavior and Voltammetric Determination of Insulin at a Gold Electrode Modified With a Nanoparticles of Mo.

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In this work, the Fe_3O_4@SiO_2@schiff-base of Mo(MNPs) was synthesized a multistep procedure and was simultaneously doped in to electropolymerizedpolypyrrole (PPy) film using the cyclicvoltammetry (CV) technique. Scanning electron microscopy (SEM), electrochemical impedance spectroscopy (EIS) and CVs were used to characterize the composite films. Fig.1, shows that the PPy–(MNPs) modified gold (Au) electrode has the highest response towards insulin than with the other constructed electrodes (curve sa.c) and it could be used for further studies with more confidence. As is seen, no electrochemical response to insulin was observed at the surface of Au bare electrode (curve.a). In addition, a pair of smaller redox peak (in comparison to the final modified electrode, curve.c) with weak electrochemical response to insulin was observed when the Au/ PPyelectrode. Enhanced peak current of insulin on the Au/PPy– MNPs film is probably due to the d^0 metal complexes of Mo.

It was found that the prepared nanoparticles have excellent electrocatalytic activity towards insulin oxidation due to special properties of magnetic nanoparticles (MNPs). The common coexisting substances showed no interferences on the response of modified electrode to Insulin. The modified electrode indicated reproducible behavior and a high level stability during the experiments, making it particularly suitable for the analytical purposes.

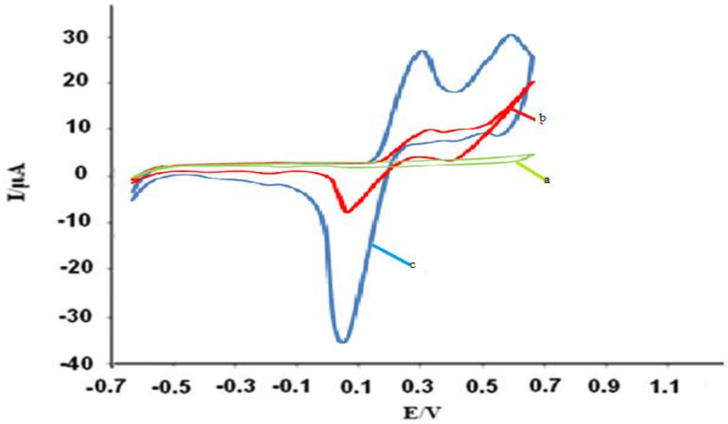

Fig1. Cyclic voltammograms of Au bare electrode (curve. a), Au/PPy electrode (curve. b) and Au/PPy–MNPs electrode (curve. c) in 20 nM of insulin solution (pH= 6) at and scan rate 100 mVs^{-1}.

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Crystal Structure of Bis(dipropylammonium) Tetrachloro-Dimethyl-Tin(IV)

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The property of organotin compounds, R_2SnX_2 (X = halogen), as Lewis acids has been utilized to prepare tetrahalodiorganoastannates, $[R_2SnX_4]^{-2}$.[1] A search of the Cambridge Structural Database (CSD) shows that 17 structures including $[R_2SnX_4]^{-2}$ anions were deposited. Some examples are as follows: bis(dimethylammonium) tetrachloro-dimethyl-tin(IV) (CSD refcode ERIPIF; Diop *et al.*, 2011)[2], bis(4-nitroanilinium) tetrachloro-dimethyl-tin(IV) (CSD refcode HAXQIH; Gholivand *et al.*, 2005)[3] and bis(2-aminopyridinium) dimethyl-tetrachloro-tin(IV) (CSD refcode GEKDEF; Valle *et al.*, 1988)[4]. Here, the structure of a new organotin(IV) compound with formula $[(C_3H_7)_2NH_2^+]_2[Sn(CH_3)_2Cl_4]^{-2}$ is reported. The crystal belongs to space group $P2(1)/n$ with cell dimensions $a = 10.9199(3)$ Å, $b = 13.1459(3)$ Å, $c = 17.8167(5)$ Å, $\alpha = 90.00°$, $\beta = 107.328(3)°$, $\gamma = 90.00°$; the final R value is 0.0306. The cations and anions are aggregated in a two-dimensional arrangement along the *ab* plane, produced by intermolecular $[N—H]_2\ldots Cl$ hydrogen bonds. Each $[Sn(CH_3)_2Cl_4]^{-2}$ anion is connected to four dipropylammonium cations trough the hydrogen bonds noted (Fig. 1).

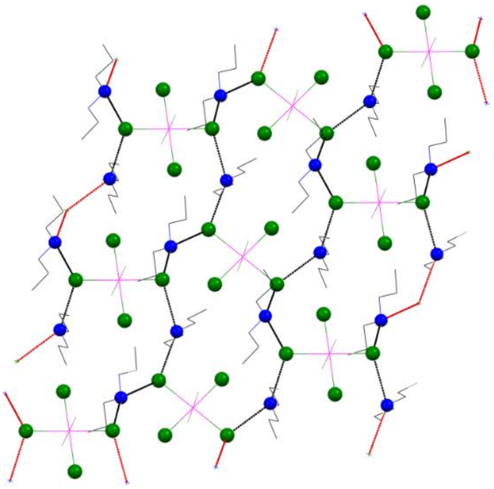

Fig. 1 The 2-D arrangement of cations and anions in the title structure is represented, produced by intermolecular $[N—H]_2\ldots Cl$ hydrogen bonds.

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Synthesis of Nano-Mn_2O_3 from Nanostructures of Mn(II) Supramolecular Complex

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The expanding applications of nano-sized metal oxides in different areas such as super-capacitors [1], catalysts for oxygen reduction [2] and epoxidation of alkenes [3] and *etc*, encouraged us to prepare nano-manganese oxide. The present paper focuses on the synthesis and characterization of a very rare form of manganese oxide, Mn_2O_3, with a novel morphology. Nano-sized Mn_2O_3 particles have been prepared from the nano-supramolecular compound of $[Mn(hpydc)_2(H_2O)_4]$ (**1**) (where hpydc is 4-hydroxy-pyridine-2,6-dicarboxylic acid) upon calcination at 650 ºC under air atmosphere. The size and morphology of nano-structures of manganese oxide were examined by scanning electron microscopy (SEM). It was found that these particles were formed with two types of morphologies, rod and particle, with sizes ranging from 50 to 150 nm. The XRPD pattern of the residue also confirms the formation of nano-Mn_2O_3, as matches well with the standard pattern of Mn_2O_3 (JCPDS card No. 31-0825).

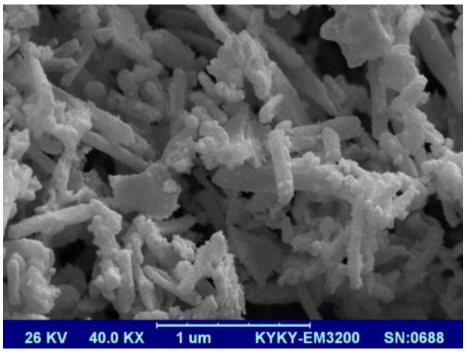

Figure 1. SEM image of Mn_2O_3 nanoparticles prepared by calcination of **1** at 650 ºC.

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Preparation of a titania-supported palladium in water: An efficient heterogeneous catalyst for the Suzuki cross-coupling reaction

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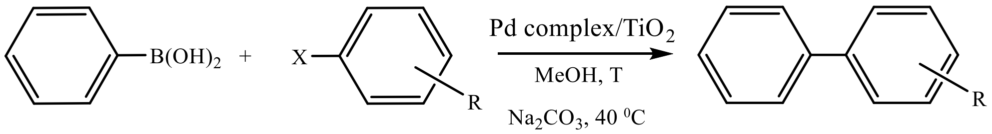
In the recent years Palladium nanoparticles (Pd NPs) have been investigated as efficient catalysts. Among them, the palladium-catalyzed Suzuki cross-coupling reaction has been recognized as powerful and versatile method for the selective construction of carbon–carbon bond formation and widely applied to organic and fine chemical synthesis such as pharmaceuticals, herbicides, natural products, and advanced materials. [1-3] Currently Suzuki cross-coupling reaction is performed mostly with homogeneous palladium salts and complexes, which bring about concerns of high cost and environmental issues at large scale. Therefore, it is highly desirable to develop the recovery of expensive ligands and complexes by immobilization of various complexes on support surfaces. [4] Titania is readily available, cheap, non-flammable and non-toxic, which is very promising support for preparation of green catalysts. In this work, Palladium complex nanoparticles were supported on titania by a very simple method using water as the medium. This catalyst showed excellent activity and stability in Suzuki cross-coupling reaction with different arylhalides (scheme 1). It was found that for aryl halides with various electron-donating and electron-withdrawing groups the coupling reaction of substrate with arylboronic acid proceeded smoothly at low catalyst loading (0.1 mol% Pd). Short reaction times associated with good to excellent yields also expressed the effectiveness of this catalyst in these reactions. Recycling test showed that the catalyst can be used many times in repeating cycles without decreasing in the activity. Hot filtration test confirms the heterogeneous character of the catalytically active species.



Scheme 1

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Efficient Adsorption of Hg^{2+} in a New metal-organic Nanocapsule

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Mercury, in both inorganic and organic forms, is a significant public health and environmental concern because of its toxic, and bioaccumulative properties.[1] So removal of mercury compounds from the environment is so important. The field of infinite coordination polymer particles (ICPs) is rapidly growing due to their potential use in a variety of important applications. These structures, which consist of repeating ligands interconnected by metallic nodes, are appealing because they can be made from readily available and highly tailorable metal and ligand precursors, often have chemically adjustable porosities and high internal surface areas, and provide the researcher with a network structure that can be deliberately and easily modified for many applications, including catalysis, gas storage , separations, photonics, drug delivery and elimination of pollutants from the environment.[2] Herein, we report the application of a ICP, $Fe_3O_4@Zn(btb)_n$, (btb:1,3-bis(tetrazol-5-ylmethyl)benzene) with spherical shape morphology for adsorption of Hg^{2+} from the environment. Experiments showed that these nanocapsules can adsorb Hg^{2+} from the solution effectively.

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Synthesis of TiO_2 @ Zn-Al LDH nanocomposite and its application in dye sensitized solar cells

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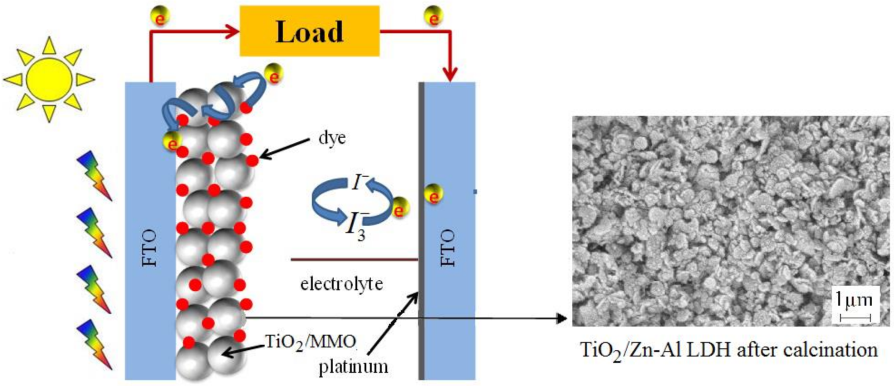
Among the different technologies, solar energy has the unique potential to meet the energy demands. [1] In order to replace the use of fossil fuels and petroleum, the conversion of Sunlight energy into electrical energy seems as one of the most promising solutions for the energy tension problem. Today, Dye-sensitized Solar Cells have attracted much attention because of their low cost. [2]

layered double hydroxides (LDHs), have been a subject of numerous investigations during last three decades. Calcined LDH always produced mixed metal oxides (MMOs) which is considered to be a good electrode material to make the dye-sensitized solar cell (DSSC) because of high purity and good quality control in manufacture on a large scale.[3]

In this study, the TiO_2/ Zn-Al- LDH nanocomposite was prepared by co-precipitation method. Our prepared solids were characterized by chemical analysis, X-ray diffraction (XRD), Scanning electron microscopy (SEM), Fourier transform infrared (FT-IR), Thermo gravimetric analysis (TGA) and UV–vis diffuse reflectance spectra (DRS). The TiO2@Zn-Al LDH was employed as a photo anode in dye-sensitized solar cells (DSSCs). For solar cell device based on TiO2@Zn-Al LDH, the open circuit voltage was 0.81, and the short-circuit current was 2.63 V and a fill factor (FF) of 0.7, and the solar-to-electricity conversion efficiency of 1.51%.



TiO_2/Zn-Al LDH after calcination

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Palladium complexes with 3-phenylpropylamine ligand: synthesis, structures and application in the aerobic oxidation of alcohols as a catalyst via palladium nanoparticles

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Selective oxidation of alcohols to corresponding carbonyl compounds is an important transformation in the chemical industry .[1,2] The most important organic reactions have been performed with homogeneous palladium catalysts, that these catalysts possess many merits such as high turnover number, high activity and selectivity and excellent yields, but from economic and environmental standpoint, heterogeneous catalysts are highly desirable .[3-6] For this purpose, researchers have immobilized palladium complexes and nanoparticles on various supports. CB[6] is a family of macrocyclic molecules that can act as both support and capping agent.

In this work three complexes, *trans*-$[Pd(C_6H_5(CH_2)_3NH_2)_2(OAc)_2]$(**1**), *trans*-$[Pd(C_6H_5(CH_2)_3NH_2)_2(Cl)_2]$(**2**) and *trans*-$[Pd(C_6H_5(CH_2)_3NH_2)_2(PPh_3)_2]2Cl^-$ (**3**) were synthesized. All the complexes **(1–3)** of palladium (II) were fully characterized by IR and NMR spectroscopies. In addition, the crystal structures of **1, 2** were determined by single-crystal X-ray diffraction analysis. Palladium nanoparticles derived from complexes (**1-3**), were supported on cucurbit[6]uril (CB[6]) and identified by X-ray powder diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM) and inductively coupled plasma analyzer (ICP). CB[6]-supported palladium nanoparticles (NP) were used as heterogeneous catalysts for the aerobic oxidation of alcohols to corresponding aldehydes or ketones without over oxidation (scheme 1). CB[6]-Pd NPs (**3**) (prepared from complex **3**) shows better catalytic activity than CB[6]-Pd NPs (**1**), (**2**), as higher yield was observed with it in a relatively short time. This catalytic system showed high activity and selectivity toward alcohols in mild conditions. The catalyst was reused five times without any significant loss in the catalytic activity.

$$\text{Alcohol} \xrightarrow[\substack{\text{Toluene, } K_2CO_3 \\ 40\ ^{o}\text{C, t}}]{\text{CB[6]-Pd NPs}} \text{Aldehyde/Ketone}$$

scheme 1.

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Shynthesis, characterization and application of aluminium doped ZnO@Fe_3O_4 nano-particles as an magnetic sorbent for removal of Cd(II) ions from water samples

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In this research, aluminium doped ZnO@Fe_3O_4 nanoparticles were synthesized by a simple co-precipitation method with controlled pH. The size, morphology and surface coating of the obtained material were characterized by powder X-ray diffraction, scanning electron microscopy and Fourier transform infrared spectroscopy. The feasibility of using aluminium doped ZnO@Fe_3O_4 as a magnetic solid phase extraction sorbent was explored for the separation of Cd(II) ions from aqueous solutions. The important parameters influencing the removal efficiency were studied and optimized. To study of the removal efficiency, the extracted Cd(II) ions were eluted and determined by flame atomic absorption spectrometric detection. Under the optimum removal conditions (mass of nano-sorbent; 200 mg, pH 7.0, sample solution; 100 mL and eluent; 2.0 mL of 2.0 mol L^{-1} acetic acid), a linear range between 0.1 and 60 ng mL^{-1} (R^2= 0.9866) with detection limit of 0.02 ng mL^{-1} for Cd(II) ions were observed. The accuracy of the method was confirmed by analyzing a standard reference material (NIST SRM 1643e). The method was applied for the determination of Cd(II) ions in natural waters.

Synthesis and characterization of new mercury (II) iodide complexes containing carboxamide ligand based on thiazole ring with two different synthetic methods

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Crystal engineering is an emerging field of research that is concerned with the rational design of molecular building blocks and preparation of crystalline materials with the desired properties. In this regard, crystal engineering is closely related to supramolecular chemistry and non-covalent interactions play a key role in the supramolecular chemistry. Hydrogen bond, halogen bond and π-based interactions are the most important non-covalent interactions used in various self-assembly of supramolecular aggregates.[1-4] In the present work the synthesis of new mercury (II) iodide complexes including carboxamide ligand (N-(1,3-thiazole-2-yl)-2pyrazinecarboxamide using two different synthetic methods were performed and characterized by IR spectroscopy, elemental analysis and x-ray crystal structure analysis. X-ray crystallographic analysis of complex $[Hg_2I_4(L)_2]$ (1) obtained from the conventional solution-based method, indicated that the complex (1) has a polymeric structure and iodine atoms are located as a bridge between the mercury atoms. Also according to the data obtained from x-ray diffraction analysis, complex $[Hg_2I_4(L)_2]$ crystallizes in orthorhombic $Pna2_1$ space group and the asymmetric unit of this compound consists of two metallic mercury(II) and two carboxamide ligands. Powder X-ray diffraction has been exploited to investigate the structure of mercury (II) iodide complex prepared by the environmentally friendly solvent-free method (2) and the results showed that the complex (2) has a different crystal structure.

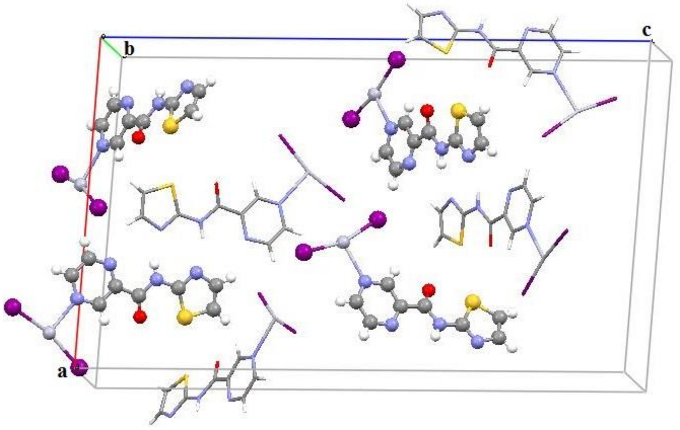

Fig. 1. Representation of unit cell of $[Hg_2I_4(L)_2]_n$

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Synthesis, spectral characterization, crystal structure studies and biological activities of novel Zn- (II) complexes of NOON tertadentate Schiff bases

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Schiff base ligands have received more and more attention, mainly because of their wide application in the fields of synthesis, catalysis, solid phase extraction of metal ions and various types of polymerization. Schiff base with donors (N, O, etc) have structure similarities with neutral biological systems and due to presence of imine group are utilized in elucidating the mechanism of transformation of rasemination reaction in biological system. They show biological activities including antibacterial antifungal, antidiabetic, antitumor, antiproliferative, anticancer, herbicidal, anticorrosion and anti-inflammatory activities.[1-3]

Novel mononuclear Zn (II) complexes were synthesized from the reactions of $Zn(OAc)_2.2H_2O$ with neutral NOON donor tetradentate Schiff bases. The new complexes were fully characterized by using micro analyses (CHN), FT-IR, ^1H NMR, UV–Vis spectra and their solid state structures were determined using single crystal X-ray diffraction.

As a potential application, the biological activity (e.g., antimicrobial action) of the prepared ligands and complexes were assessed by in-vitro testing of their effect on the growth of various strains of bacteria. All tested compounds were very active against both gram-positive and gram-negative bacteria.

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Metal oxides doped with vanadium as efficient catalyst for green oxidative degradation of methylene blue

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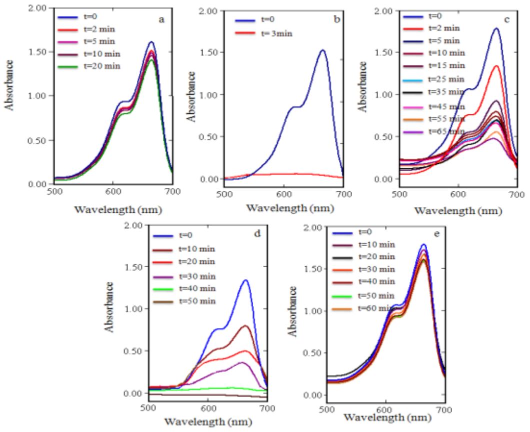
Methylene Blue (MB) as a deep blue colour pigment is one of the most commonly used substances for dyeing cotton, wood and silk.[1] It is potentially harmful to the eco-environment due to its non-biodegradability and high toxicity to aquatic creatures and carcinogenic effects on humans, therefore the degradation of MB dye has attracted much attention.[2]

Nanoparticles of the vanadium doped on ZrO_2, CeO_2 and TiO_2 were synthesized and the physicochemical properties of compounds were characterized by X-ray diffraction (XRD), X-ray absorption near edge structure (XANES), energy dispersive X-*ray* analysis (EDX), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The catalytic degradation of methylene blue (MB) as an organic dye in the presence of these materials and hydrogen peroxide (H_2O_2) as a green oxidant was studied at room temperature. Effects of solution *pH*, catalyst composition and radical scavenging agents on the degree of degradation of MB were also studied. Finally, recoverability and reusability of the V-doped ZrO_2 catalyst was check.



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TiO_2 and ZnO nanoparticles as an efficient catalyst for photocatalytic degradation of some organic dyes under solar light irradiation

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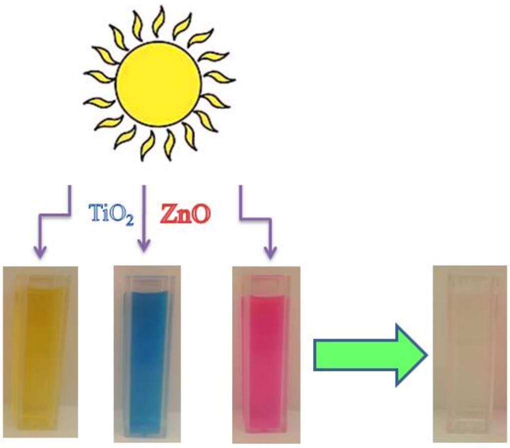
With the development of the textile industry, intense concerns were focused on the contamination of the environment caused by dye pollutants, which caused severe environmental pollution and health problems due to the variety, toxicity and persistence characteristics.[1] Therefore degradation of the dyes in industrial wastewaters has generated considerable attention due to their huge volume of production, slow biodegradation, low decoloration and high toxicity .[2]

Nanoparticles of the ZnO and TiO_2 were synthesized and the physicochemical properties of compounds were characterized by IR, X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). These nanoparticles were used for photocatalytic degradation of various dyes, Rhodamine B (RhB), Methylene blue (MB) and Acridine orange (AO) under solar light irradiation at room temperature. Effect of the amount of catalyst on the rate of photodegradation was investigated.



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Synthesis and Characterization of mixed ligand Cd (II) complex

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Studying the coordination nature of saccharin and determining the binding site(s) to metal ions are perhaps a key to understand the bioinorganic chemistry of saccharin. A lot of saccharin binary and ternary complexes have been reported and investigated. The data obtained indicate that saccharin acts either as a monodentate anion, coordinating via the nitrogen or carbonyl oxygen atoms. [1]

The mixed ligand complex of Cd (II), [Cd (bpy)$(Sca)_2$], where bpy= 2,2' bipyridine and Sca= saccarinato, has been synthesized and characterized by elemental analysis, ^{1}H NMR, FT-IR, UV-visible spectroscopy.

The UV-Vis spectrum shows peaks at 256 nm, 340 nm and 362 nm assigned to ($\pi \rightarrow \pi^*$) and (n $\rightarrow \pi^*$) electronic transitions. The FT-IR spectrum of free ligand saccharin (Hsac) exhibits a weak band at 3441 cm^{-1} due to the υ (N-H) vibration. This band is not present neither in the spectra of its sodium salt nor of the saccharinato complexes. This observation suggests that saccharin reacted with these metal ions in the anionic form. The υ_{as} (CNS) lies a 962 cm^{-1}.

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Differences in the geometries of compounds with $[O]_nP(O)[N]_{3-n}$, $[O]_nP(S)[N]_{3-n}$ and $[C]_mP(O)[N]_{3-m}$ (n = 0, 1, 2, 3; m = 1, 2, 3) segments: A Cambridge Structural Database analysis completed with fourteen new structures

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Recently, we reported on the analysis of hydrogen bond pattern in different families of phosphorous(V) compounds, considering the structure determination of some derivatives and the study of analogous structures deposited in the Cambridge Structural Database.[1,2] These efforts led to find some "empirical rules" which are benefit to prediction of hydrogen bond patterns for such molecules with limited numbers of H-bond donor and H-bond acceptor sites. In continuing, we are interesting to study of the geometry at the P, N, C, O and S atoms in structures with $[O]_nP(O)[N]_{3-n}$, $[O]_nP(S)[N]_{3-n}$ and $[C]_mP(O)[N]_{3-m}$ (n = 0, 1, 2, 3; m = 1, 2, 3) segments. This survey on the CSD was completed with reporting of fourteen new structures belonging to different families of P(V) compounds within a tetrahedral environment and updated our previous studies. The new structures are $[CH_2FC(O)NH]P(O)[NHC_6H_4\text{-}4\text{-}CH_3]_2$ (1), $[C_6H_5]P(O)[NHCH_2C_6H_4\text{-}4\text{-}CH_3]_2$ (2), $[C_6H_5]P(O)[NHC_6H_4\text{-}4\text{-}CH_3][NHCH_2C_6H_5]$ (3), $[4\text{-}Cl\text{-}C_6H_4NH]P(O)[N(CH_3)(C_6H_{11})]_2$ (4), $[4\text{-}Cl\text{-}C_6H_4NH]P(O)[NC_4H_8O]_2$ (5), $[4\text{-}Cl\text{-}C_6H_4NH]P(O)[NC_5H_9\text{-}4\text{-}CH_3]_2$ (6), $[4\text{-}CH_3\text{-}C_6H_4NH]P(O)[NC_5H_9\text{-}4\text{-}CH_3]_2$ (7), $[4\text{-}Cl\text{-}C_6H_4NH]_3P(O)$ (8), $P(S)[NH^tBu]_3$ (9), $[CH_3O]_2P(S)[NHNHC_6H_5]$ (10), $[4\text{-}Cl\text{-}C_6H_4O]P(O)[NHC_6H_{11}]_2$ (11), $[4\text{-}Cl\text{-}C_6H_4O]P(O)[NHC_6H_5]_2$ (12), $[4\text{-}Cl\text{-}C_6H_4O]P(O)[N(CH_3)(C_6H_{11})]_2$ (13) and $[4\text{-}Cl\text{-}C_6H_4O]P(O)[NHC_6H_4\text{-}4\text{-}CH_3]_2$ (14). The main topics of investigation are as follows: (i) the study of histograms of $P{=}X$ (X = O & S) and $P{-}Y$ (Y = O, N & C) bond lengths in order to a comparison of each bond length in different families of structures involving it, (ii) the analysis of bond-angle sums at the nitrogen atoms bonded to phosphorous in a three-coordinated $[P]N[Z][W]$ environment [Z and W atoms are any atoms from CSD, including H and C] and a comparison between different families including nitrogen atoms, (iii) the analysis of the vector of lone electron pair (LEP) located at the non-planar nitrogen atoms with respect to the $P{=}X$ bond vector and (iv) evaluation of the acceptor directionalities in $N{-}H\ldots X{=}P$ (X = O & S) hydrogen bonds with considering the $H\ldots X{=}P$ angles.

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Determination of metronidazole using citrate-capped CdS quantum dots

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In this work, a novel , ultrasensitive and simple method for the determination of metronidazol was proposed based on the quenching of the fluorescence intensity of citrate capped CdS QDs. CdS quantum dots capped by citrate were prepared at one step. The size, shape, components and spectral properties of Cit-capped-CdS QDs were characterized by transmission electron microscopy (TEM), infrared spectrometry and spectroflourometry. The Cit-capped CdS QDs fluorescent probe offers high sensitivity and selectivity for detecting metronidazol. A good linear relationship was obtained from 1.6×10^{-8} molL^{-1} to 3.0×10^{-4} molL^{-1} for metronidazol. The detection limit was calculated as $5.3\times10^{-9}\mathrm{molL}^{-1}$. When adding other drugs to the Cit– CdS QDs solution, fluorescence spectra of Cit–CdS QDs did not change significantly revealing good selectivity of the sensors towards metronidazol. There is no significant wavelength shift on the fluorescence-quenched signals in the presence of metronidazole at the pH 6. Compare to the organic dyes, these nanoparticles are brighter and more stable against photoble aching. The method presented here is simple, rapid, inexpensive, sensitive and suitable for practical application.

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L-Cysteine-coated CdS quantum dots as selective fluorescence probe for Ceftriaxon determination

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In this work, a novel, sensitive and convenient application based on the quenching of the fluorescence intensity of Cysteine capped CdS QDs by Ceftriaxon was proposed. The modified CdS QDs are water-soluble, stable and highly luminescent. The size, shape, components and spectral properties of Cys-capped-CdS QDs were characterized by transmission electron microscopy (TEM), infrared spectrometry and spectroflourometry. When Ceftriaxon was added into the CdS QDs colloid solution, the surface of CdS QDs generates the electrostatic interaction in aqueous medium, which induces the quenching of fluorescence emission. Under optimum condition, the fluorescence intensity versus concentration showed a linear response according Stern–Volmer equation with an excellent correlation coefficient 0.99. The linearity range of the calibration curve was 1.6×10^{-8} $molL^{-1}$ to 1.0×10^{-3} $molL^{-1}$. The limit of detection is 5.3×10^{-9}M. Result demonstrated that other drugs can not change the intensity fluorescence of CdS quantum dots in the same conditions. The proposed method manifested several advantages such as high sensitivity, short analysis time, low cost and ease of operation.

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Synthesis and characterization of photocatalytic properties of cadmium Sulfide nanoparticles doped with some lanthanide cations.

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Contamination of water resources is one of the most important problems in the world today. With the increasing expansion of industries, significant amounts of pollutants, including pharmaceutical compositions, agricultural pesticides and organic dyes into water resources are. Textile dyes are an important source of environmental pollution. These dyes not only are important colors to water sources but also damages living organisms by blocking sunlight, stopping photosynthesis and therefore disturbing the aquatic life. Conventional biological and physical methods do not degrade this type of pollutants as environmental standards, but chemical methods such as advanced oxidation process in recent years become increasingly desirable. One of the processes used to remove pollutants resistant to biological oxidation is photocatalytic process. By using semiconductors such as TiO_2 , ZnO , ZnS and CdS in the presence of UV light and aqueous solution, power oxide OH radical produced and the radical OH destroys organic pollutants and convert them to CO_2 and H_2O. In this research work, CdS nanoparticles produced by hydrothermal method and used as photocatalyst for the destruction of Red 43 dye. To reduce the band gap of energy, CdS doped with some lanthanide cations and evaluated its effectiveness in removing organic dye. These photocatalysts in visible light are efficient. Because of the doping efficiency, bandgap of energy decreases and reaches into visible light and ultraviolet light is not needed. By using a hydrothermal method, doped CdS with some lanthanide cations synthesized under conditions of various time and temperature and identified by means of XRD, SEM, EDX and DRS.

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Electronic aspects of hydrogen bonds of a new Phosphonylurea

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N-phosphinylureas are some important instances of phosphoramidates that little attention has been given to their biological properties [1] and structural studies. [2] These compounds can cause attractive biological activities due to having urea and peptide moieties. The hydrogen bond plays a key role in the chemistry of life such as protein-ligand interactions and enzymatic activity. [3,4] Moreover, the physico-chemical properties of compounds depend on the presence of intermolecular hydrogen bonds. Hence, the electronic aspects of hydrogen bonds in a new phosphonylurea with formula $4\text{-}FC_6H_5NHC(O)NHP(O)NHCH_2C(CH_3)_2CH_2NH$ have been investigated by NBO and AIM analyses. The weak intramolecular CH…OC hydrogen bond between the *ortho*-proton of the $4\text{-}FC_6H_4NH$ and the carbonyl O atom creates a six-membered ring via the O-C-N-C-C-H bond paths. Furthermore, intramolecular $4\text{-}FC_6H_4N\text{-}H\ldots O{=}P$ hydrogen bond creates a six-membered ring *via* the O-P-N-C-N-H bond paths. In addition, the titled molecule was modeled as clusters in which the target molecule is surrounded by two neighboring conformers and a similar molecule on the basis its solid-state structure (Fig.1). The results of NBO showed that the electronic delocalizations Lp(OC) → σ*(C-H_{ortho}) and Lp(OP) → σ*(N-H) in monomer, LP(O_C) → σ^*(N-H) and Lp(OP) → σ*(N-H) in cluster model well as. AIM analysis revealed the decrease in the ρ value at the bcp of the N-H bond from the monomer to its corresponding cluster due to the titled electronic delocalizations.

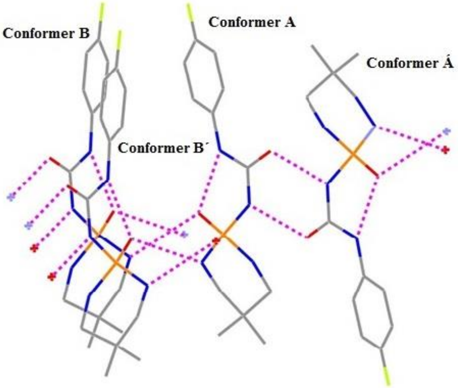

Fig. 1 Model hydrogen-bonded cluster for DFT calculations

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DNA binding and BSA studies of Cu (II) complex containing novel Schiff-base ligand gabapentin derivated: The effect of metal on the mode of binding

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Gabapentin [1-(aminomethyl) cyclohexaneacetic acid, Neurontin, Gpn] is structurally related to the neurotransmitter gamma-aminobutyric acid (GABA) which has been widely studied for its significant inhibitory action in the central nervous system.[1] Gpn has been advanced for the treatment of neuropathic pain, it is a new generation antiepileptic drug that is used as add-on therapy as well as monotherapy in patients with partial seizures [2] new antiepileptic drugs, safe and effective seizure control may become a reality for an increasing number of adults with epilepsy. Epilepsy also poses a considerable economic burden on society. [3] A novel schiff base ligand of gabapentin derivative $[C_{20}H_{23}NO_3]$($\mathbf{L^1}$) has been synthesized by condensation reaction of 2hydroxy1-naphtaldehyde and Gpn. This ligand $\mathbf{L^1}$ is allowed to react with Cu (II) complex. We characterized ligand and complex by elemental analysis, UV–visible, FT-IR, Single crystal X-ray crystallography. The Cu(II) complexe; $[Cu(C_{20}H_{23}NO_3)_2]$ and ligand investigated by their intraction of calf thymus DNA and BSA by electronic absorption spectroscopy, fluorescence spectroscopy. The experimental evidences indicated that the two compounds could parcial bind to CT-DNA via an intercalation mechanism The experimental results also indicate that the probable quenching mechanism of fluorescence of BSA is mainly a static quenching procedure.

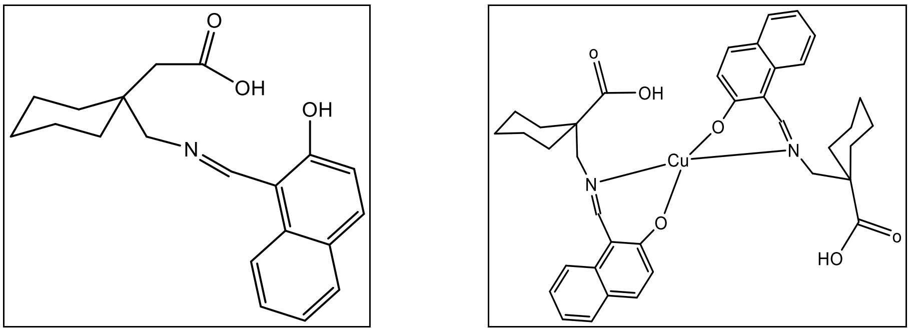

Fig. 1. struchers of the ligand and Cu (II) complex

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Copper (II) complex with a new Unsymmetric Schiff base Immobilization of onto Montmorillonite-K10: As an effective catalyst for aerobic oxidation of alcohols unde air in water solvent

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Unsymmetric Schiff base complexes have attracted more attention in recent years their diverse effects in catalytic reactions. Due to their high dissymmetry, unsymmetric metallosalen complexes are harder to prepare than symmetric ones.[1] The oxidation of alcohols into aldehydes and ketones is a significant transformation in organic chemistry with recognized industrial importance. Selective oxidation of benzyl alcohol to benzaldehyde is a practically important reaction for the production of chlorine-free benzaldehyde required in the perfumery and pharmaceutical industries.[2] copper-catalyzed aerobic alcohol oxidations have gained enormous attention and many efforts have been made to develop efficient oxidation systems. Although homogeneous catalysts exhibit excellent activity and selectivity, technical problems as the difficulty in product separation have slowed their industrial applications. On this way, the studies on the heterogeneous catalytic activities of copper active sites. [3]
A novel Unsymmetric schiff base ligand (L^1) has been synthesized by condensation reaction of reacting 2,4dihydroxy acetophenone and 2pyridine carbaldehyde and 1,2phenylendiamine. This ligand L^1 is allowed to react with Cu (II) complex. We characterized ligand and complex by elemental analysis, UV–visible, FT-IR, H^1-NMR. The obtained complex were incorporated into Montmorillonite-K10 nanoclay via simple ion-exchange reaction and were identified by FT-IR, XRD, TGA/DTA, SEM and TEM techniques. we used this catalyst in aerobic oxidation of alcohols and investigated by gas chromatography. Based on the XRD results of the new nanohybrid materials, the Schiff base complexes were intercalated in the interlayer spaces of clay. SEM and TEM micrographs of the clay/complex shows that the resulting hybrid nanomaterials has layer structures.

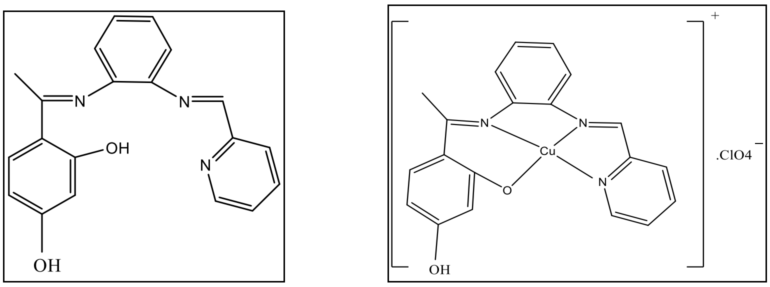

Fig. 1. struchers of the ligand and Cu(II) complex

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Oxidative addition of allylbromide to a cyclometalated organo platinum(II) complex

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Oxidative addition reaction of carbon-halogen (C-X) bonds to low valent transition metal complexes has extensively been studied during the past several decades.[1] In the case of oxidative addition reactions of MeI with cyclometalatedplatinum(II) complexes [PtMe(C^N)L] to form [$PtMe_2I$(C^N)L], good second-order kinetics are observed, first order with respect to both reactants. The entropy of activation, $\Delta S^{\neq}$, has a large negative valuein each reaction consistent with an S_N2-type mechanism. The operative mechanism involves nucleophilic attack of platinum(II) on the carbon atom of MeI to give the transient cationic platinum(IV) intermediate, [$PtMe_3$(C^N)L]$^+$I$^-$, which rapidly rearranges to [$PtMe_3I$(C^N)L] . [2] Recently, It has been shown that oxidative addition reactions of allylichalides(Br, Cl) to [$PtMe_2$(bpy)] complex (bpy = 2, 2'-bipyridine) both follow second-order, except for the substituted ally Chloride (CH_2=CHCHMeCl) which follows a third-order kinetics with S_N2 or S_N2' mechanism respectively.[3] In this research, we have studied oxidative addition reaction of [PtMe(C^N)L](C^N = deprotonated 2-phenylpyridine (ppy) and L =PPh_3) with allylbromide to form [Pt(allyl)MeBr[(C^N)L]. This reaction follows good third-order kinetic, first-order in [PtMe(C^N)L] and second order in allylbromide. The third-order reaction has a large negative value inentropy of activation, $\Delta S^{\neq}$, with a potential mechanism which is controlled by both the pre-equilibrium and the rate-determining step inaccord with the Curtin−Hammett principle.

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Synthesis and Characterization of mono- and di-insertion of symmetric alkynes into the Pd-C σ bond of cyclopalladated complexes.

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The insertion of alkynes into the Pd-C bond of cyclopalladated complexes has received great attention. In some cases the palladation reaction and the insertion of the alkyne form part of a catalytic cycle yielding interesting organic compounds.[1] Most reactions of palladacycles with alkynes give stable complexes because of intramolecular stabilization of the coordinated atom. However, sometimes the resulting cyclopalladated complex is unstable and gives interesting organic products[2] or a noncyclopalladated aryl palladium complex forms a stable cyclopalladated derivative after the insertion of the alkyne.[3] It is well known that the nature of the final product formed by the insertion of alkynes depends on a wide variety of factors including the nature of the metalated carbon, the electron withdrawing or -donating ability of the substituents on thealkyne, the stoichiometry of the reaction, the remaining ligands bound to the palladium, etc.[4] In this context, the reaction between internal alkynes with electron-withdrawing substituents and cyclometalladated compounds favors the production of mono-inserted products, while internal alkynes with electron-donating substituents promotes the synthesis of di-inserted products. [5] The mechanism of these insertion reactions show that monoinserted derivatives are difficult to prepare if the rate of the second insertion is much greater than the first one. [6] In this paper, the synthesis of new mono- and di-inserted palladacycles of Schiffbasesalong with their characterization is reported. Complexes react with dimethylacetylenedicarboxylate and diphenylacetylene producing monoanddi-nuclearpalladacyclesderived from single and double insertion of the corresponding alkynes intothe Pd-C σ bonds.

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A New Zinc Complex of an Iminophenol-iminopyridine Ligand as a Catalyst for Synthesis of Cyclic Carbonates

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The use of carbon dioxide as a building block for the synthesis of useful chemicals and as a fluid in numerous applications can serve to contribute to a sustainable chemical industry and concomitantly reduceCO_2 emissions into the atmosphere.[1-3] _ENREF_1In nature, CO_2 is captured, converted and/or reduced tocarbohydrates by a series of cascade reactions carried out by specific metalloenzymes present in photosynthetic organisms.[4, 5] _ENREF_4In the present work, the treatment of iminophenol-iminopyridinehybrid ligand (HL^{IPIP})with zinc acetate afforded the new zinc complex, L^{IPIP}ZnOAc as a transition metal-based catalyst for CO_2 conversion. The structure and physical properties of the synthesized complex have been examined in detail by X-ray, ^{1}HNMR, FT-IR, UV-Vis spectroscopy. It is evident from X-ray crystallography analysis that L^{IPIP}ZnOAc exists as a distorted square-pyramidal in which Zn^{II}coordinated by pyridine, imine as well as one phenolate. The acetate group occupies the fifth positions in L^{IPIP}ZnOAc.The mononuclear zinc complex in combination with tetrabutyl ammonium bromide (TBAB) as a co-catalyst is capable of efficient coupling of epoxides and carbon dioxide (Fig. 1). Various epoxides were converted into the corresponding cyclic carbonates under mild and solvent free conditions within short reaction time. The catalytic system and reaction conditions represent a readily available and an atom-efficient route for the conversion of CO_2, which is an inexpensive, widely available, renewable and non-toxic feedstock, into value-added products.

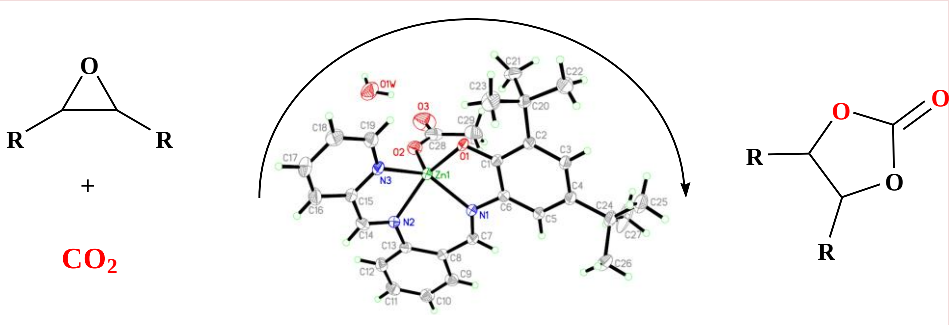

Fig. 1. Molecular structure of L^{IPIP}ZnOAcand its CO_2conversion activities

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Copper Complex of a New Redox-Active Ligand of Aminophenol-Benzimidazole Incorporating N_2O_2 Donor Atoms: Aerobic Alcohol Oxidation

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Redox interactions between a transition metal ion and a redox-active amino acid side chain such as the phenol group of tyrosine have been recognized to play a crucial role in several biologically important processes.[1] Galactose oxidase (GO) is one of the widely studied tyrosyl-radical containing metalloproteins which catalyzes the aerobic oxidation of primary alcohols to aldehydes.[2-5] In this work, the reaction of o-aminophenol-benzimidazol ligand with $CuBr_2$ afforded the new copper complex of $L^{APIM}Cu^{II}$ incorporating N_2O_2 coordination environment, as a model for galactose oxidase enzyme. ESI-MASS analysis in combination with spectrophotometric titration clearly indicated the formation of 1:2 complex of copper to ligand (Figure 1). Aerobic alcohol oxidation experiments were conducted to evaluate the oxidase reactivity of this complex towards different alcohols. This new copper complex is capable of efficient aerobic alcohol oxidation under mild conditions. Kinetic studies using the initial rate method exhibited the first-order dependence of the rate on the complex and substrate. The intriguing features of this catalytic system include the efficient use of oxygen as the green oxidant, high yield, high selectivity, KOH as a low cost base and the oxidizing of benzyl alcohol to bezaldehyde with a good turnover number of 480 after 9 h.

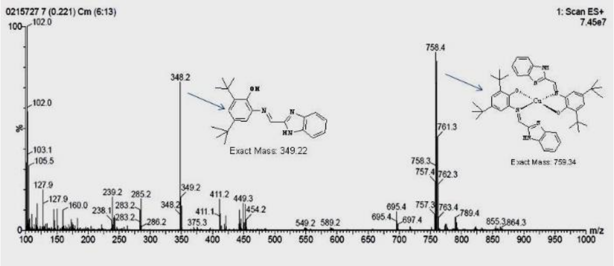

Fig. 1. Mass analyses of $L^{APIM}Cu^{II}$ complex

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Some nanostructure cadmium complexes of a new N_3-Schiff base ligand: spectral characterization, in vitro antimicrobial activity, DNA cleavage and their thermolysis to CdO nanoparticles

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Although cadmium is a widespread environmental contaminant and human carcinogen but studies indicate that its organic complexes are capable of inhibiting tumor cellular proteasome activity and consequently induce cancer cell-specific apoptotic death.[1] On the other hand, cadmium oxide is a promising candidate for optoelectronic applications and other applications including solar cells, photo transistors, photodiodes, transparent electrodes and gas sensors.[2] In this investigation, we report the synthesis of some new nanostructure cadmium complexes with a new tridentate Schiff base ligand obtained by the condensation of 2-aminoethylethylenediamine and 3-(2-nitrophenyl)-2-propenal. All compounds have been characterized using various physicochemical techniques such as FT-IR, ^{1}H NMR, ^{13}C NMR, UV–Vis. The spectral data revealed that Schiff base ligand acts as tridentate and metal center is five-coordinated. Nanostructure Cd(II) complexes have been synthesized by sonochemical method and characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Also, the CdO nanoparticles were synthesized by direct thermolysis of cadmium complexes and characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The in vitro antimicrobial activity of compounds was screened against four pathogenic bacteria (*Staphylococcus aureus* and *Bacillus subtilis*) as Gram-positive bacteria, and (*Escherichia coli* and *Pseudomons aeruginosa*) as Gram-negative bacteria and two pathogenic fungi (*Candida albicans* and *Aspergillus orayzea)* by disc diffusion method. The activity data showed that the metal complexes to be more potent/antimicrobial than the parent Schiff base ligand. Also, DNA cleavage ability by agarose gel electrophoresis method was studied for all the complexes (Fig. 1).

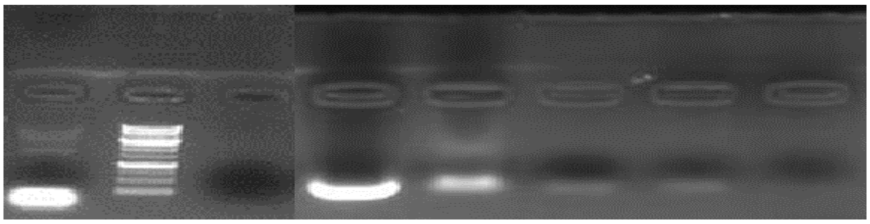

Fig. 1. Gel electrophoresis picture for DNA cleavage ability of cadmium complexes.

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Determination of molecular geometry in two new cadmium complexes of NO_2-donor ligand by spectral and theoretical studies

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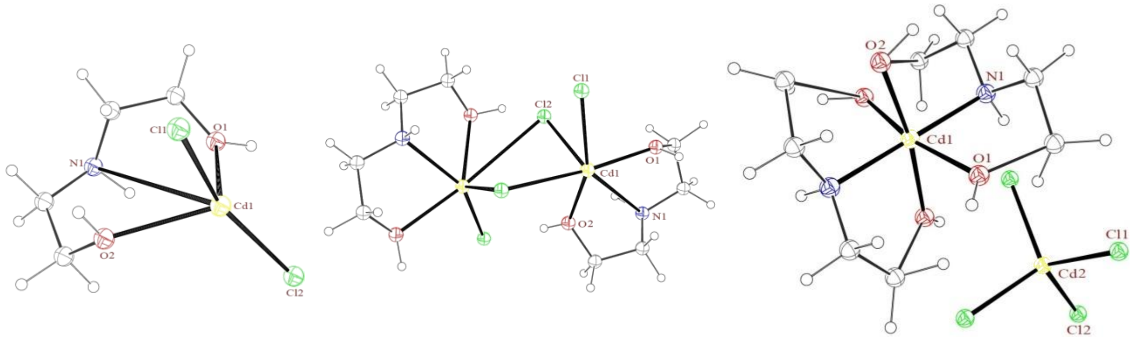
In this paper, two new complexes of cadmium, [$CdLCl_2$] and [$CdLI_2$], with 2,2'-azanediyldiethanol was prepared and identified by elemental analysis, FT-IR and ^{1}H NMR spectroscopies. Structures of two complexes were evaluated by density functional theory (DFT) at B3LYP/DGDZVP level. All possible structures of 1:1 M:L complexes in Cambridge Structural Database (CSD)[1]for cadmium chloride and iodide with tridentate ligands were extracted and then optimized to definition of the most stable structure. Three possible and optimized structures of cadmium chloride complexes are shown is figure 1. Possible structures of cadmium iodide complexes are similar to structures of cadmium chloride complexes. Combination of spectral data and optimized structure of complexes reveals that ligand acts as tridentate. In these structures, the cadmium atom has three different geometries including tetrahedral, disordered square planar and octahedral with coordination numbers 4, 5 and 6 respectively.[2,3] The frequency calculation results show that the predicted vibrations compare well with the experimental results. Molecular orbital energy diagrams of complexes and related HOMO and LUMO orbitals were performed and discussed.



Form 1 Form 2 Form 3

Figure 1. All possible structures of 1:1 M:L complexes in CSD for cadmium chloride with tridentate ligands.

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Synthesis and characterization of two new complexes of mercury(II) with bis(2-hydroxyethyl)amine and structural evaluation by DFT calculation

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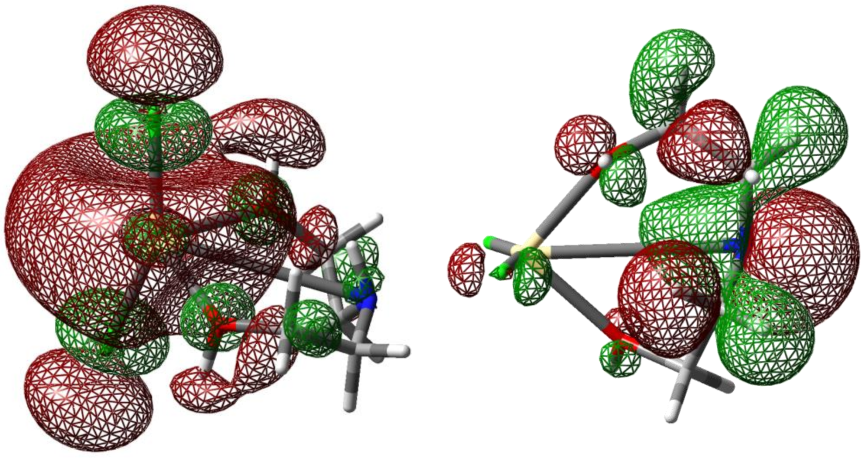
In this work, two new mercury(II) chloride and iodide complexes of bis(2-hydroxyethyl)amine (L), [$HgLCl_2$] and [$HgLI_2$] were prepared and identified by elemental analysis, FT-IR and ^{1}H NMR spectroscopies. Structures of two complexes were evaluated by density functional theory (DFT) at B3LYP/DGDZVP level. All possible structures of 1:1 M:L complexes in Cambridge Structural Database (CSD)[1] for mercury chloride and iodide with tridentate ligands were extracted. Then structures were optimized and the most stable structure was determined. The optimized structures of complexes reveals that the ligand acts as tridentate. Same result was observed in ^{1}H NMR spectroscopy by shifting of all amine and alcohol groups to lower magnetic field.[2] The frequency calculation results show that the predicted vibrations compare well with the experimental results. Molecular orbital energy diagrams of complexes and related HOMO and LUMO orbitals were performed. HOMO depicted in figure 1 for one of the possible structures, essentially located on the ligand and LUMO is delocalized on the mercury and two chloride ions without any significant participation of the ligand.[3]



LUMO HOMO

Figure 1.Comparison of HOMO and LUMO of [$HgLCl_2$].

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A database analysis of P—O—C bond angles in the structures with P(O)[O—C]$_2$[N] and P(S)[O—C]$_2$[N] segments: a comparison with P—S—C bond angles and completed with three new structures

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In the previous published papers, some structural features of phosphoramides[1,2] and thiophosphoramides[3,4] were considered through diffraction study of some derivatives and also analysis of analogous structures deposited in the Cambridge Structural Database.[5] Among these systematic studies, some of them concern the analysis related to the nitrogen atom (s) bonded to phosphorous, in compounds containing N—P(=O) and N—P(=S) segments. Here, we focus on the oxygen atom (s) bonded to phosphorous, considering the structures with P(O)[O—C]$_2$[N] and P(S)[O—C]$_2$[N] segments deposited in the CSD and two new structures reported here: P(O)[OC$_6$H$_5$]$_2$[NHNHC$_6$H$_5$] and P(S)[OCH$_3$]$_2$ [NHCH(CH$_3$)$_2$]. So, the his tograms of P—O—C bond angles were considered in the noted structures. The result of this analysis for the structures with a P(S)[O—C]$_2$ [N] segment is given in Fig. 1. Moreover, for a comparison of the geometry at the oxygen atom bonded to phosphorous atom with the geometry of the sulfur atom bonded to phosphorous, one novel salt structure is studied: [2-Cl-C$_6$H$_4$CH$_2$NH$_3$]$_2$ [(CH$_3$S)P(O)—O—P(O)(SCH$_3$)] and compared with a few analogous structures deposited in the CSD.

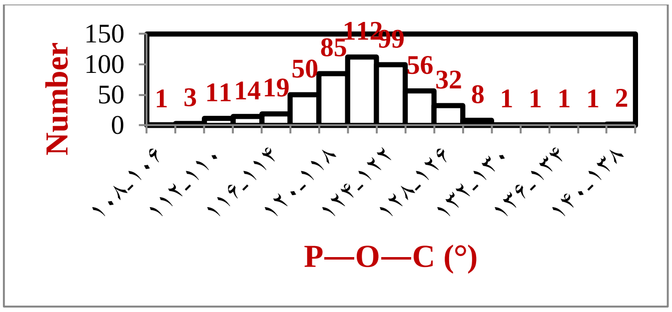

Fig. 1. A histogram of P—O—C bond angles (°) is given for the structures with a P(S)[O—C]$_2$[N] segments deposited in the CSD.

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Quantifying intermolecular interactions of a Hg(II) coordination compound by using Hirshfeld surface analysis

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Recently, the prediction and computation of molecular crystal structures through the aspect of intermolecular interactions, for the purpose of studying the crystal structural features, crystal design and crystal engineering, also have aroused much attention.[1,2] The main approach was through Hirshfeld surfaces, which serves as a powerful tool for elucidating molecular crystal structures.[3,4] In this work, crystal structure and Hirshfeld surface analysis of $HgLI_2$ complex was investigated. $HgLI_2$ complex was synthesized by template reaction of diethylenetriamine, 4-nitrobenzaldehyde, and mercury(II) iodide. The molecular structure of $HgLI_2$ complex was analyzed by single crystal X-ray diffraction. The results reveal that the mercury complex crystallizes in the triclinic system with space group of $P\bar{1}$. The Hg(II) center is five-coordinated in a trigonal–bipyramidal configuration. The Hirshfeld surface and 2D fingerprint plot (Fig. 1) of $HgLI_2$ complex were calculated and visualized for investigation of intermolecular interactions. The O···H interactions are observed as two bright red spots and several light red spots on d_{norm} surface. These interactions are the main intermolecular interaction by 26.7% and are seen as two sharp spikes in the 2D fingerprint plot. The high proportion of H···H interaction (23.5%) is due to existence of abundant hydrogens in molecular structure. H···I interactions comprise 16.8% of Hirshfeld surface and are observed as wings on the top left (H···I interaction) and bottom right (I···H) of the 2D fingerprint plot. The proportion of H···C and C···C interactions in this compound is considerable (10.4% and 6%, respectively). The relative contribution of the interactions is shown in Fig.1.

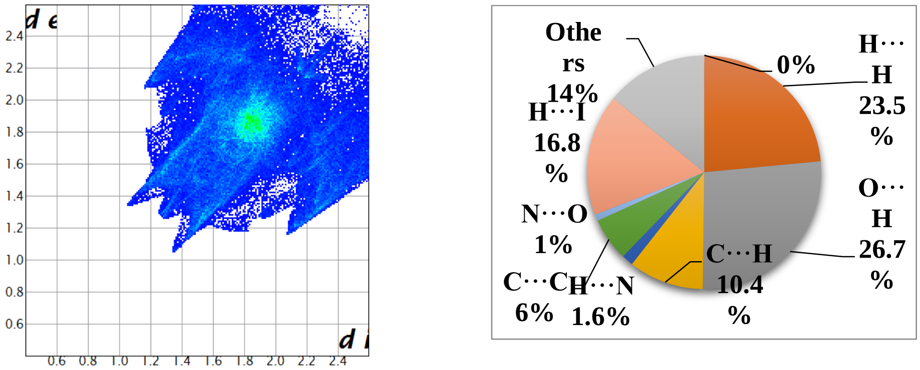

Fig. 1. (left) 2D fingerprint plot, (right) relative contribution of various intermolecular interactions.

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Crystal Structure, Hirshfeld Surface Analysis, and DFT Calculations of new four-coordinated cadmium compound

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Cd(II) ion is capable of adopting a wide variety of geometries and coordination numbers permitted by its d^{10} configuration.[1] Most Cd(II) complexes are octahedral while four- and five-coordinated complexes are limited to few cases.[2-4] also, Hirshfeld surface based tools represents a unique approach to the crystal structure prediction and this method offers a facile way of obtaining information on trends in crystal packing. We report here the synthesis of a new four-coordinated Cd(II) complex. The compound was characterized by single crystal X-ray diffraction and analyzed for its crystal packing. $CdLI_2$ complex crystallizes in a triclinic system with space group $P\bar{1}$. Cd(II) is coordinated by a bidentate Schiff base ligand (L) and two iodide ions. The Hirshfeld surface is illustrated in Fig. 1 showing surface that has been mapped over d_{norm}. The visible red spots on d_{norm} surface are due to H···H close contacts. Other contacts are observed as white and/or blue color areas. There are three distinct spikes in the 2D fingerprint plot (Fig. 1). H···H interactions are the main intermolecular interaction by 46.4% and are presented as one distinct spike with $d_e+d_i \approx 2$. Two other distinct spikes are related to I···H/H···I interactions that comprise 17.7% of Hirshfeld surface and are observed as wings on the top left (H···I interaction) and bottom right (I···H) of the 2D fingerprint plot. The interactions related to phenyl rings (H···C and C···C) comprise considerable distribution of fingerprint plot (18.7% and 6.7%, respectively).

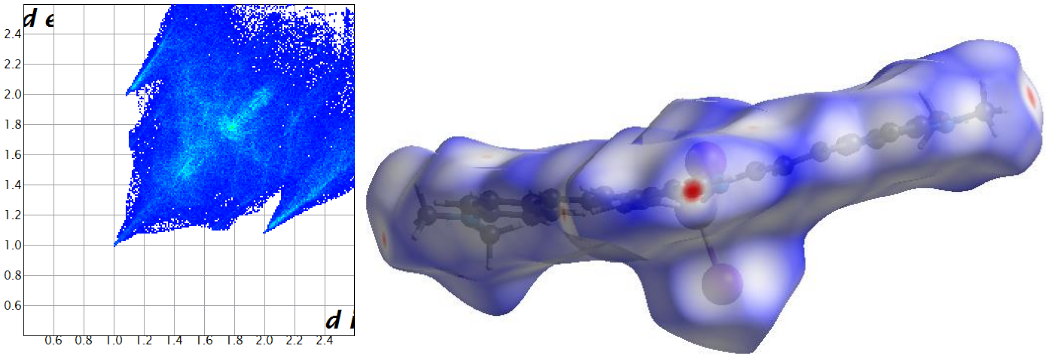

Fig. 1. (left) 2D fingerprint plot, (right) d_{norm} surface of $CdLI_2$.

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Effect of Particle Size on the Adsorption of carbon monoxide on Cobalt: A Density-Functional Theory Study

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In recent decades metal clusters have received particular attention both on the theoretical and experimental level due to their potential application in catalytic processes and electronic materials.[1] The mechanisms of surface reactions are very complex and any discover in recognize of these reactions increase the ability of design new active catalytic species. The study of the interaction of molecules with surfaces is the important step in surface reactions. The interaction of CO with metal surfaces has been studied extensively with great academic and industrial interest because it is an indispensable step in many surface and catalytic reactions like Fischer-Tropsh synthesis (FTS).[2,3,4]

An enormous body of experimental data on the effect of the particle size of the active component of a catalyst on the specific catalytic activity. This parameter is not related to the total surface of the catalyst active phase or to the number of active sites; therefore, they characterize the properties of the active site itself. As a step toward understanding how the structure of catalyst particles affects these functions, we have studied the effect of the size of Cobalt clusters, including the infinite Co (100) surface, on the energy of adsorption of carbon monoxide. The calculated results show that adsorption energy of carbon monoxide increase by decreasing of cluster size.

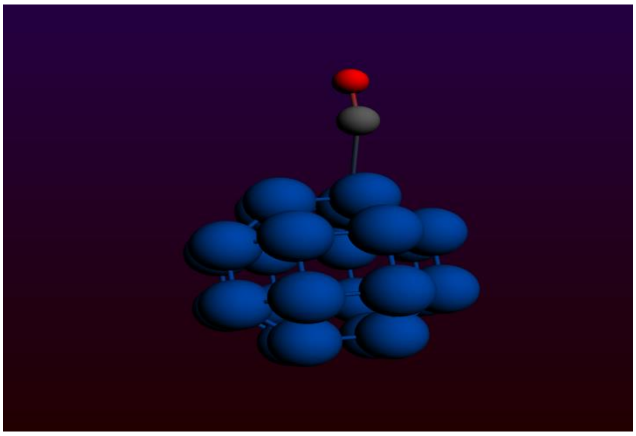

Fig. 1. adsorption of carbon monoxide on Co_{24} .

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Synthesis and characterization of a new Ag(I) complex containing 1,2,4-triazole derivative and oxalic acid as a co-ligand.

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Thiosemicarbazone and thiosemicarbazide derivatives are of considerable interest due to their antibacterial, antimalarial, antiviral and antitumor activities. Heterocycles derived from thiosemicarbazide in form of 1,2,4-triazoles were also found to possess significant antifungal, antibacterial and insecticidal properties. Metal complexes of ligands such as S,N-heterocycles, amino acids and proteins often exhibit enhanced biologicalactivities compared to the uncomplexed ligand. In the present work, we wish to report the synthesis and characterization of a new Ag(I) complex containing AMTT (AMTT= 4-amino-5-methyl-2H-1,2,4-triazole-3 (4H)-thione) as ligand and an organic diacid (oxalic acid) as co-ligand. The complex has been characterized by NMR, FTIR spectroscopy, UV-Vis, powder X-ray diffraction (XRD), EDX , thermal gravimetric analysis (TGA) elemental analysis. according to mass spectrometry diagram (564 m/z) exhibits Ag(I) complex.

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A new organotin(IV)-phosphoric triamide complex: $[(2\text{-Cl-}C_6H_4CH_2NH)_3P(O)]_2SnMe_2Cl_2$

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The ligands with an N—P(O) segment, especially phosphoric triamides with the oxygen-donicity property, were used for preparation of metal complexes.[1,2] Here, the phosphoryl donor ligand $(2\text{-Cl-}C_6H_4CH_2NH)_3P(O)$ was applied for the synthesis of a new organotin(IV) complex, $[(2\text{-Cl-}C_6H_4CH_2NH)_3P(O)]_2SnMe_2Cl_2$. The Sn coordination geometry is octahedral with the pairs of similar ligands in a *trans* orientation. The Sn atom is located at the inversion center, making half of the molecule related by the symmetry. In the crystal structure, adjacent molecules are linked *via* pairs of equivalent N—H…O═P hydrogen bonds into a chain running parallel to the *b* axis. From the two other N—H units in the structure of phosphoric triamide ligand, one of them takes part in an intramolecular hydrogen bond interaction with the carbon-bonded chlorine atom; whereas, the other one doesn't take part in any hydrogen bond (Fig. 1). The spectroscopic features of ligand and complex were discussed.

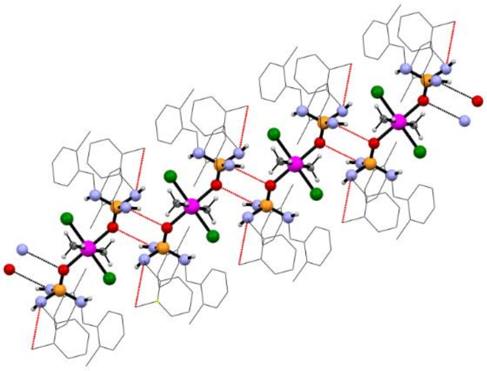

Fig. 1. A view of the crystal packing of the title complex is represented.

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Biomimetic alkene epoxidation with peracetic acid in mild condtions catalyzed by Mn (III) meso-tetraphenylporphyrin acetate [Mn(TPP)OAc]

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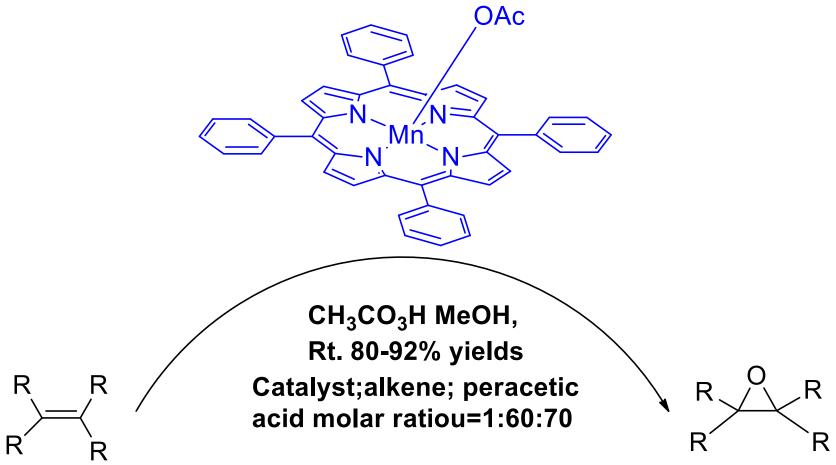
Metalloporphyrins are well-known catalysts for the oxidation of various organic substrates such as alcohols [1], alkenes [2], alkanes [2] and arylacetic acids. [3] In these catalytic reactions the nature of porphyrin, central metal atom and the kind of oxidant used have dramatic influence on the yields and selectivity of the reactions. We wish here to report our results on the catalytic epoxidation of simple alkenes by peracetic acid as an oxidant in the presence of Mn (III) meso-tetraphenylporphyrin acetate [Mn(TPP)OAc]. Mn(TPP)OAc was prepared using free base H_2TPP and Mn(OAc).4H_2O and purified by column chromatography(CHCl3/EtOAc, 1: 3). The epoxidation reactions were achieved with Mn(TPP)OAc, alkene, peracetic acid in a molar ratio of 1:60:70 in MeOH at room temperature and the products were analyzed by GC. We have found that the epoxidation were accomplished with high selectivities and 80-92% yields with peracetic acid.



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Synthesis, characterization and luminescence properties of Pr(III) and Sm(III) Complexes with Novel Schiff Base Derivatives

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Nowadays, luminescent lanthanides complexes have interested much attraction due to their application in imaging and high resolution magnetic resonance imaging (MRI).[1] Besides, they have many interesting application in fluorescent sensor molecules and luminescence probe.[2] As some lanthanide ions, e.g. Sm(III) and Pr(III) possess good luminescence properties based on the transitions between the 4f energy levels anda series of schiff base compounds by mentioned lanthanides have been investigated for luminescence probe materials.[1] The study of relationship between the structures of schiff base ligands and the luminance properties of lanthanide ions could be the intelligent way for designing new luminescent species for biomedical application.[2] In this work, two novel schiff basederived ligands, (E)-2-(((2-hydroxyphenyl)imino)methyl)-6-methoxyphenol (L^{SAL}) and 2,2'-((1E,1'E)-(1,4-phenylenebis (methanylylidene)) bis(azanylylidene))diphenol (L^{TPH}) were prepared by 2-aminophenol. Their complexes with praseodymium(III) and samarium(III) were synthesized. The complexes were characterized by elemental analysis, UV-Vis spectroscopy, infrared spectra, ^{1}H NMR and TGA. The luminescence properties of these complexes were investigated. Theresults suggested that Pr(III) and Sm(III) complexes exhibit efficient luminescence and the two ligand (L^{SAL}) and (L^{TPH}) areexcellent sensitizers to Pr(III) and Sm(III) ion.

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Immobilization of new iron complex supported on silica coated magnetic Fe_3O_4 nanoparticles:Magnetically recyclable catalyst systems for the high selective oxidation of sulfides

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Recoverable catalysts have attracted a great deal of interest in both academic and industrial research because, in addition to environmental concerns, there are beneficial effects of decreasing the cost of the final product.[1] Immobilization of the catalytically active molecules onto the surface of magnetic nanoparticles is a suitable way to separatethe catalyst from the reaction mixture.[2, 3] Herein we have synthesized a new magnetically separable catalyst consisting of iron complex supported by amine-bis (phenolate) ligand, covalently supported onsilica-coated Fe_3O_4 nanoparticles. The mentioned catalyst characterized by thermo gravimetric analysis (TGA), Fourier transform infrared spectroscopy (FT-IR), scanningelectron microscopy (SEM), Transmission electron microscopy (TEM) and vibrating sample magnetometry (VSM) techniques. Our synthesized catalyst with iron center could be particularly attractive because of readyavailability, low cost and low toxicity of this metal. This catalyst exhibited high catalytic activity in selective oxidation of aromatic and aliphatic sulfides with H_2O_2. Interestingly, the novel catalyst could be recovered in a facile manner from the reaction mixture by applying an external magnetic field without any significant loss in activity.

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Synthesis of novel nano magnetic schiff base ligand with phosphate spacer for the preparation of various metal complexes

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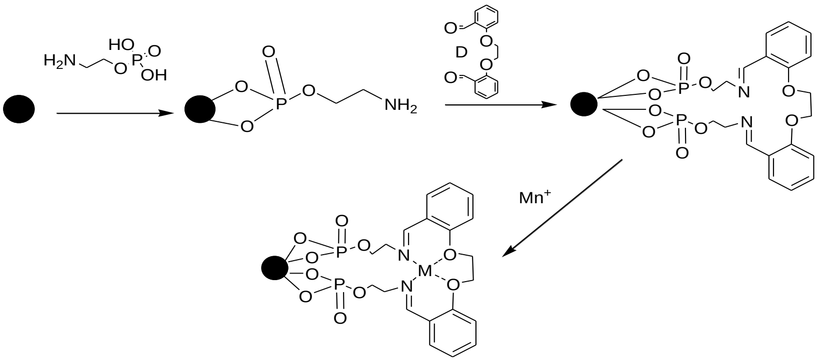
Nowadays, recycling and reusing of heterogeneous catalysts is employed in the various area such as industrial and green chemistry. Heterogeneous supports allow efficient recycling by filtration, but the application of heterogeneous catalysts is limited because of their less active site than their homogeneous counterparts. [1-4] In this regard, nano materials have emerged as useful and sustainable alternatives to the immobilization of homogeneous catalysts. [5] Since, when the size of the support is decreased to the nanometer scale, the surface area is substantially increased, which is combined with excellent accessibility of the surface-bound catalytic sites.[6] Among the various nano materials, Inorganic nanoporous materials have recently been used in various fields, such as catalysis, adsorption, extraction, energy, drug delivery systems and so on.

Herein, we wish to report the synthesis of taske-specific novel nano magnetic schiff base ligand with phosphate spacer for the preparation of various metal complexes. With this aim, 2-aminoethyl dihydrogen phosphate has been used instead of TEOS and 3-aminopropyl triethoxysilane for coating of nano magnetic Fe_3O_4. Synthetic procedure, characterization and their applications will be discussed.



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Synthesis, characterization and electrochemical studies of Ni (II) and Co (II) complexes with ligands based on salicylidene

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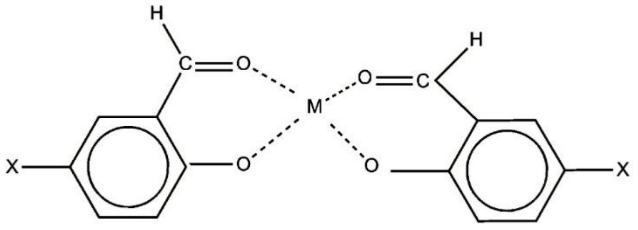
The new complexes of Nickel (II) and Cobalt(II) with two ligands, [bis(salicylidene) Nickel(II)]-oleylamine (Ni C_{32} O_4 $H_{38}N$), [bis(salicylidene) Cobalt(II)]-oleylamine (Co C_{32} O_4 $H_{38}N$), [bis(5 -phenylazo-salicylidene) Ni(II)]-oleylamine (NiC_{49} $O_2H_{84}N_4$) and [bis (5 -phenylazo-salicylidene)Cobalt (II)]- oleylamine($CoC_{49}O_2H_{84}N_4$) were synthesized and characterized by elemental analysis , UV-Vis spectroscopy, FT-IR spectra and cyclic voltammetry. Elctronic spectra of the Ni^{+2} and Co^{+2} copmlexes in the region 300 -800 nm are investigated. The difference of absorption maxima from the complexes to their was discussed. Cyclic Voltammetry indicates that Nickel and Cobalt complexes have a quasi –reversible redox behavior (at a scan rate 0.1VS^{-1}) under the experimental conditions. On the basis of FT-IR results it can be deduced that in complexes, the ligands are coordinated to metal atom as tetradentate O_4ligands.



X=H , N=N—Ph

M=CO^{+2}, Ni^{+2}

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Synthesis and characterization of copper metal organic frameworks with bis-tetrazole and 2-cyanoguanidine ligands

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Metal organic frameworks (MOFs) are a class of organic –inorganic hybrid materials made of metal clusters interconnected through organic linkers. There has been extensive interest in porous metal-organic framework (MOF) materials because of their intriguing molecular topologies and their potential applications in several technological areas, such as gas storage, size-selective separation, molecular recognition, heterogeneous catalysis, and ion exchange. Copper metal organic frameworks are amongst well studies MOFs with promising industrialization potential. Tetrazoles belong to a class of molecules that are found to be useful in various sectors as drugs, explosives, sensors, and even for pancreatic cancer treatment.[1,2] In this work, new metal organic frameworks (MOF) of copper metal were synthesized by using bis-tetrazole and 2-cyanoguanidine linkers via solvothermal and microwave-assisted method.

Synthesized materials were characterized by X-ray diffraction (XRD) for phase purity and crystal structure, scanning electron microscopy (SEM) for morphology and size distribution and thermogravimetric analysis (TGA) for thermal stability. The experimental results showed that samples synthesized by the microwave-assisted method have smaller particle size with relatively more uniform particle size distribution.

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The Compare of Effect of Two Kind of Iron Salts on Synthesis of Fe_3O_4 Nanoparticles by Co-precipitation Method

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Magnetite (Fe_3O_4) is a common magnetic Iron Oxide and it has a cubic inverse spinel structure with oxygen forming a FCC closed packing and Fe cations occupy the interstitial tetrahedral sites and octahedral sites.[1] The synthesis of magnetite nanoparticles has been intensively developed not only for its great fundamental scientific interest but also for many technological applications in biology, such as extraction of genomic DNA,[2] ultrahigh density magnetic storage media, medical applications (such as targeted drug delivery, labelling, separation).[3,4]

In this study, magnetite (Fe_3O_4) nanoparticles were synthesized by chemical co-precipitation from the solution containing iron salts (iron chloride and iron sulfate) in alkaline medium under atmosphere of N_2 and temperature of 45 °C. Magnetite nanoparticles were characterized by X-ray diffraction (XRD), Fourier transform infrared spectrometer (FTIR) and scanning electron microscopy (SEM). The size of particles was calculated by Sherrer᾽s formula, and then compared with the size of nanoparticles obtained from Sem images .The results from the SEM images, show the formation of spherical nanocrystal Fe_3O_4 particles with the average diameter of 39 nm for used iron chloride and 30 nm for used iron sulfate salts.

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Theoritical study of the adsorption of carbon dioxide on nanostructured nickel catalysts

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An explosion of interests in nanocatalysis is to be able to adjust the structure of catalytic materials to obtain the optimal electronic properties for desired chemical reactivity. The mechanisms of surface reaction are very complex and any discover in recognize of these reactions increase the ability of design new active catalytic species. The study of the interaction of molecules with surfaces is the important step in surface reactions. In the process reforming with carbon dioxide in the process of synthesis gas with a ratio of hydrogen to carbon monoxide is equal to 1, according to the following reaction:

$$CH_4+CO_2 \leftrightarrow 2CO+2H_2 \qquad \Delta H=247\ {}^{kj}/_{mol}$$

This process was introduced in 1928 for the first time, today, due to increased emission o greenhouse gas carbon dioxide in the industry as one of the chemical processes taking carbon dioxide considered. If the process is exactly according to the above reaction without the presence of water is raised as dry reforming.

Given the importanc of high-performance Ni catalysts in industrial processes, methane dry reforming, knowing the exact behavior of the surface reactions on the catalyst in order to improve their capabilities are highly regarded.

That's why we think the carbon dioxide adsorption on different levels of Ni catalysts discussed and how adsorption of carbon dioxide on the active sites on different pages of Ni metal that looked full of cubic structure funds centers.

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Synthesis and characterization of novel organometallic complexes containing 1,2,4-triazine moiety

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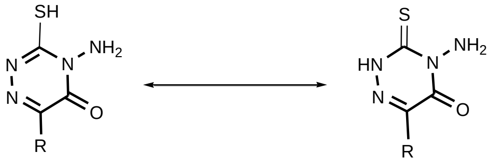
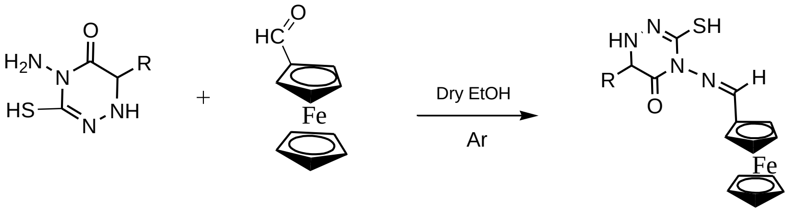
Among heterocycles, 4-Amino-3-mercapto-6-methyl-5-oxo-1,2,4-triazine (AMTTO) and its derivatives, as the most important member in amino-thione-1,2,4-triazine family, exhibit two different tautomeric forms as shown in scheme 1. They have attracted considerable attention in coordination chemistry since they contain soft (S) and hard (N) donor atoms, simultaneously. It is also known that Schiff-bases show catalytic activities. On the other hand, incorporation of a ferrocene fragment into such Schiff bases provides unique geometries and electronic properties. In this work, a series of novel Schiff-bases containing ferrocene and 1,2,4-triazine moieties were synthesized in accordance to Equation (1). The new compounds were characterized by FT-IR, ^{1}H-NMR and MS spectroscopy and elemental analysis as well. Also electrochemical properties of the ferrocene containing Schiff bases were investigated by cyclic voltammetry. Furthermore, the new compounds were graftedon different supports like nano Al_2O_3 and silica gel and their photocatalytic activity was investigated in decolorization of organic dyes from solution.



Scheme 1. The thione-thioltautomeric forms in 1,2,4-triazines



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Synthesis and characterization of Zn-MOFs based on 2-cyanoguanidine and 5-aminotetrazole

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Metal Organic Frameworks, or MOFs, are crystalline materials consisting of metal ions or clusters, coordinated to rigid or flexible organic linkers to form two or three dimensional porous structures. Metal organic frameworks (MOFs) have many characteristics including structural adaptivity and flexibility, ordered tridimensional pores, and multiple coordination sites. There are an enormous number of MOFs that can be synthesized with various combinations of organic linkers and metal centers, which provide an opportunity to tailor surface area, pore size, and surface functionality.[1] They have attracted wide scientific interest due to their extremely high surface area and pore volume, and have potential applications in gas storage, separation, and heterogeneous catalysis. In this research, Zn-MOFs based on 2-cyanoguanidine ($C_2H_4N_4$) and 5-aminotetrazole (CH_3N_5) were successfully synthesized with both solvothermal and microwave-assisted method for rapid synthesis. These MOFs samples were characterized with scanning electron microscopy (SEM) for morphology and particle size, powder X-ray diffraction (XRD) for crystal structure and phase purity, as well as thermal gravimetric analysis (TGA) for thermal stability.

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Study of electronic effects of carbene derived from purine, 2-aminopurine, and adenine on the platinum-based anticancer drugs

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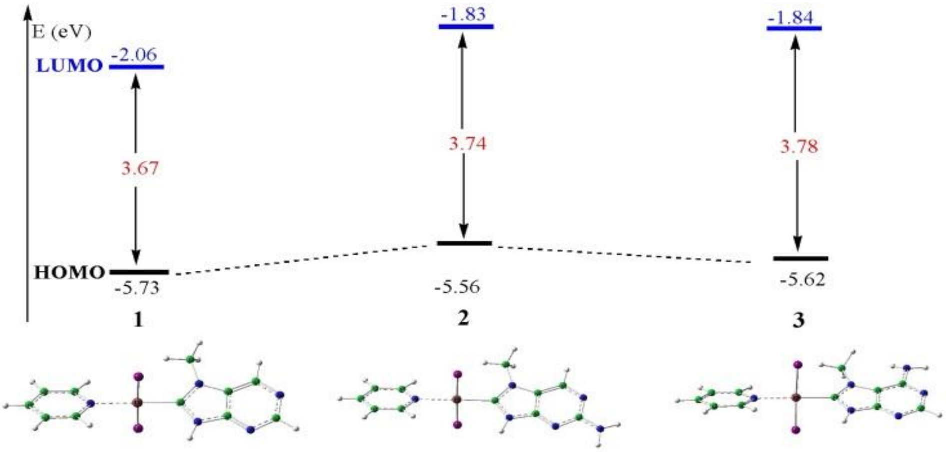
Platinum-based anticancer drugs are one of the leading agents in modern medicine for clinical applications. These drugs contain a square-planar Pt(II) center coordinated with four ligands.[1] On the other hand, the *N*-heterocyclic carbenes (NHCs), which are stable compounds of a divalent carbon atom, may provide an interesting class of ligands with electron-donating properties. In this study, the effects of the electronic properties of purine (**1**), 2-aminopurine (**2**), and adenine (**3**) carbene ligands on the nature of the transition metal–carbon atom bond in the platinum complexes were examined using computational chemistry.[2,3] The results show that the highest occupied molecular orbital (HOMO) energy level of **1** is –5.73 eV. Therefore, this complex has the highest nucleophilic character as shown in scheme 1. A replacement of either the 2-aminopurine or adenine ligands to form **2** or **3** leads to a decrease in the HOMO levels (to –5.56 and –5.62 eV), respectively. In addition, the HOMO–LUMO energy gap ($\Delta E_{\text{HOMO–LUMO}}$) of carbene **3** is higher than the gaps in complexes **1** and **2,** implyinga higher kinetic stability for carbene **3**. The value of $\rho_b$for compound **2** is the highest (0.457) among the three counterparts, which indicates a relatively stronger Pt–C: bond.[4]The larger$\nabla^2\rho_b$value (3.876) in complex **2**, which involves2-aminopurine, confersa stronger electrostatic nature on the metal–carbene bond in this carbene.



Scheme 1. Graphical illustration of HOMO–LUMO gaps.

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Synthesis of graphene oxide for the stabilization of palladium nanoparticles application for a heterogeneous catalyst toward aerobic alcohol oxidation

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Graphene, a two-dimensional sheet of sp^2-hybridized carbon atoms arranged in a honeycomb lattice, has heralded a versatile material due to its amazing properties and enormous potential for applications in advanced electronic devices and composite materials .[1,2] Furthermore, the use of graphene as support for developing novel heterogeneous catalysts with enhanced activity is desired due to its huge surface area (theoretical value 2600 m2/g) and excellent chemical stability. In this work, novel trinuclear Pd (II) complex with benzophenone oxime ligand, $[Pd_3(C_{12}H_{11}C{=}NO)_6]$ was synthesized and structurally characterized by elemental analysis, IR and resonance signals in the NMR. We have developed an efficient method to generate highly active Pd nanoparticles supported on grapheme (Pd/G) and characterized by XRD, TEM and SEM. We used this heterogenous catalyst for aerobic oxidation of alcohols with investigated by gas chromatography and exhibited high and stable activity.

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Airbag bag fuel containing of nano composits

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Nano composits becuase of their high surface area compared to micro materials has attracted great attentions. In gas producing system, this materials application in fuel and energy resource for satellite and automobiles, propellant. Also, thermal degradation kinetic of nano composits which determine their aplications, is improved by using of devices of TGA/DSC date and temperature of degradation. In this project 3 kinds of nano composits of nitroguanidine, sodiumazid and cyanoguanidine with 3 diffrent kinds of additives produced and these nanocomposites were studied for rate of burn.our aim is using nanocomposit that through passing the time nanohydrolysied, preserve its basic property and product non toxic gas such as nitrogen.

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The effect of nano oxidant on the gas kinetic of Airbag

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The kinetic of airbag is an important factor for evaluating of its applicability which the best result is 0.4-0.7 second. The fuel of air bag consist of potassium chlorate ($KClO_4$) and sodium Azide (NaN_3) which by adding of various oxidant, the kinetic of burn raised. In this study, we tried to get the shortest time and the most favorable result for inflating the airbag. For this purpose, we used Nano copper oxide and nano iron oxide was used and good result obtained. This results approved by sensor that determiner the pressure of gas producted versus time.

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Synthesis, characterization of an orthopalladated complex and investigation of its interaction with DNA and BSA

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Due to resounding success of cisplatin, as antitumor drug, and closely related platinum complexes, alarge number of platinumand palladium complexes containing amine based ligands and various other ligands have become the subject of intensive research.[1]
Palladium(II) complexes have been investigated for developing the new antitumor agents, because palladium(II) has a similar coordination mode and chemical properties to platinum(II).[2] NC palladacyclic complexes have reasonable cytotoxic effects against some tumor cell lines and good DNA/BSA binding affinity.[3]In this work, we synthesized a palladacyclic complex containing NC, NN ligands and characterized by NMR, IR and single crystal X-ray crystallography, then studied the ability of the complex to interact with DNA and investigated its interaction mechanism using UV-Vis and fluorescence spectroscopy, thermal denaturation, and circular dichroism (CD) spectra, monitored the protein binding ability by UV absorption and tryptophan fluorescence quenching experiment in the presence of the complex using BSA as a model protein; the molecular dynamics (MD) performed on the structure of BSA and DNA simulations.All the experimental evidences indicated that this complex could strongly bind to CT-DNA via a partial intercalation mechanism. Further, the albumin interactions of complex were investigated using fluorescence quenching spectra and synchronous fluorescence spectra. The result of fluorescence titration suggested that the fluorescence quenching of BSA by complex was a static quenching procedure. The site marker displacement experiments suggested the location of complex binding to BSA was Sudlow's site I in the subdomain IIA. Finally, the molecular docking experiment supported the above results and effectively proved the binding of Pd (II) complex to BSA and DNA.

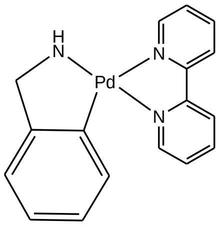

Fig.1.structure of the complex

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Synthesis, characterization of an orthopalladated complex and investigation of its catalytic properties in oxidation of alcohols

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Heterogeneous catalysis is a key enabling technology, which has significant impact on modern life(1). Palladium(II) complexes have shown significant potential as catalysts for a variety of oxidation reactions.The oxidation of alcohols to carbonyl compounds is of paramount importance in synthetic organic chemistry because of their use in a wide range of products, such as drugs, agro-chemicals, and fragrances. The smectite-type clays, such as montmorillonite (MMT), contain negatively charged silicate layers and intercalated cations. Clay has been widely studied as the host of catalytic noble metals in its interlamellar space, and generally the ion-exchange property was utilized.In this work, we synthesized a palladacycle complex; containing NC and NN ligand and characterized by NMR and IR spectroscopy, then intercalated cationic complex in the MMT and studied by XRD, TEM and SEM.We used this heterogenous catalyst for aerobic oxidation of alcohols andwith molecular oxygene and investigated by gas chromatography, finally we obtained very good resultsfor oxidation of alcohols.

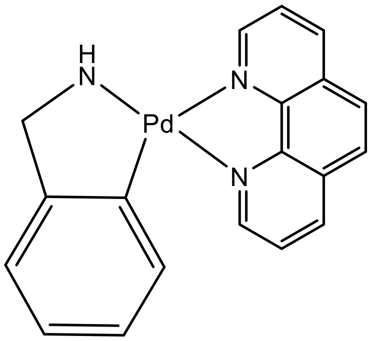

Fig.1. structure of the complex

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Glucose biosensing via a new titanium oxide nanostructure doped by copper ion.

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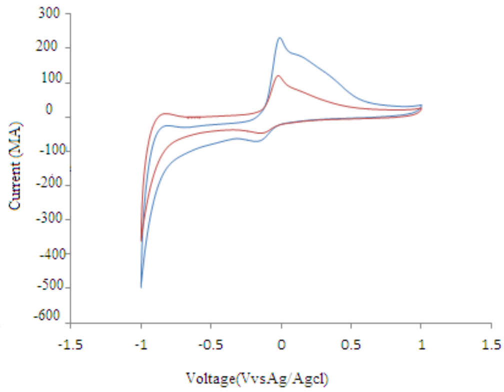
Glucose is an essential biomolecule that is important in our life. Excess amount of this molecule in the blood can cause many diseases. Development of glucose sensors has been reached to cheap and selective ones. There are many electrochemical methods for detecting the glucose such as cyclic voltammetry and chronoamperometry. Enzymatic biosensing of glucose by glucose oxidase has many problems such as highly cost and instability of this compound.
Nowadays fabricating non enzymatic sensor is developing. [1-4]
In this article, glucose was sensed by a nonenzyatic method in buffer phosphate medium. The main part of the glassy carbon electrode is made of f rom titanium oxide nanostructure which was doped with copper ion. The nano composite was synthesized by a solvothermal method and characterized with FT-IR, XRD and SEM. Results showed that sensitivity of the sensor is 132μA/cm mM Also the sensor detected the glucose without interference from dopamine and uric acid.



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Cuonanostructures as an efficient catalyst for the decolorization of a diazo dye.

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Synthetic are very pollutants for the environment. These poisonous materials can destroy ecosystems and waters. Many industries produce such a compound and sent it to the nature. Among these dyes, azo compounds are consisted 70 % of portion in environmental pollution. Purification of the wastes are very expensive and take long time. Active catalysts can decompose the dyes via several routes. Catalytic and photocatalytic processes are the most well-known ones.[1-3]

Copper oxide as an active catalyst can decolorize the dyes. In this study, congo red was decolorized by CuO that was synthesized by solvothermal method. The product was calcinated at 550 °C and was characterized by FT-IR, XRD and SEM. Congo red was decolorized only after 30 min without using any oxidizing agent or UV-light. These results confirm that nano-CuO is an active catalyst for this reaction.

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A Facile Synthesis of PdNPs/CNTs Catalyst Hybrids by Spontaneous Reduction Method

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Supported noble metal nanoparticles are the most important catalysts for many application, including petroleum refining, automobile exhaust treatment, fuel cells, and environmental protection.[1] The catalytic performance strongly depends on the size, composition, and structure of the metal nanoparticles, as well as the underlying support. Suitable and frequently used support materials are alumina, silica and carbon, all being compounds with high melting and decomposition temperatures.[2] Functionalized carbon nanotubes (FCNTs) with many oxygen-containing functional groups (such as carboxyl and hydroxyl groups) are getting more attractive as a support material for noble metal nanoparticles.[3] The immobilization of metal nanoparticles to carbon nanotubes is of interest to obtain nanoparticles/nanotubes hybrid materials with useful properties.[4] Previous methods to attach metal nanoparticles on CNTs include physical evaporation, electrochemical deposition, grafting after functionalizationof carbon nanotubes (CNTs) and electroless depositionfrom metal salt solutions with the aid of reducing agents or catalyst.[5] In this work, the synthesis of Pd nanoparticles/FCNTs catalyst hybrids has been achieved by spontaneous deposition in alcohol-water solution at room temperature. In the presence of carboxyl group functionalized multi wall carbon nanotube (FMWCNT) and functionalized single wall carbon nanotube (FSWCNT), Pd nanoparticles (PdNPs) were in situ generated from H_2PdCl_4 aqueous solution, without any additional reducing agent or irradiation treatment, and readily attached to the FCNTs surfaces, leading to the PdNPs/FMWCNT and PdNPs/FSWCNT nanohybrids. In this process, $PdCl_4^{2-}$ ions were spontaneously reduced though a galvanic cell effect between them and the FCNTs. The prepared nanohybrids were characterized by scanning electron microscopy (SEM), high resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDX) techniques.

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Synthesis and Characterization of Silver Nanoparticles by Phytosynthesis Method

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Nowadays different methods for the synthesis of metal nanoparticles are under consideration due to their useful applications in different fields.

These include physical and chemical methods but both of these are time-consuming, expensive and environmentally toxic. Biological methods are of great advantage due to their non-toxic and large scale synthesis. In the present study, fruit extract of *Ammicopticum* was used as a reducing agent of silver ions to silver nanoparticles. Bio-reduction was monitored by colour change using UV-Visible spectroscopy which revealed absorption peak at λ_{max} 460 nm. Scanning electron microscopy and energy dispersive X-ray spectroscopy were utilized to identify characteristics of synthesized particles. The synthesized particles were spherical with size ranging from 20 to 40 nm. FTIR spectrum evidences the presence of different functional groups of biomolecules participated in encapsulating Ag NPs and the possible mechanism of Ag NPs formation was also suggested. The results confirmed that the *Ammicopticum* is a very good eco friendly and nontoxic source for the synthesis of Ag-NPs as compared to the conventional chemical/physical methods. [1,2]

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Activation of C-I bond by Cycloplatinated Complexes Containing 1-Phenylpyrazolate

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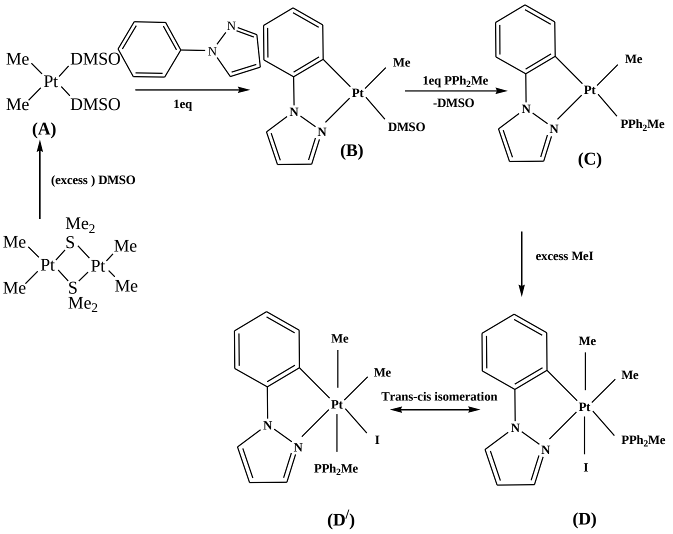
The study of the cyclometallation reaction is of considerable interest from a mechanistic point of view[1] because of its role in the functionalisation of C–H bonds, and because of the use of the derived complexes.[2] Cyclometallated compounds of late transition metals with nitrogen ligands are well-known. During the years they have been the subject of continuous research, due to their numerous potential applications in areas such as organic synthesis, homogeneous catalysis, medicinal and biological chemistry and the design of novel materials with attractive properties. Square-planar platinum(II) species were also used as "building blocks" for complex systems such as supramolecular entities or dendrimers.[3]

In this work, the organoplatinum(II) complex[PtMe(ppz-H)(L)] (L = DMSO, PPh_2Me and ppz-H =1-Phenylpyrazol) was synthesized and characterized by microanalysis and multinuclear NMR spectroscopy [Scheme 1]. The kinetic of oxidative addition of MeI to [Pt(ppz-H)(PPh_2Me)(Me)] was studied by using UV-vis spectroscopy at different temperatures and the structure of the final product [$PtMe_2I$(ppz)(PPh_2Me)] complex determined by multinuclear NMR studies.



Scheme 1

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Synthesis, characterization, electrochemistry and catalytic activity of two Ni(II) Schiff base complexes

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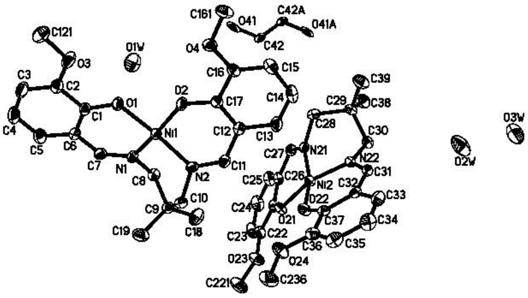
Transition metal complexes with Schiff base ligand have been widely studied in the past few years because of their application in electrochemistry, analytical and catalical fields. [1,2] In this work two Schiff base ligands and their Ni(II) Schiff base complexes derived from 2-hydroxy-3 methoxy benzaldehyde and 2,2-dimethyl-propylenediamine have been synthesized and characterized. The Ni(II) Schiff base complexes have been characterized by different spectroscopic methods and the crystal structure of one of them has been determined.

The electrochemical properties of the Ni-Schiff base complexes were investigated in DMF and CH_3CN by cyclic volatmmetry. Also the catalytic properties of the prepared complexes in the oxidation of olefins has been investigated.



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Synthesis, characterization and catalytic performance of the oxovanadium Schiff base complex supported onto magnetic nanoparticles

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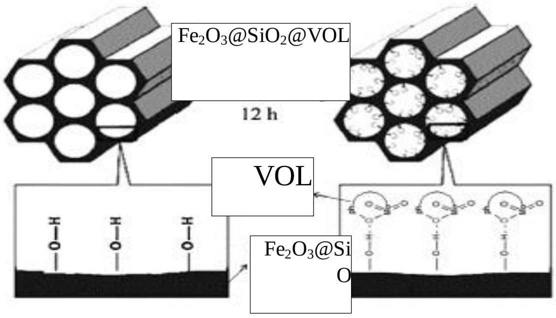
The discovery of efficient method for catalytic oxidation is an important goal in synthetic chemistry. The use of transition metal complexes as catalyst has been receiving increasing attention during past two decades due to many reasons: (1) the requirement for the functionalization of lower alkenes formed as by products in the manufacture of gasoline, (2) the need for partial selective oxidation and (3) the preparation of compounds with a specific structure. The transition metal complexes seem to fulfill some of these requiremens. Vanadium oxide was probably one of the first transition metal complex used in oxidation rections1. So, for this propose a Schiff base ligand derived from 2-hydroxy-3 methoxy benzaldehyde and 2,2-dimethyl-propylenediamine (H2L) an dits corresponding oxovanadium(IV) complex (VOL) has been synthesized and characterized by X-ray crystal structure.

Then adsorption of VOL on the surface of silica-coated magnetite nanoparticles via hydrogen bonding led to the formation @VOL as a heterogeneous catalyst 2. FT-IR and atomic absorption spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used to characterize and investigate the magnetic nanocatalyst . We have performed the oxidation reaction of various olefins using Fe2O3@SiO2@VOL as the catalyst. The heterogeneous catalyst can be recover-ed easily and reused many times without significant loss in catalytic activity and selectivity.



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Synthesis of amino functionalized magnetic nano-particles and its application for magnetic removal of benzoic-acid from aqueous solution: Kinetics, equilibrium and thermodynamic studies

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In this research, Fe_3O_4 magnetic nano-particles were synthesized and then functionalized with amino group (alanine) by a simple and cost-effective approach to prepare a novel adsorbent for the removal of benzoic acid (BA) . [1-3] The adsorbent was characterized using powder X-ray diffraction, Fourier transform infrared spectroscopy and field emission scanning electron microscopy. The studies were carried out under various experimental conditions such as pH, contact time, BA initial concentration and temperature to assess the potentiality of the adsorbent regarding the removal of BA from water samples. It was observed that the adsorption of 30 mg L^{-1} BA is favored at pH around 6 with equilibrium time of 30 min. To determine the adsorption capacity, the equilibrium data were analyzed using linear form of Langmuir, Freundlich and Temkin isotherm equations. Langmuir equation showed higher conformity than the other equations with a maximum adsorption capacity of 119.95 mg g^{-1}. Kinetic adsorption data were analyzed using the Lagergren pseudo-first-order kinetic model and the pseudo-second-order model. The regression results showed that the adsorption kinetics was more accurately represented by pseudo-second-order model. The calculation of the thermodynamic parameters such as Gibbs free energy, entropy and enthalpy indicated that the adsorption process was spontaneous and exothermic in nature.

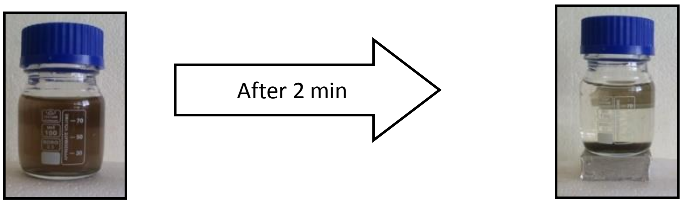

Fig. 1. nano-hybrids without/in the presence of the magnet

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Study on Ultrasound Assisted Co-precipitation as a New Method for Synthesis of NiMo Hydrodesulfurization Catalysts

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In this paper, NiMo catalysts dispersed on multi-walled carbon nanotubes (MWCNT) and γ-Al_2O_3 were synthesized by using new method of ultrasound assisted co-precipitation. The samples were characterized by BET, FTIR and XRD techniques and tested in HDS process at 160°C and atmospheric pressure. BET surface area were higher in ultrasound assisted co-precipitated catalysts which confirmed using ultrasound irradiation during precipitation resulted in formation of small and well-dispersed particles. [1] Comparing MWCNT and alumina supported catalysts showed more surface area for carbon-based catalysts. XRD analysis showed that the active phase peaks have higher crystallinity in MWCNT supported catalyst due to the hydrophobic surface of carbon nanotubes [2] that makes the interaction between the support and the active phase weak enough to allow forming a more structured crystals. Sulfur reduction in HDS was higher in catalysts synthesized with ultrasound assisted co-precipitation method which shows surface area has more positive influence on reactivity of the HDS catalyst than negative effect of active phase crystallinity.

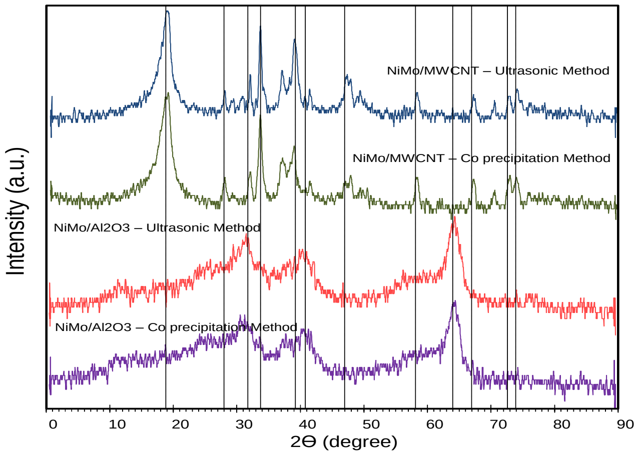

Fig. 1. XRD Patterns for NiMo nanocatalysts with different synthesis methods

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Comparison of different carbon nanotubes as support in new trimetallic Ni Mo W catalysts for HDS process

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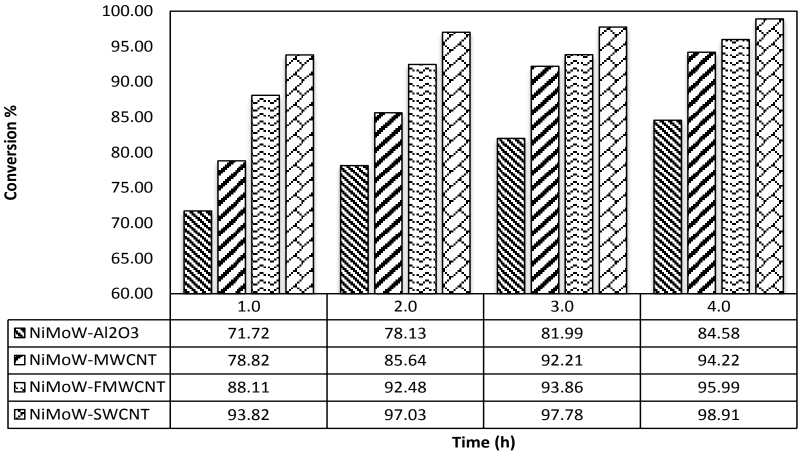
A series of new trimetallic Ni Mo W catalysts supported on multi-walled carbon nanotubes, functionalized multi-walled carbon nanotubes and single-walled carbon nanotubes were prepared and compared with conventional support of γ-Al_2O_3 in hydrodesulfurization process. The prepared catalysts were characterized by XRD, BET, FTIR and TGA and tested at atmospheric pressure and 160 °C. XRD patterns showed that active phase crystals are in nano-metric scale and the crystallinity of active phase were less in single-walled due to porosity and surface properties of the support .[1] Maximum surface areas was related to single-walled and functionalization of multi-walled with acid increased its surface area. All catalysts indicated weight loss during TGA analysis which can be attributed to the elimination of physisorbed water and decomposition of deposited metal salts of active phase .[2] Catalytic studies indicated that the HDS activity and selectivity was the highest in the case of single-walled carbon nanotubes. The highest sulfur reduction in this catalyst is attributed to the high surface area and less crystalline structure of active phase which increased the amount of active sites and their dispersion over the support suitable for HDS activity.



	1.0	2.0	3.0	4.0
▧ NiMoW-Al2O3	71.72	78.13	81.99	84.58
▨ NiMoW-MWCNT	78.82	85.64	92.21	94.22
▤ NiMoW-FMWCNT	88.11	92.48	93.86	95.99
▩ NiMoW-SWCNT	93.82	97.03	97.78	98.91

Fig. 1. Conversion of Ni Mo W nanocatalysts on different supports

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Effect of Tungsten Loading in New Trimetallic NiMoW Catalysts for HDS Process

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The deep desulfurization of fossil fuels has been attracted many researches due to the environmental regulations for decrease of the sulfur content.Today, utilization of low sulfur content fuels (less than 10-15 ppm) is considered in the most of countries.[1] In this paper, modified Iranian Clinoptilolite was utilized as the support of NiMoW and synthesized by the ultrasound-assisted precipitation method. The optimum amount of tungsten and operational parameters such as thiophene concentration and reaction time were investigated. Characterization analyses such as XRD, FTIR and BET were applied and the activity of catalysts in the hydrodesulfurization process was tested at 160 ˚C and one atmosphere. XRD results proved the existence of WO_3, NiO and MoO_3 crystals in synthesized catalysts. The HDS catalytic tests considered the sample with 6%wt of tungsten was the highest activity which leaded to 91% removal of thiophene from n-decane solution. Study on reaction time showed that at the beginning the rate of thiophene removal was high which gradually decreased.

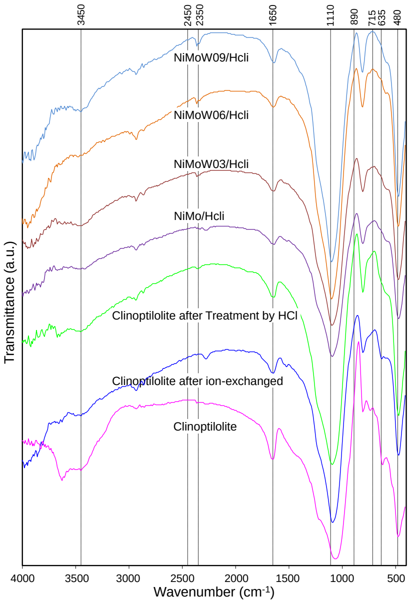

Fig. 1. FTIR Patterns for NiMo/Hclin nanocatalysts with different tungsten loading, and after treatment of clinoptilolite

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TrimetallicNiMoW/Mordenite Synthesized byUltrasound Assisted Co-precipitationMethodas Hydrodesulphurization Catalyst

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Regarding environmental issues,hydrodesulfurization of cruel oil for reduction of sulphur content is an important process .[1]_ENREF_2_ENREF_3 In this paper, the modified Iranian mordenite, a natural zeolitewas applied as the support of tungsten promoted molybdenumandnickel catalysts. Tungsten has electrical and surface properties like nickel and can be applied for modification of dispersion and interaction between Ni and Mo particles. These catalysts were fabricated by the conventional precipitation and ultrasound assisted precipitation methods. Various analyses such as XRD, BET and FTIR were utilized to investigate the physicochemical properties of synthesized catalysts. The XRD patterns proved that presence of tungsten in catalyst reduced the Ni and Mo crystal size in comparison to tungsten free catalyst leading to more active sites.Furthermore, there was an optimum amount of 6%wt of tungsten in which 95% of thiopheneremoval from n-decane solution was observed. In loadings of tungsten more than 6%wt there was a sensible reduction in HDS activity probably due to sintering and agglomeration of active sites. This trend was similar to trend was observed for BET analysis which proves direct effect of surface area in HDS activity. HDS activity also is higher for catalyst synthesized by ultrasound assisted precipitation compared to the conventional precipitation method.

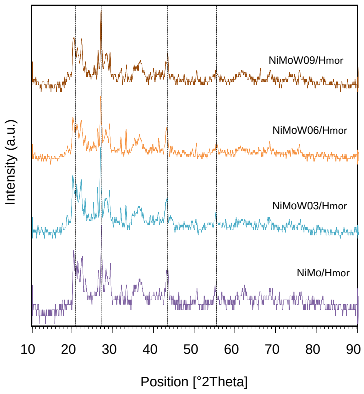

Fig. 1.XRD Patterns for NiMo nanocatalystssynthesized by ultrasound assisted co-precipitation method

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Synthesis, characterization and biological evaluation of new α-aminophosphate as AChE and Urease inhibitor

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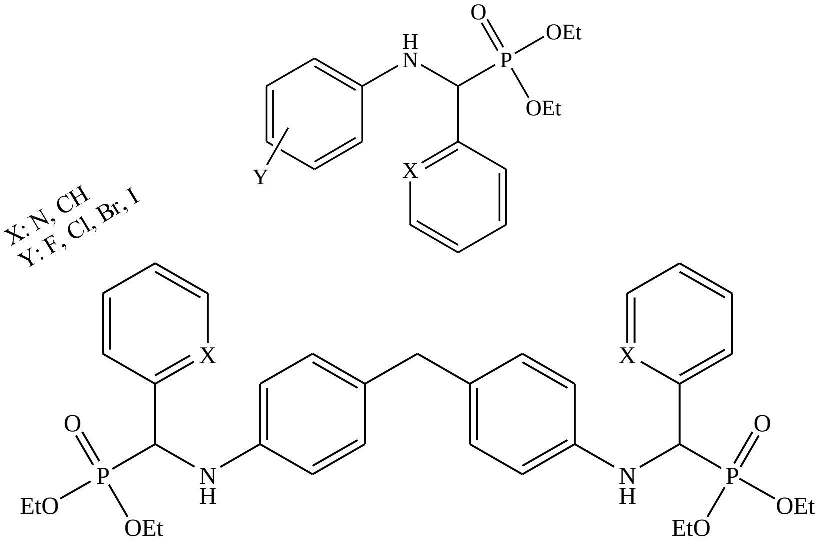
Aminophosphonic acid derivatives constitute an important class of organophosphorus compounds on account of their versatile biological activity. The general low mammalian toxicity of these compounds made them attractive for use in agriculture and medicine. The pharmacological importance and utility of aminophosphonic derivatives have stimulated extensive studies on various aspects of chemistry: synthetic routes, structural and spectral characterization and evaluation of their biological properties. From the above consideration, and in connection with our current works in the biological activity of phosphous(IV) compounds,[1-3] here we synthesized novel *mono* and *bis* *α*-aminophosphonates. All compounds were characterized by ^{31}P, ^{13}C, ^{1}H NMR and IR spectroscopy. A comparable study on the inhibitory effects of the *mono* and *bis* derivatives on AChE and Urease activity were performed using a modified Ellman's method and their inhibition mechanisms were evaluated by obtaining Line weaverBurk plots.



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Homogeneously catalyzed synthesis of aldol derivatives from Isatins and ketones

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Catalysts are currently widely used in industry, but the search for improved efficiencies, stereo selectivities, or recycling is still a matter of intense researches. Metal-catalyzed reactions have made a great contribution to the recent growth of organic synthesis, and a variety of synthetic methods have been reported using ruthenium complexes in catalytic amounts.[1]
On the other hand, C-C bond formation reactions are the essence of organic synthesis used extensively in many important syntheses. The aldol reaction is a powerful method of creation of new C-C bonds. The reaction has proven to be a powerful and general method for the stereo controlled construction of β-hydroxy ketone derivatives and has relevant application in the synthesis of carbohydrates, amino sugars, steroids and natural heteroatomic molecules. Aldol reaction frequently provides an easy access for compounds which plays an important role as an intermediate for the design of pharmaceuticals. There are several approaches to synthesis of aldols. However, only few reports described the use of catalyst to perform the aldol reactions in the mild conditions. As part of our continuing studies toward Ru-catalyzed aldol reactions[2], we found that isatin derivatives react with unactivated ketones in the presence of ruthenium catalyst to afford β-hydroxy ketones. This approach may provide access to a wide range of aldol adducts in moderate to good yields with excellent diastereo selectivities.

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Syntheses and structural properties of a new tricoordinated mercury(II) compound: X-ray structure, Hirshfeld surface analysis and DFT calculations

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The chemistry of mercury and its compounds has attracted the interest of both the chemistry and chemical engineering communities over the years, due to its potential applications in the paper industry, in sensors, as well as for mercury batteries.[1,2] The versatility of this chemistry is evident from the ample variations in the coordination environment of Hg(II), and the formation of a plethora of coordination frameworks.[3,4] in this work, synthesis and structural investigation of a new mercury(II) complex with a ligand based on isonicotinohydrazide were reported. The molecular structure of complex was analyzed by single crystal X-ray diffraction. The results reveal that the mercury complex crystallizes in the monoclinic system. The Hg(II) center is tricoordinated by one nitrogen atom of ligand and two iodide anions. The theoretical studies on the molecular structure and vibrational spectra of complex were investigated by FT-IR and DFT calculations. The recorded X-ray diffraction bond parameters are compared with theoretical values calculated at B3LYP/LANL2DZ level. The observed vibrational patterns were compared with the computed wave numbers. Also, Hirshfeld surface analysis has been used for investigation of intermolecular interactions. The Hirshfeld surface and 2D fingerprint plot of mercury complex have been shown in Fig. 1. The visible red spots on d_{norm} surface are due to the O···H/H···O interactions. These interactions are the main intermolecular interactions by 20.9% and are presented as two distinct sharp spikes ($d_e+d_i \approx 2.2$) in the 2D fingerprint plot. Other important contacts are H···H and H···I interactions.

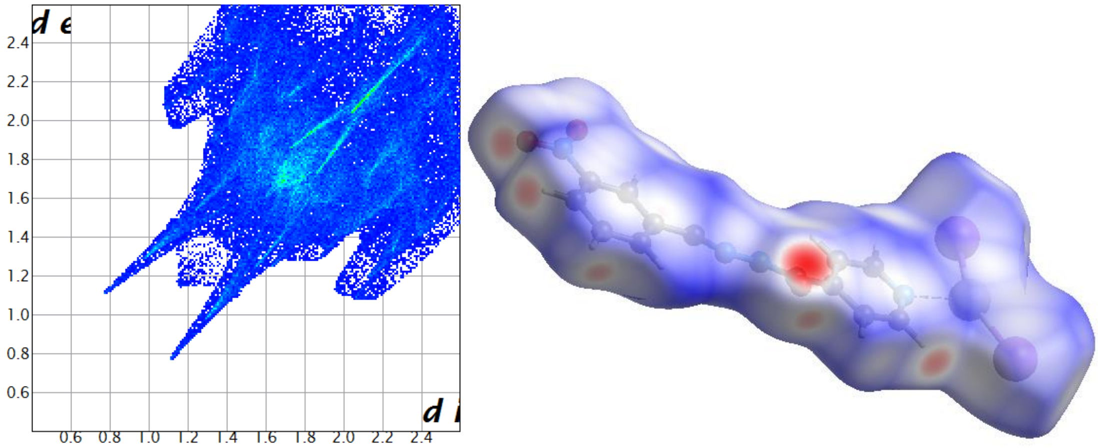

Fig. 1. (left) 2D fingerprint plot, (right) 3D Hirshfeld surface mapped with d_{norm}.

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Synthesis of nano core-shell Fe3O4@SnO2

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This study is about synthesis, characterizaion and application of SnO_2 nano catalysts in the synthesis of polyolester oils. The nano catalyst was synthesized by core-shell method. In this method, $SnCI_4$ salt was used in alkalin media in the presence of Fe(II) and Fe(III) salts for the formation of $Fe_3 O_4$ Nano particals as the core in two thermal steps. First step is preparation of Tin hydroxide and second is converting Tin hydroxide to SnO_2 by remove of water. This nano coreshell is $Fe_3O_4@SnO_2$.Nano catalyst was characterized with XRD, SEM, TEM and thermal analysis of synthetic was carried out by Differential Scanning Calorimetry(DSC)/Thermal Gravimetry Analysis (TGA). the presented method has some advantages such as low cost and easy access.

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Zinc(II) complex with 2,2'-bipyridine and 4-pyridincarboxylichydrazid dithiocarbamato ligands: synthesis and characterization

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Dithio carbamates are S, N containing ligands, which display a rich and varied coordination chemistry with a wide range of transition and main group metal complexes. Dithio carbamates have also found important use in medicine as anti-alcoholic drug, anticancer, and recently as co-adjuvant in AIDS treatment.[1] In this study we report the synthesis of a new dithio carbamate ligand and its complex with zinc(II) to the following formula [Zn(py-dtc)(bpy)]Cl (where py-dtc = 4-pyridincarboxylichydrazid dithiocarbamat and bpy = 2,2'-bipyridine) (Fig.1).Solid state FT-IR spectroscopy of the above complex shows three characteristic stretching bands at 1502, 766 and 690 cm^{-1} assigned to ν(N-CSS), ν(CSS)$_{as}$ and ν(CSS)$_{s}$ modes respectively.[2] ^{1}HNMR (500 MHz, DMSO-d$_6$, ppm): 7.29 (m, 2H-a), 7.65 (m, 2H, H-b), 12.25 (sb, H, H-c), 13.11 (sb, H-d), 8.43 (m, 2H, H-3,3′), 8.13 (m, 2H, H-5,5′), 8.55 (m, 2H, H-4,4′) and 8.95 (m, 2H, H-6,6′). Electronic spectra exhibit four bands. The bands at 210 (logε = 2.14), 245 (logε = 2.75), 301 (logε =2.55) and 333 nm (logε =2.01) may be assigned to intraligand π→π* and n→π* transitions of 2,2'-bipyridine ligand as well as CSS^{-} group.[3]

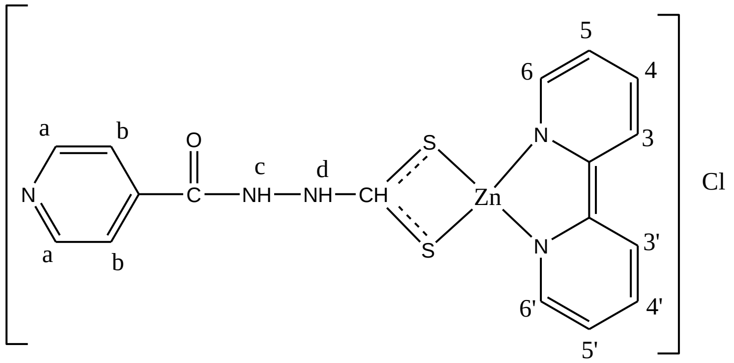

Fig. 1 Proposed structures and nmr numbering scheme of [Zn(py-dtc)(bpy)]Cl

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Synthesis, X-ray structure and catalytic activity of oxovanadium(V) complex with N,N,O-donor ligand

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A new mono oxidovanadium(V) complex, [$VOCl_2L$], of the tridentate Schiff base hydrazone-type N,N,O-donor ligand (HL = (E)-N′-(phenyl(pyridin-2-yl)methylene)isonicotinohydrazide), has been synthesized starting from the reaction of $VOCl_3$ with H_2L in methanol. The ligand was synthesized by condensation of 4-pyridine carboxylic acid hydrazide with 2-benzoyilpyridine in methanol.[1] These compounds were characterized by spectroscopic methods (^1H NMR, ^{13}C NMR, IR and UV-Vis) and elemental analyzes. The structure of complex was determined by single crystal X-ray analysis. Structural studies revealed that this complex has a slightly distorted octahedral $N_2O_2Cl_2$ coordination environment around the metal centre, which the hydrazone ligand acting as N,N,O-donor tridentate, mononegative ligand.[2]

The catalytic potential of this complex has been tested for the oxidation of *cis*-cycloocten using H_2O_2 as the cheap and environmentally safe oxidant. In order to achieve the maximum oxidation of cyclooctene, the effects of various parameters including the molar ratio of oxidant to substrate, temperature and solvent have been studied. The results of these studies showed that this complex has high potential for the catalytic and selective oxidation of cis-cyclooctene with aqueous H_2O_2.

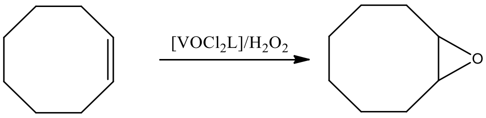

Fig 1. Schematic representation of cycloocten oxidation in the presence of [$VOCl_2L$]

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Synthesis and characterization of new zinc(II) complex containing phenyl acetic hydrazide dithiocarbamate as potential anticancer agent

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Many metal ions are known to play very important roles in biological processes in the human body. For example, zinc (II) ion is the third most abundant transition metal in humans. This ion found either at the active sites or as structural components of a good number of enzymes.[1] Based on these evidences, we report here in the synthesis and characterization of a newly-created water-soluble of zinc(II) complex [Zn(ph-dtc)(bpy)]Cl (where ph-dtc= phenyl acetic hydrazide dithiocarbamate and bpy = 2,2'-bipyridine) (Fig. 1). Solid state FT-IR spectroscopy of the above complex shows three characteristic stretching bands at 1536, 841 and 710 cm^{-1} assigned to ν(N-CSS), $\nu(CSS)_{as}$ and $\nu(CSS)_{s}$ modes respectively.[2] ^{1}HNMR (500 MHz, DMSO-d_6, ppm): 6.98 (m, H-a), 7.13 (m, 2H, H-b), 7.35 (m, 2H, H-c), 11.02 (sb, H-e), 13.11 (sb-H-d), 8.02 (t, 2H, H-3,3′), 8.19 (m, 2H, H-5,5′), 8.33 (m, 2H, H-4,4′) and 8.65 (m, 2H, H-6,6′). Electronic spectra exhibit four bands. The bands at 213 (logε = 2.09), 239 (logε = 3.61), 289 (logε =2.93) and 340 nm (logε =2.33) may be assigned to intra ligand $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions of 2,2'-bipyridine ligand as well as CSS^- group.[3]

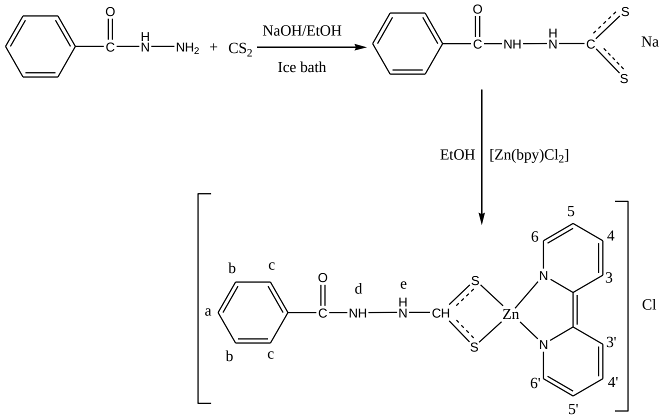

Fig. 1

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Synthesis, X-ray structure and catalytic activity of manganese complex with keto form N,N,O-donor neutral ligand

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A new manganese(II) complex, [Mn(HL)Cl_2(CH_3OH)], of the tridentate Schiff base hydrazone-type N,N,O-donor ligand (HL = (E)-2-cyano-N'-(phenyl(pyridin-2-yl)methylene)acetohydrazide.), has been synthesized starting from the reaction of $MnCl_2$ with HL in methanol. The ligand was synthesized by condensation of 2-cyanoacetohydrazide with phenyl(pyridin-2-yl)methanone in methanol.[1,2] These compounds were characterized by spectroscopic methods (^{1}H NMR, ^{13}C NMR, IR and UV-Vis) and elemental analyzes. The structure of complex was determined by single crystal X-ray analysis. Structural studies revealed that this complex has a slightly distorted octahedral $N_2O_2Cl_2$ coordination environment around the metal centre, which the hydrazone ligand acting as N,N,O-donor tridentate. In addition, the ligand is coordinated in keto form as neutral ligand.

The catalytic potential of this complex has been tested for the oxidation of *cis*-cycloocten using H_2O_2 as the inexpensive and environmentally safe oxidant. In order to achieve the maximum oxidation of cyclooctene, the effects of various parameters including the molar ratio of oxidant to substrate, temperature and solvent have been studied. The results of these studies showed that this complex has high potential for the catalytic and selective oxidation of cis-cyclooctene with aqueous tert-butylhydroperoxide (TBHP).

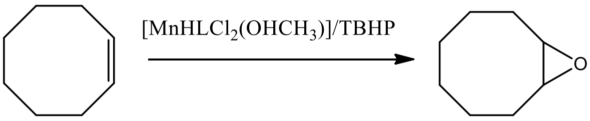

Fig. 1. Oxidation of Cycloocten in the presence of

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Indanol dehydration based on B/Al_2o_3nano reactors

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Catalytic technologies are critical to present and future energy,chemical process, and environmental industries. Conversion of crude oil, coal and natural gas to fuels and chemical feedstock,production of a variety of petrochemical and chemical products,and emission control of CO, hydrocarbons, and NO, all rely on catalytic technologies. In the era of nanotechnology where size of every object is going to smaller and smaller with their enhanced properties; catalysts of nano size are also used in several chemical processes and beneficial for human being. A key objective of nanocatalysis research is to produce catalysts withmaximum selectivity, extremely high activity, low energy consumption, and long lifetime. This can be achieved only by precisely controlling the size, shape, spatial distribution, surface composition and electronic structure, and thermal and chemical stability of the individual nanocomponents.In recent years, Al_2O_3–B_2O_3compounds have attracted considerable interests due to their strong acidity and high catalytic activity in different types of reactions. [1,2] Alumina as an amphoteric compound has attracted many attentions for such a reaction. Modification of the alumina can change the conversion and yield of the reaction. Boron atom is smaller than aluminum. Therefore, doping this atom can change the alumina oxide acidic properties. In this study, Boronoxide supported onγ-alumina catalyzed dehydration of indanol.The catalyst characterized by N2- sorption, XRD, SEM and FT-IR.Results showed that the boron oxide is doped in the alumina matrices. Catalytic activity exhibited that the indene is the main product.

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Starch and poly (acrylic acid)-based hydrogel as efficient and reusable catalyst in oxidation of olefin

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For first time, we have developed the starch and poly (acrylic acid)-based system for oxidation of olefin. The composite hydrogels were synthesized by free radical crosslink copolymerization of acrylicacid (AA) and N_methylenebis-acrylamide (MBA) in the presence of starch. During polymerization starch was incorporated in situ in the crosslinked polyacrylicacid gel to produce composite hydrogels.[1] the structure and properties of the hydrogels were characterized by FTIR, DTA–TGA and XRD.

Starch-PAA particles were loaded with Cu (II) ion from $CuCl_2$.[2] The starch-PAA-Cu^{II} Composite was used in oxidation of *cis*-cycloocten in the presence of H_2O_2 as an oxidant and $NaHCO_3$ as a co-catalyst. The effects of various parameters, including the molar ratio of oxidant to substrate, the temperature and the solvent, have been studied. The catalyst shows high activity and selectivity toward production of cyclohexne epoxide in acetonitrile at 60 °C with $[H_2O_2]/[C_6H_{10}] = 4$ molar ratio and 0.25 mmol $NaHCO_3$ as co-catalyst. Starch-PAA-Cu^{II} composite catalyst system had better catalytic performances in the oxidation reactions and it could be used for ten times without any loss of activity.

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Oxidation of organic compounds in the presence of silver compounds incorporated in clinoptilolite materials

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Oxidadation of a cycloocten was studied using silver nano-particles incorporated in clinoptilolite (CP). The Ag^+/CP was prepared by a conventional ion-exchange method[1] in silver acetate aqueous solution (0.5M) for 24 h and the solid portion was subsequently filtered, washed with deionized water and dried at 100 °C overnight to obtain Ag^+/CP. Then Ag^+/CP calcined at 450 °C for 12 h for preparation of the Ag_2O/CP catalyst.[2] The modified samples were characterized by X-ray diffraction (XRD), Fourier transformation infrared (FTIR) and inductively coupled plasma–atomic emission spectrometer (ICP). Oxidation reaction of the cycloocten was determined by gas chromatography (GC).

The catalytic potential of Ag^+/CP has been tested for the oxidation of *cis*-cycloocten using H_2O_2 as the terminal oxidant. The effects of various parameters, including the molar ratio of oxidant to substrate, the temperature and the solvent, have been studied.

The catalyst shows high activity and selectivity toward production of cyclooctene epoxide in acetonitrile at 60 °C with $[H_2O_2]/[C_8H_{14}] = 3$ molar ratio. Comparison of the Ag^+/CP catalyst with Ag_2O/CP catalyst showed that the Ag^+/CP catalyst had higher activity than the other one.

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Design and synthesis of clay composite for the stabilization of silver nanoparticles application for a heterogeneous catalyst toward reduction of nitro group

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Clay minerals occur widely in nature and their high surface area and ion exchange properties make them suitable for use as solid supports. The smectite-type clays, such as montmorillonite (MMT), contain negatively charged silicate layers and intercalated cations .[1] Clay has been widely studied as the host of catalytic noble metals in its interlamellar space, and generally the ion-exchange property was utilized. Various methods are employed for the reduction of nitro compounds .[2-4] Hence, attention has been focused on to develop suitable heterogeneous catalyst for catalytic reduction reactions. In recent years Nanostructures of silver have been gaining significant research interest due to their unique shape and size dependent optical, antimicrobial, and catalytic properties.

In this work, novel Ag (I) complex with ylide-phosphonium ligand, $[PPh_3CH_2C(O)CH_2Cl]$ [5] was synthesized and structurally characterized by IR and resonance signals in the NMR, then intercalated cationic complex in the MMT and studied by XRD, TEM and SEM. We used this heterogeneous catalyst for reduction of nitro compounds with investigated by gas chromatography and exhibited high and stable activity.

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Quantitative Insights into the Crystal Structure of a new four-coordinated zinc compound: X-Ray crystallography and Hirshfeld Surface investigation

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Hirshfeld surface analysis represents unique quantitative and qualitative tools to decode intermolecular interactions and offer a facile way of obtaining information from comparable structures.[1] The molecular Hirshfeld surfaces reflect intermolecular interactions in a novel visual manner as a triangulation surfaces, and breakdown of the corresponding 2D fingerprint plot provide a convenient means to show the significant similarity and/or differences between related moieties.[2] in present study, crystal structure and intermolecular interactions of a new four-coordinated zinc compound were investigated. The complex crystallizes in the triclinic system and space group $P\bar{1}$ with with two crystallographically independent molecules noted as A and B per asymmetric unit cell. The crystal structure of the complex reveals the presence of a structure consisting of a N_2-donor Schiff base, two bromide anions and a zinc(II) center in the discrete monomeric species. Both molecules are in distorted tetrahedral environments. Theoretical analysis of intermolecular interactions was performed within the Hirshfeld surfaces approach. Fig. 1 shows Hirshfeld surface of molecule B and relative contribution of various intermolecular interactions in molecule A. relative contributions of interactions in both molecules is almost identical. H···H interactions comprise the majority of the Hirshfeld surface, making up 52.1% for each molecule in the asymmetric unit. Red spots on d_{norm} surface of molecules are due to H···Br and H···C interactions that comprise 19.9% and 21.8% of Hirshfeld surface in molecule A.

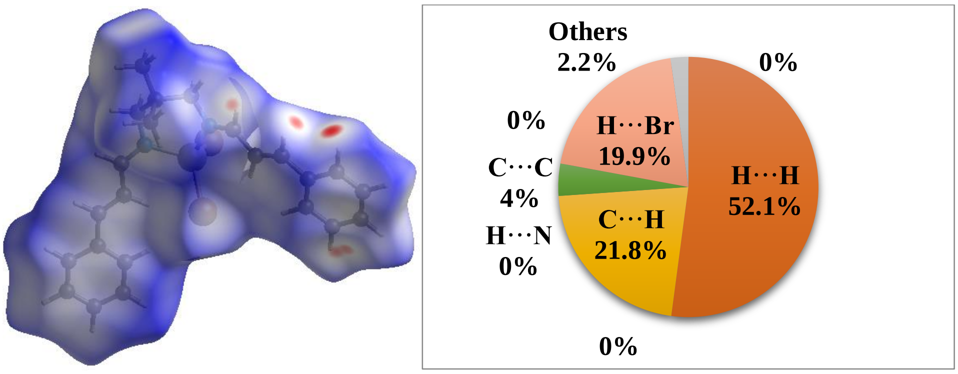

Fig. 1. (left) 3D Hirshfeld surface mapped with d_{norm} of molecule B, (right) relative contribution of various intermolecular interactions in molecule A.

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Magnetic removal of gemfibrozil from pharmaceutical wastewater effluents utilizing a β-cyclodextrin grafted graphene oxide-magnetite nano-hybrid

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A β-cyclodextrin (β-CD) grafted graphene oxide (GO)/ magnetite (Fe_3O_4) nano-hybrid was synthesized and used as an innovative adsorbent for magnetic removal of gemfibrozil (Gem) from pharmaceutical wastewater effluents .The sorption media was characterized using powder X-ray diffraction, Fourier transform infrared spectroscopy and field emission scanning electron microscopy. The as-prepared nanohybrid was used for studying the mechanism of magnetic removal of gemfibrozil from aquatic media. The studies were carried out under various experimental conditions such as pH, contact time, Gem initial concentration and temperature to assess the potentiality of the adsorbent regarding the removal of Gem from waste water samples. The equilibrium adsorption data were analyzed using Langmuir, Freundlich and Tempkin isotherms. The thermodynamic parameters such as $\Delta G°$, $\Delta H°$ and $\Delta S°$ were computed from the vant hoff equation. Freundlich equation showed higher conformity than the other equations with a maximum adsorption capacity of 48.3 mg g^{-1}. The regression results for kinetic adsorption data showed that the adsorption kinetics was more accurately represented by pseudo-second-order model. The calculation of the thermodynamic parameters such as Gibbs free energy, entropy and enthalpy indicated that the adsorption process was spontaneous and exothermic in nature.

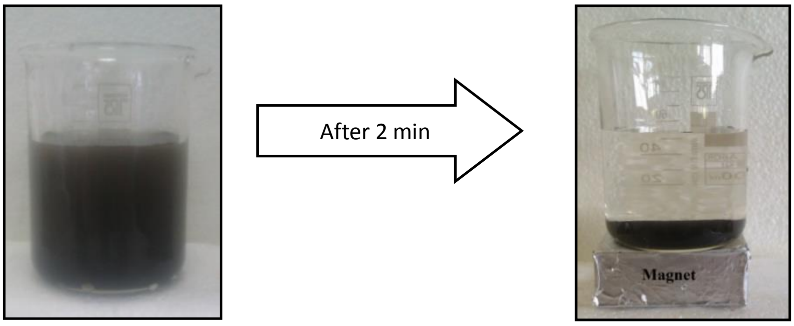

Fig. 1. Nano-hybrids without/in the presence of the magnet

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Synthesis, characterization and catalytic properties study of new yttrium sandwich-hetropolyoxometalate

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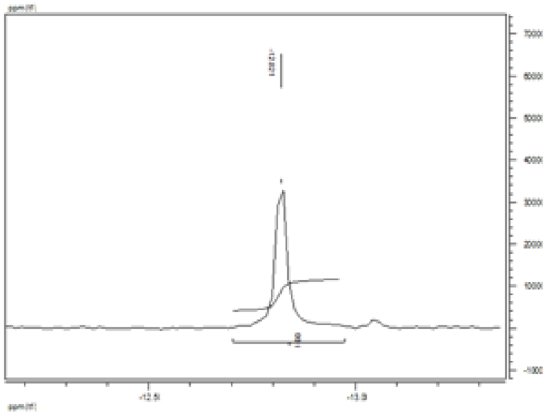
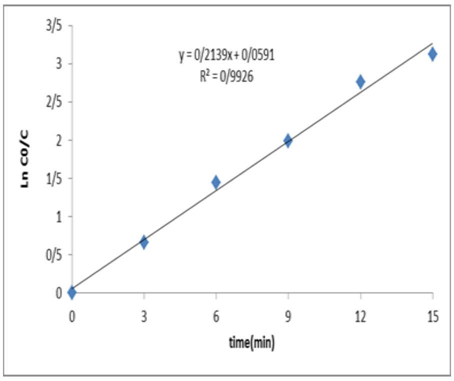
The potassium salt of new sandwich-type polyoxometalate $[\{Y_3O_3(OH_2)_2\}(PW_9O_{34})_2]^{15-}$ has been synthesized by the reaction of the trilacunary $[A\text{-}PW_9O_{34}]^{9-}$ ligand with Y(III) in an acidic solution, and characterized by Fourier transform infrared spectroscopy (FT-IR), powder X-ray diffraction (XRD), cyclic voltammetry (CV), ^{31}P NMR, UV–Vis spectroscopy and Thermogravimetric analysis (TGA).

To improve the photocatalytic efficiency of TiO_2, $[\{Y_3O_3(OH_2)_2\}(PW_9O_{34})_2]^{15-}$-Y-$TiO_2$ nanocomposites with different $[\{Y_3O_3(OH_2)_2\}(PW_9O_{34})_2]^{15-}$ loading levels (10%–40%) were prepared by impregnation method. Y-TiO_2 support, doped with yttrium, was synthesized via sol-gel technique.

The effects of $[\{Y_3O_3(OH_2)_2\}(PW_9O_{34})_2]^{15-}$ loadings, catalyst dose and initial pH of dye solution on the degradation kinetics of methyl orange under UV light ($\lambda \geq 365$ nm) were discussed. Kinetics studies showed that the photocatalytic degradation of methyl orange fitted the apparent first-order reaction. Methyl orange was totally degraded in 11 min under optimum conditions: 10% loading, 0.01 g dose and pH 3. The catalyst was stable and easily to be separated from reaction system for recovery.





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Graphene–Copper Complexes Hybrid Catalyst for the Preparation of Various Aryl Azides

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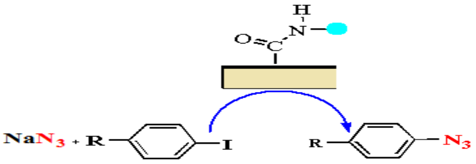
Graphene,[1] with its distinctive two-dimensional structure,[2] huge surface area,[3] and excellent mechanical[4] and electrontransfer[5] properties, has emerged as a promising support for heterogeneous catalysis. A new hybrid complex based on covalent interaction between of copper (II) complex of 1,2-bis(4-aminophenylthio)ethane and graphene oxide(GO), was prepared. This new copper (II) complex–graphene oxide, Cu(II)-GO, was characterized by XRD, IR, TGA and ICP-AES which confirmed the successful incorporation of the Cu(II) complex onto the graphene oxide. N_2 adsorption–desorption and SEM showed the intact structure of the graphene oxide. Aryl azides have found growing applications in organic transformations, especially for the assembly of various heterocycles and metal complexes.[6] Direct coupling of inactivated aryl halides with sodium azide catalyzed by Cu^{2+} was reported to be possible but gave low yields, mainly because completion of the reaction needed a higher reaction temperature, which caused decomposition of the aryl azides. In the present study, catalytic results showed that the immobilized Cu (II)-GO catalyst was more active in for efficient conversion of aryl halides to aryl azides. The reaction parameters were optimized. The catalyst was reusable without loss of its catalytic activity.



Scheme 1. Cu -catalyzed conversion of aryl halides to aryl azides.

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Copper(II) Complex Immobilizedon to Graphene Oxide as Efficient Catalyst for Epoxidation of Alkenes

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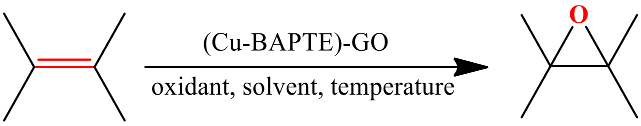
Multifunctional hybrid materials that take advantage of both the superior properties of graphene and a functionalizing material have been largely unexplored. Graphene oxide (GO), derived from the oxidation of graphite, possesses abundant oxygen-containing functional groups, which not only render GO moderate water-dispersibility but also offer reactive sites for further modification.[1] Graphene oxide due to its outstanding surface properties has emerged to be a matter of choice for supporting various homogeneous catalysts for various applications. For this reason, noncovalent[2] and covalent[3] methods for the functionalization of graphene have been developed. A new graphene-based hybrid material was prepared directly by covalent linkage between grapheme oxide and copper (II) complex of 1,2-bis(4-aminophenylthio)ethane. The catalyst, Cu(BAPTE)-GO was characterized by TGA, UV-Vis, FT-IR, SEM, BET, ICP-AES, and XRD. The synthesized catalyst was found to be highly efficient for conversion of alkenesto epoxides under mild conditions. The identification of products and their quantitative determination was done using GC. After completion of the reaction, the catalyst was easily recovered by filtration and reused for several runs without loss in activity and no leaching was observed during the reaction.



Scheme 1. Epoxidation of alkenescatalyzed by Cu(BAPTE)-GO

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Modified Nano-Manganese Oxide by Molybdenum as a robust Catalyst in Water Oxidation Reaction

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Designing a high efficient, cheap and green catalyst in water oxidation (WO) reaction has become one of the most important challenges in the sustainable energy field. Since, the structure of calcium-manganese ($CaMn_4O_4$) cluster in WO centre of photosynthesis was characterized; many researches focus on modelling of this centre by many metal complexes and different ligands as models for this metalloenzyme.[1] Manganese element has a main role in the catalytic activity of$Ca_4Mn_4O_4$ cluster. By this way, finding a method for modifying the efficiency of manganese oxides in water oxidation reaction could be the wisely rout to produce a robust catalyst in WO reaction.[1,2] In this work, a modified manganese oxide by molybdenum (MoMn) as an efficient WO catalyst was synthesized and characterized by X-ray diffraction (XRD), thermogravimetry (TG), Fourier transform infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM). The catalytic activity of MoMn oxide in chemical WO reaction in the presence of Ce(IV) was performed. Besides, the electrochemical behavior of MoMn oxide in WO reaction and the effect of molybdenum ion in the activity of manganese oxide were studied.

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A novel copper(II) complex containing *N*,N,N,O,O-donor ligand and Its electrochemical behavior studies at GC electrode

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The present study aimed to investigate the synthesis and electrochemical behavior of a new copper(II) Schiff-base complex. The electrochemical behavior of this complex was investigated by using cyclic voltammetry technique in the potential range between -0.1 and +1 V (*vs.* Ag/AgCl), at the surface of a glassy carbon electrode.

The copper(II) complex $[Cu(L_1)(H_2O)]$ of the five dentate Schiff base *N*,N,N,O,O-donor ligand (H_2L_1 = 2-{(E)-[(6-{[(1E)-(2- hydroxyphenyl)methylene] amino}pyridin-2-yl)imino]-methyl}phenol), has been synthesized starting from the reaction of $Cu(NO_3)_2$ with H_2L_1 in methanol. The ligand was synthesized by condensation of 2,6-diaminopyridine with salicylaldehyde in methanol. This compound was characterized by spectroscopic methods (^{1}H NMR, IR and UV-Vis). The structure of complex was determined by FTIR, AA and UV-Vis analysis. Structural studies and same papers revealed that this complex has a slightly distorted octahedral $N_3O_2OH_2$ coordination environment around the metal centre, which the Schiff base ligand acting as five dentate, dinegative ligand.

The electrochemical behavior of this compound was studied using cyclic voltammetry in DMF and tetrabutylammoniumperchlorate as solvent and supporting electrolyte. The anodic oxidation peak potential of copper(II) complex at the glassy carbon electrode occurred at about 0.4 V *vs.* Ag/AgCl with a current intensity of 1.82 µA which can be attributed to the Cu^{1+}/Cu^{2+}.

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Synthesis and Electrochemical Studies of Oxovanadium Complex with *N*,N,O,O - Donor Ligand

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A new mono oxidovanadium(V) complex, [VOL(OCH_3)], of the four dentate Schiff base hydrazone-type N,N,O,O-donor ligand (H_2L_1 = 2-{(E)-[(6-{[(1E)-(2-hydroxyphenyl)methylene]amino}pyridin-2-yl)imino), has been synthesized starting from the reaction of VO(acac)$_2$ with H_2L in methanol. The ligand was synthesized by condensation of 2,6-Diaminopyridine with salicylaldehyde in methanol.[1] These compounds were characterized by spectroscopic methods (^{1}H NMR, ^{13}C NMR, IR and UV-Vis) and elemental analyzes. The structure of complex was determined by FTIR, AA and UV-Vis analysis. Structural studies and same papers revealed that this complex has a slightly distorted octahedral $N_3O_2OH_2$ coordination environment around the metal centre, which the Schiff base ligand acting as four dentate, dinegative ligand.

The redox behavior of vanadyl complex was studied by cyclic voltammetric technique in the potential range between -0.5 and +1 V (*vs.* Ag/AgCl), in DMF and tetrabutylammoniumperchlorate as solvent and supporting electrolyte respectively. In the light of these results, it is suggested that this ligand acts as di anion and four dentate and coordinates to metal atom by azomethine nitrogen and oxygen atoms of hydroxyl group of the salicylaldehyde. The anodic peak potential of the ligand is about 0.7 V vs. Ag/AgCl while the vanadium complex shows an irreversible anodic peak at about 0.45 V vs. Ag/AgCl at the glassy carbon electrode with a current intensity 1.73 µA which can be attributed to the VO^{4+}/VO^{5+}.

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Ag(I) complexes of sulfonium ylide: Synthesis, characterization and NMR study

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Sulfonium ylide are important reagents in organic chemistry, this being especially true in the synthesis of naturally occurring products with important biological and pharmacological activities [1]. The synthesis of complexes derived from ylides and Ag(I) began in 1975 by Yamamoto et al. [2]. Other types of ylide complexes of silver(I) have been reported [3,4]. In 2013, Sabounchei et al. reported the crystal structures of Ag(I) complexes of sulfonium ylides [5]. It is well known that silver ions and silver-based compounds are highly toxic to micro organisms. For this reason, there is an urgent need to develop novel antimicrobial agents with difficult mechanisms of action aimed ata better understanding of the antimicrobial resistance. Herein we report the synthesis of stable silver(I) complexes, which are belongs to carbonyl stabilized sulfur ylides. The reaction of sulfonium ylide $(Me)_2SCHC(O)C_6H_4R$ (R = *m*-OMe) with Ag(I) in dry dichloromethane leads to the formation of C-coordinated polymeric complexes of the type Ag(NO3) and Ag(OTF). Characterization of the obtained compounds was also performed by elemental analysis, IR, MS, ^1H and ^{13}C NMR that indicated a 1:2 stoichiometry between the silver(I) nitrate and ylide *m*-OMe. (**Fig. 1**).

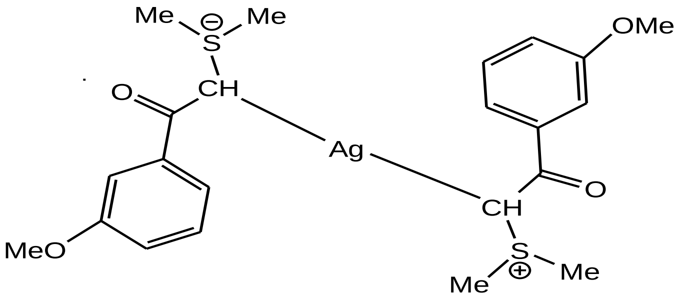

Fig. 1.Cα coordinated M(II) complexes.

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New Cu(I) complex containing α-keto stabilized sulfonium ylide: Synthesis, characterization and behavior toward Mizoroki-Heck reaction

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The coordination and organometallic chemistry of α-keto stabilized sulfonium ylides has been investigated extensively. [1] Copper complexes as well as palladium homologous combined with a ligand (phosphorous ylide) is one of the commonly used catalytic system in the Mizoroki-Heck cross-coupling reaction. [2] In view of the economy, the use of cheaper metals such as copper instead of palladium as catalyst precursor provides another attractive route. In this work, we report the synthesis, characterization and application of new Cu(I) complex $[CuCl_2((Me)_2SCHC(O)C_6H_4R)_2]$ (R=*m*-OMe) toward the Mizoroki-Heck cross-coupling reaction. Reaction of α-keto stabilized sulfonium ylides $(Me)_2SCHC(O)C_6H_4R$ (R = *m*-OMe) with $CuCl_2$ in 2:1 ratios leads to mononuclear products of the type $CuCl_2(ylide)_2$. Characterization of the complex by IR, MS, ^1H and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom. Well-defined sulfonium ylide Cu(I) complex was found to be an effective catalyst for the Mizoroki-Heck coupling of various aryl halides including with styrene and ethyl acrylate (**Fig. 1**). The reaction yielded the desired coupling products with good to excellent yields. Moisture/air-stability, High efficiency and low catalyst loadings are important features of these homogeneous reactions.

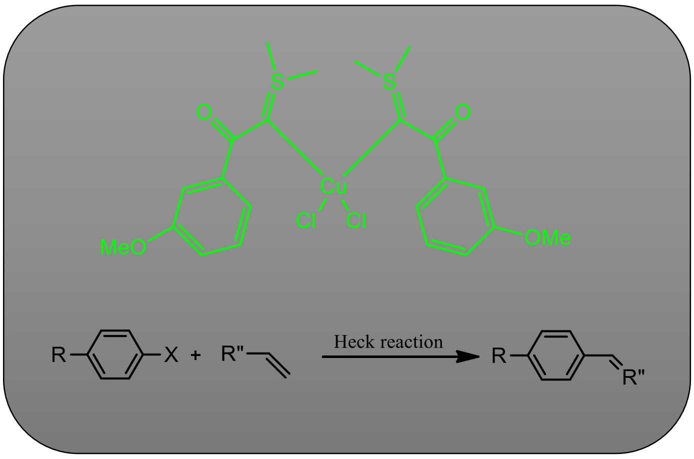

Fig. 1. The Heck cross-coupling reaction.

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Structural elucidation and Hirshfeld surface analysis of a new cadmium thiocyanate complex

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Coordination chemistry of cadmium(II) compounds is of great interest owing to their potential applications in various fields.[1,2] The d^{10} configuration and softness of cadmium(II) permit a wide variety of geometries and coordination numbers.[3,4] Additionally, pseudohalide anions such as thiocyanate (SCN^-) represent a familiar type of inorganic building blocks for creating metallosupramolecular complexes.[5] In this work, crystal structure and Hirshfeld surface investigation of a new octahedral Cd(II) complex were reported. $CdL_2(NCS)_2$ complex crystallizes in Orthorhombic system with space group *Pbca*. The molecular structure of complex is shown in Fig. 1, where atom Cd lies on an inversion center and is hexacoordinated by four N atoms from two Schiff base ligands, located in the equatorial plane, and two N atoms from the two isothiocyanate ligands in the apical sites. Two Schiff base ligands coordinate the cadmium center as a bidentate through the nitrogen atoms of iminic groups. The Hirshfeld surface and 2D fingerprint plot (Fig. 1) were calculated and visualized for investigation of intermolecular interactions. The majority of the Hirshfeld surface is related to H···H interactions, comprising 55% for each molecule in the asymmetric unit. These interactions are observed as several deep red spots on d_{norm} surface. S···H/H···S interactions arise from noncoordinated sulfur atom of thiocyanate groups comprise 13.2% of Hirshfeld surface and are observed as wings on the top left (H···S interaction) and bottom right (S···H) of the 2D fingerprint plot. Also, there are some visible red spots belong to H···C close contact, making up 29.7% of Hirshfeld surface.

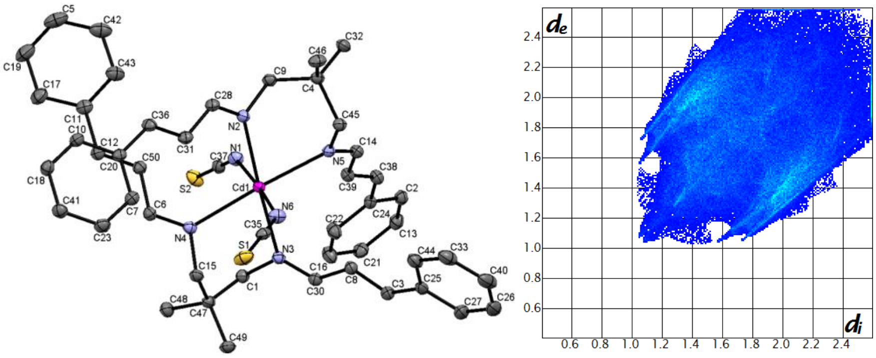

Fig. 1. (left) Crystal structure and (right) 2D fingerprint plot of $CdL_2(NCS)_2$ complex.

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Breathing Interpenetrated Metal−Organic Frameworks for CO_2 Storage Application

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A breathing 2-fold interpenetrated microporous metal−organic framework was synthesized with a flexible organic linkers and zinc metal. Self-assembly of ligands with zinc nitrate hexahydratein dimethyl formamide resulted in MOF-P1. Crystallographic measurements on MOF-P1 confirm the fumaric acid was connected to two zinc atoms ina paddle-wheel fashion.The paddle wheels are further pillared by 4-bpdb (1,4-bis(4- pyridyl)-3,4-diaza-1,3-butadiene) molecules occupying the axial sites of the Zn_2 paddlewheels to form a three-dimensional (3D) structure. Gas sorption experiments using CO_2 were performed using an HPVA-100 volumetric device at room temperature. The CO_2 sorptionplot at 0.1 p/p_0 suggests that sample does not reach a saturationpoint; therefore high pressure experiments with CO_2 were conductedat ambient conditions. Figure 1 shows the absorption isotherm of CO_2 at high pressures that indicate a type I relationship with a stepin the absorption at ~0.3 p/p_0. At 195 K, which exhibits two consecutive hysteretic breathing transitions between lp (large pore) and np (narrow pore) phases. We also propose an explanation for the experimentally observedcoexistence of np and lp phases in MOF-P1.

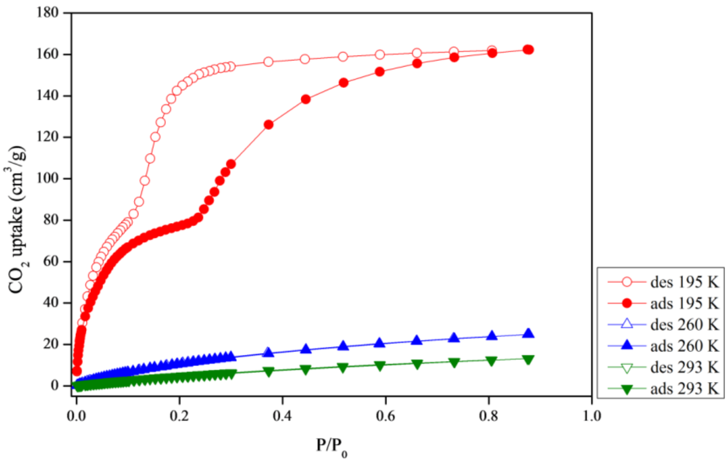

Fig. 1. CO_2 uptake isotherm of MOF-P1 in different temperatures

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Synthesis and characterization of new mononuclear and polymeric complexes $M(NO_3)_n$ derived from α-keto stabilized sulfoniumylide

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Metal carbene complexes are of much interest in syntheticchemistry. [1] One of the most abundant carbine complexesareCα coordinated Hg(II) and Cd(II)complexes, $[((Me)_2SCHC(O)C_6H_4\text{-m-}OMe)_2.Hg(NO_3)_2]$ and $[((Me)_2SCHC(O)C_6H_4\text{-m-}OMe)_2.Cd(NO_3)_2]$. Sulfur ylides $R_2S = C (R') (R'')$ (R, R′, R″ = alkyl or aryl groups) arevery reactive species with interesting applications in organic synthesis. [2] These compounds can behave as ambidentateligands, because the carbanion located at the Cα of the ylide or the enolate oxygen is able to donate electron density to a transition metal.[3] Considering the importance of metal carbenes, and particularlysulfoniumylide, synthetically simple and general routes fortheir preparation are highly desirable. Herein, we report the synthesis andcharacterizationof new mononuclear and polymeric complexes of M(II)derived from α-keto stabilized sulfoniumylide. Reaction of α-keto stabilized sulfoniumylides $(Me)_2SCHC(O)C_6H_4R$ (R = *m*-OMe) with $Hg(NO_3)_2.H_20$and $Cd(NO_3)_2.4H_2O$in 1:1 ratios leads to mononuclear andpolymeric products of the type $[HgX_2(ylide)]_2$. Also, The reaction yielded the desired M(II) complexes in excellent yields. Characterization of the complexes by IR, ^1H and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom (**Fig. 1**).

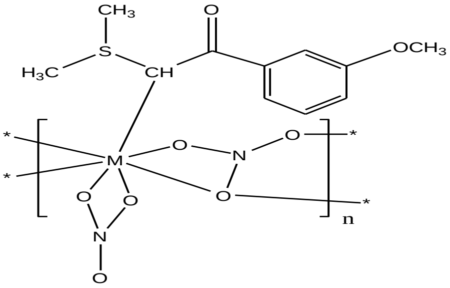

Fig. 1.Cα coordinated M(II) complexes.

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Synthesis of Fe -Mn oxide nanoparticles by hydrothermal method and Study of the effects of calcination conditions on their structures

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Fe- Mn oxide nanoparticles with high reactivity are suitable for ground water cleanup and treatment of industrial effluents. These nanoparticles have applications such as anti-scratch, catalyst, pigment and removal of arsenic. In other hand manganese oxide has no environmental problems and physical activity that lead using in industrial different sectors. When Fe and Mn metals combine to each other, the efficient catalyst will be obtain to use in industry. Recently Scientists studied the effect of preparation conditions on activity of Fe-Mn oxide catalysts to change the synthesized gas to ethylene and propylene by using different methods and checked the parameters like molar ratios, reactive, pH, and the time on the nanoparticle structures. In this study Fe-Mn nanoparticles prepared by hydrothermal method and calcinated at various times and temperatures. These nanoparticles characterized by X-Ray diffraction and SEM analysis. The time of reaction was 2h and the products were calcinated in range of 2-5 hours and the temperature varied between 400°-750°C). The lowest size of these nanoparticles obtained in 500°C and 3 h with tetragonal morphology. X-ray diffraction analysis (XRD) and scanning electron microscope analysis (SEM) showed in fig1. and fig 2.

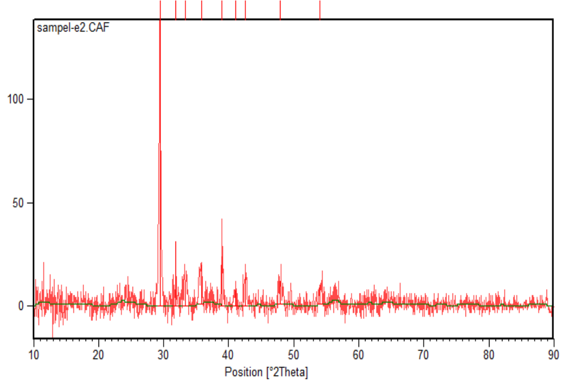

Fig.1. The XRD spectrum obtained for Fe-Mn nanoparticles calcinated in 3h and 500°C

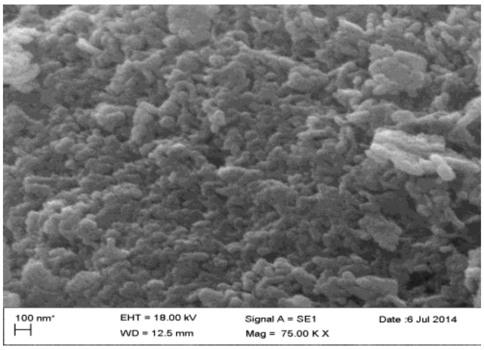

Fig.2. The SEM image of Fe-Mn nanoparticles calcinated in 3h and 500°C

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Computational Prediction of L-carnisine as a Drug-Likeness Ligand

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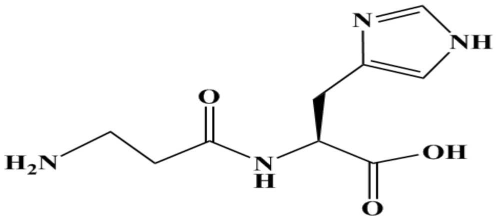
What's probably the most exciting result of the studies is that it was discovered that carnosine can actually reverse the signs of aging in senescent cells .[1,2] Carnosine has the remarkable ability to throttle down bodily processes that are in a state of excess, and to ramp up those that are under expressed . [3]

Lipotropic compounds are those that help catalyze the breakdown of fat during metabolism in the body. We have predicted L-carnisine produces modest short-term weight loss in some people, on the other hand because of the potential for insignificant side effects (1.3 to 6.9 %) and good pharmacological activity (56.7 %), this compound can be introduced as a suitable in obesity. There are many conditions, diseases, and disorders include sleep apnea, teeth grinding, allergies and colds, snoring, frequent urination, fibromyalgia, nightmares and etc. that can cause sleep disturbances which treatment for its depends on the causes but L-carnisine with 54.2 % pharmacological effects can be treatment sleep disorders. In fact, L-carnosine with new biological properties presented in this study can be utilized to identify numerous applications.

Table 1. A portion of the predicted probability activity spectra for L-carnisine($p_a > p_i$).



L-carnisine
Drug-Likeness: 0.916

Pharmacological Effects	**% P_a**	**Molecular Mechanisms**	**% P_a**	**Side Effects and Toxicity**	**% Pa**
Lipotropic	56.7	X-His dipeptidase inhibitor	88.7	Ulcerogenic	6.9
Sleep disorders treatment	54.2	Histidine ammonia-lyase inhibitor	78.2	Embryotoxic	5.1
Bone formation stimulant	45.4	Histidine-tRNA ligase inhibitor	77.7	Carcinogenic	1.3

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Study of the drying conditions effects on Iron-manganese oxide nanoparticles prepared by hydrothermal method

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Hydrothermal method is one of the most ideal way for synthesis of metal oxide nanostructures because of the preparation of high purity nanopowder. By this method can be controlled stoichiometric ratio, morphology and product crystallinity. The effective parameters in this method includes temperature, drying time, pressure, pH and concentration of reactants. In this study we synthesized manganese iron oxide nanoparticles supported on SiO_2 by using hydrothermal method and study the effects of drying conditions on their structures. These nanoparticles characterized by X-Ray diffraction and SEM analysis. The time of reaction was 2 h and the products were dried in range of 1-4 hours and the temperature varied between 120°-190°C). The lowest size of these nanoparticles obtained for drying in 170°C and 2 h with cubic morphology. X-ray diffraction analysis (XRD) and scanning electron microscope analysis (SEM) showed in fig.1 and fig 2.

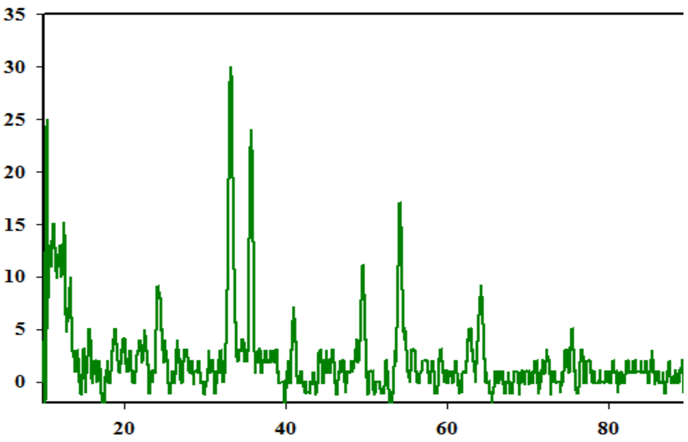

Fig 1: The XRD spectrum obtained for Fe-Mn nanoparticles dried in 170°C and 2 h 500°C

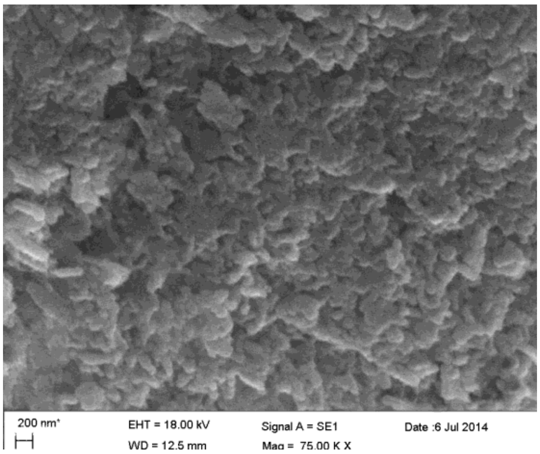

Fig 2: The SEM image of Fe-Mn nanoparticles dried in 170°C and 2 h

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Synthesis, characterization and catalytic activity of new Pd(II) complex containing α-keto stabilized sulfonium ylide in green Mizoroki-Heck reaction protocol

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Palladium-catalyzed Heck reaction is one of the most important C-C bond forming reactions for synthesis of drugs, fine chemicals, and natural products in laboratory as well as industrial scales .[1] The utility of metalated sulfonium ylides in synthetic chemistry has been well documented .[2] Mizoroki-Heck cross-coupling reaction catalyzed by palladium complex containing a ligand (usually a phosphane) is one of the most important and reliable methods for the construction of biaryls, which are present in a wide range of natural products, pharmaceuticals and functional polymer material sis the most commonly used catalytic system for the Mizoroki-Heck cross-coupling reaction. [3] In view of the economy and environmental aspects, the use of cheaper ligands such as sulfonium ylides instead of bis-phosphonium ylides as catalyst precursor and water as solvent provides another attractive route. Herein, we report the synthesis, characterization and application of new Pd(II) complex $[PdCl_2((Me)_2SCHC(O)C_6H_4R)_2]$ (R=*m*-NO_2) toward the Mizoroki-Heck cross-coupling reaction in aqueous media. Reaction of α-keto stabilized sulfonium ylides $(Me)_2SCHC(O)C_6H_4R$ (R = *m*-NO_2) with $Pd(COD)Cl_2$ in 2:1 ratios leads to mono nuclear products of the type $PdCl_2(ylide)_2$. Characterization of the complex by IR, MS, ^1H and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom. Well-defined sulfonium ylide Pd(II) complex was found to be an effective catalyst for the Mizoroki-Heck coupling of various aryl halides including with styrene and ethyl acrylatein a green protocol (**Fig. 1**). Moisture/air-stability, High efficiency, green and low catalyst loadings are important features of these homogeneous reactions.

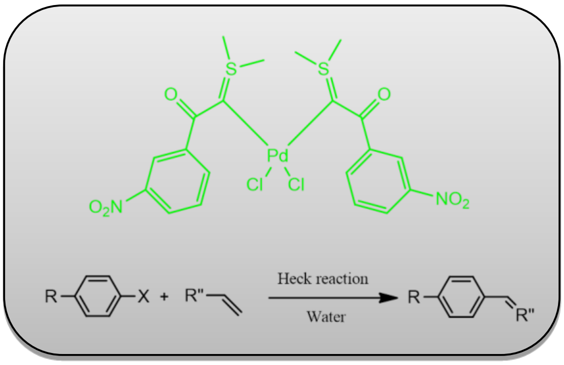

Fig. 1. The Heck cross-coupling reaction.

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Orthopalladated complexes of phosphorus ylide containing bridging diphosphine ligands: Synthesis, characterization and X-ray crystal structure

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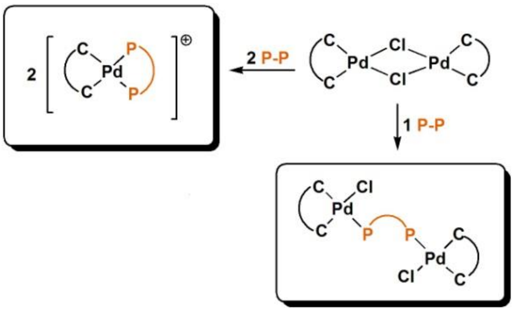
Phosphorus ylides can be used as the chiral auxiliary reagents, reaction intermediates or starting materials in a wide variety of processes due to their nucleophilic character, particular bonding properties and diverse coordination modes.[1-3] The α-stabilized phosphorus ylides can coordinate to the Pd (II) center as the bidentate ligands and undergo the orthopalladation. Herein, we report the synthesis and characterization of binuclear chloro-bridged orthometallated complex of α-keto phosphorus ylide as well as the X-ray crystal structure of corresponding complex revealing the proposed *C*,*C*-coordination of the orthometallated ylide. Furthermore, the reaction of the precursor complex with diphosphine ligands in a 1:1 molar ratio lead to preparation of binuclear complexes containing bridging diphosphine ligands while in a 1:2 molar ratio, mononuclear bischelate cyclopalladated complexes have been obtained. It is noteworthy that there are few examples of d^8 metal complexes with bridging diphosphine ligands due to their appropriate bite angles. New complexes were fully characterized by elemental analysis, IR, NMR spectroscopies and structurally determined by single crystal x-ray crystallography.



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Crystal structure and magnetic properties of a copper(II) coordination polymer

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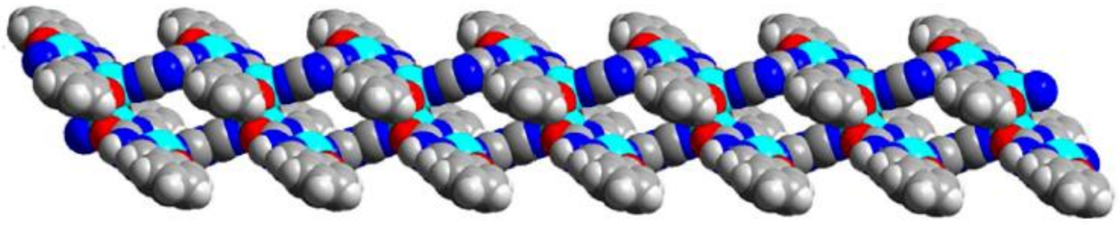
The design and synthesis of novel coordination polymers and metal–organic frameworks (MOFs) have attracted great attention in the fields of inorganic and coordination chemistry. Taking advantage of the coordination ability of ditopic bohydrazone based ligands in forming multinuclear metal complexes and the bridging ability of the dicyanamide (dca) ligand, we synthesized a new 1D coordination polymer of Cu(II) containing both phenoxido and dca bridging groups. 1D coordination polymer of Cu(II), $[Cu_4(L)_2(\text{ì-1,5-dca})_2]_n$ (**1**), has been synthesized and characterized by magnetic measurements, single crystal X-ray diffraction and other spectroscopic methods. X-ray analysis reveals that the ligand coordinates to the Cu(II) ion as a hexadentate trinegative N_3O_3-donor ligand. Tetranuclear copper(II) units with double phenoxido bridges are formed, connected and extended by two ì-1,5-dca anions, forming a 1D polymeric structure. The magnetic measurements showed global antiferromagnetic interactions with two coupling constants between ‘‘outer’’ ($J = -87 \pm 2$ cm^{-}1) and ‘‘inner’’ ($J' = -129 \pm 2$ cm^{-1}) copper pairs in tetranuclear units. The dicyanamide, adopting the end-to-end bridging mode (metal–metal separation of ca. 8.062(5) Å), has presented poor efficiency in mediating magnetic interactions.



1D polymeric chain of compound 1

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Synthesis, crystal structure and electrochemical properties of dinuclear Vanadium(V) complexes

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There is continuous interest in the chemistry of vanadium(IV/V) complexes due to their biological relevance and catalytic properties. In most cases, the active site contains either VO^{3+} or VO^{2+} coordinated by O,N-donor ligands. In this research two new dinuclear oxovanadium(V) complexes $[VO(L^1)(\mu\text{-}OCH_3)]_2$ (**1**) and $[VO(L^2)(\mu\text{-}OCH_3)]_2$ (**2**), were synthesized and characterized by spectroscopic methods and elemental analyzes where H_3L^1 and H_3L^2 are O,N-donor Schiff base ligands. These complexes were synthesized by the reaction of Schiff base ligands and $VO(acac)_2$ in methanol. The structures of complexes were determined by single crystal X-ray analyses. Single crystal studies indicated that the vanadium cores have distorted octahedral coordination environment and two vanadium ions are connected together by methoxy bridges. During the reaction, the initial vanadium(IV) ion is oxidized to vanadium(V) by aerial oxygen. Electrochemical studies by cyclic voltammetry technique indicated that these complexes are quasi-reversible electroactive (Fig. 1).

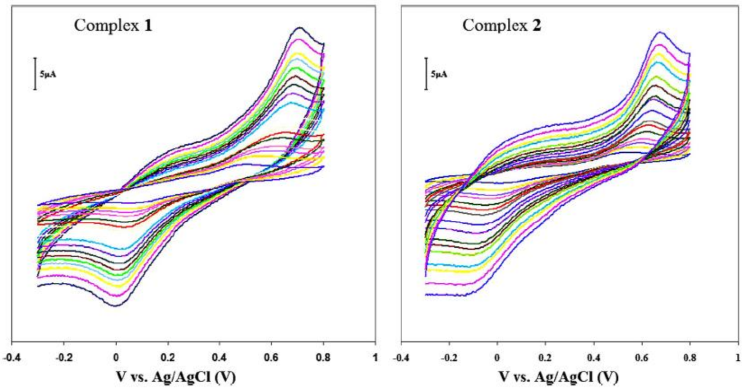

Fig. 1. Cyclic voltammograms of complexes **1** and **2** (10^{-3} mol L^{-1}) in DMSO and with TBAP as the supporting electrolyte (0.1 mol L^{-1})

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Microwave-assisted rapid green synthesis of silver nanoparticles from doremaaucheri extract and its antioxidant assay

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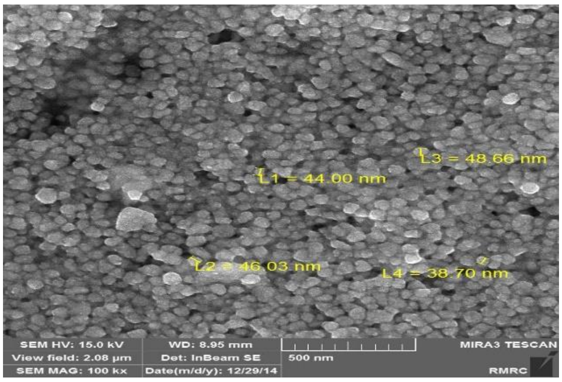
In the field of nanotechnology, development of rapid, simple, cost-effective, and ecofriendly procedures for the synthesis of nanoparticles is worth. Furthermore, the improvement of experimental processes for the synthesis of these nanoparticles of different sizes, shapes, and controlled dispersity has many important. These factors strongly affected of the physical and chemical properties and their potential application in optoelectronics, electronic, recording media, sensing devices, catalysis, biomolecular detection and medicine [1,2]. In the present study, microwave assisted synthesis of silver nanoparticles (AgNPs) has been demonstrated using aerial parts extract of Doremaaucheri reducing aqueous $AgNO_3$ solution. The synthesized nanoparticles have been characterized on the basis of fourier transform infrared spectroscopy (FT-IR), UV-Vis spectroscopy, scanning electron microscopy (SEM), transmission electron microscopy (TEM) and energy dispersive X-ray (EDX) analysis. The presence of a characteristic surface Plasmon resonance (SPR) absorption band at 458 nm in UV-Vis reveals the reduction of silver metal ions into silver nanoparticles. FT-IR analysis was carried out to probe the possible functional group involved in the synthesis of AgNPs. Further aerial parts extracts and AgNPs were evaluated for antiradical scavenging activity by 1,1-diphenyl-2-picryl-hydrazyl (DPPH) assay.



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Molybdenum (VI) complex bearingmono (phenol) amine anchored SBA-15: Anovelheterogeneous catalyst for the oxidation of organic sulfides

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Oxidation of sulfides into their corresponding sulfoxides and sulfonesis one of the most important processes from both laboratory and industrial point of view due to their role as intermediates for the synthesis of chemically and biologically significant molecules.[1,2] Nowadays, various catalytic systems based on metal complexes for the oxidation of sulfides have been reported.[3,4] In this research, an efficient molybdenum based catalyst has been synthesized by covalent grafting of (R)-1-(3,5-dichloro-2-hydroxybenzyl)pyrrolidine-2-carboxylic acid onto functionalized ordered mesoporous silica (SBA-15) followed by complexation with molybdenum salt. The catalyst was characterized by TEM, BET surface area analysis, FT-IR, atomic absorption spectroscopy and TGA analysis. The synthesized catalyst was found to be highly efficient, easy reusable for oxidation of various sulfides to their corresponding sulfonesin the presence of aqueous 25% H_2O_2 at room temperature and solvent free conditions. Furthermore, the oxidation of dibenzothiophene (DBT) as one of the most important pollutant fuels by this catalyst gave an overall yield of dibenzothiophenesulfone.

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Aminophenolate copper based complex grafting on to functionalized ordered mesoporous silica (SBA-15) for the aerobic oxidation of benzylic alcohols

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Aerobic oxidation of alcohols to the corresponding carbonyl compounds has received increas in gattention in organic synthesis.[1] Copper would seem to be a suitable active catalyst for this transformation with dioxygen in laboratory similar to that occurs at a wide variety of copper enzymes active sites., e.g. galactose oxidase, which catalyze this conversion in vivo.[2] Therefore, copper complexes have attracted significant attention for the catalytic aerobic oxidation of alcohols in recent years.[3] In this study, a novel copper based catalyst has been synthesized by covalent grafting of (R)-1-(3,5-dichloro-2-hydroxybenzyl)pyrrolidine-2-carboxylic acid ligand onto functionalized ordered mesoporous silica (SBA-15) followed by complexation with copper(II) acetate. The catalyst was characterized by TEM and BET surface area analysis, FT-IR, atomic absorption spectroscopy and TGA analysis. The immobilized catalyst was employed for the catalytic aerobic oxidation of benzylicalcohols to the corresponding aldehydes using TEMPO as co-catalyst. Moreover, this catalyst could be easily recovered by simple filtration and recycled for six times without loss of activity and selectivity.

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Synthses and study inorganic-organic nanohybrides of Mg- Al layered double hydroxides with 1,3,5 benzene tricarboxylate

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Layered double hydroxides (LDHs) or hydrotalcite-like compounds are presented by the general formula $[M_{1-x}^{II}\ M^{III}_{x}\ (OH)_2\ ]^{x+}\ [A^{n-}]_{x/n}\ .yH_2O$. The basic structure of an LDH may be derived by substitution of a fraction of the divalent cations in a brucite lattice with trivalent cations such that the layers acquire a positive charge, which is balanced by intercalation of anions (and, usually, water) between the layers.[1,2] In this role they have been used extensively as ion-exchange materials, catalysts, sorbents and halogen absorbers. 1,3,5 benzene tricarboxylate, (BTC^{3-}) , as anionic form, was selected to modify the magnesium / aluminum (Mg/Al) layered double hydroxide (LDH) using the coprecipitation method. Powder X-ray diffraction (XRD) and Fourier transform infrared (FT-IR) and elemental analyses (CHN) methods were used to identify the incorporaction of BTC^{3-} within the inorganic nanolayers of LDH. Powder x-ray diffraction pattern of BTC-Mg-Al-LDH nanohybrid shows that the interlayer distance has very small change which corresponds to a horizontal orientation of 1,3,5 benzene tricarboxylate anion (fig. 1). The interlayer structure, hydrogen bonding, and subsequent changes of LDH compounds containing trimesic acid anions will be investigated by molecular simulation.

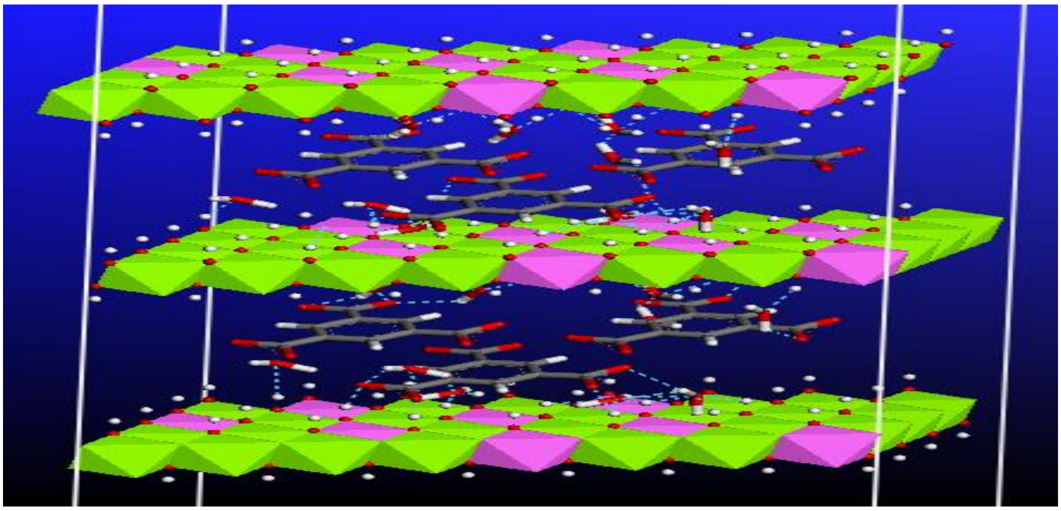

Fig. 1. Arrangement of BTC^{3-} anions within the interlayer space

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Synthesis, characterization, DFT study of Fe(III) Schiff base complex

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Schiff base ligands and their complexes have been used as biological models in understanding the structure of biomolecules and biological processes. Schiff base complexes have remained an important and popular area of research due to their simple synthesis, versatility and divers range of applications.[1]

In this work Schiff base ligand have been synthesized from condensation between an amino acid and salicylaldehyde in methanol and Fe(III) complex of this ligand were synthesis by template method in methanol (Fig.1). The ligand and related complex were characterized by elemental analysis, IR and UV-Vis spectroscopy. Density Functional Theory (DFT) study of Fe(III) Schiff base complex was performed using the GAUSSIAN 09 program.[2] B3LYP method was used to calculate the molecular structure of the mentioned complex. The geometry of this complex was fully optimized using lanl2DZ basis set for Fe and 6-311+g* for other atoms.[3] Also energy difference between the frontier orbitals (HOMO and LUMO) was calculated.

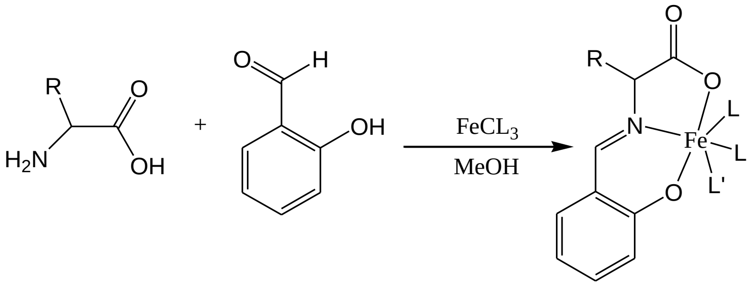

Fig.1. Synthesis of complex

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Combination of experimental methods with computational studies for predication of structural and enhanced photo-physical properties in LDHs contain large organic acidic anions

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In the present work, after investigation about experimental approach in preparation of LDHs with large organic anions and characteristic studies of synthesized LDHs compounds with XRD – FT/IR-TGA -SEM-EDX- DRS and Photoluminescence spectroscopy(PL) analyses,[1] these results are comprised with three level of computational studies involve molecular modeling, molecular dynamic simulation &quantum mechanic computation for confirmation of experiment results and proposition of exclusive structural properties: calculated X-ray diffraction pattern , proper aggregation, displacement stability of LDH contents, details of microscopic positions and distribution of nonbonding forces (Fig.1) in LDHs environment through trajectory analysis file,[2] and study of opto-physical activities: band structure analyses for band gap energies suggestion , density of state(DOS) results for electronic structure evaluates, molecular orbital modeling(Fig.2) and photo-optical investigation contain simulated edge absorption and appropriate aggregation make–photoluminescence efficiency, were explored. This kind of combined research can introduce *Large Organic Acidic Anions –LDH (LOA-LDH)* as advanced applied materials in broad range of nanotechnology.

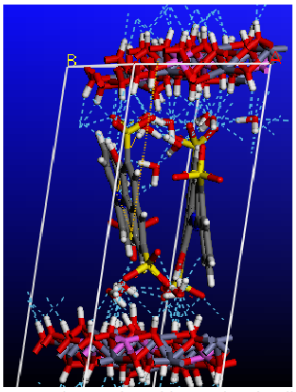

Fig. 1. Microscopic positions and nonbonding forces in the LOA-LDHs as nanohybrid systems.

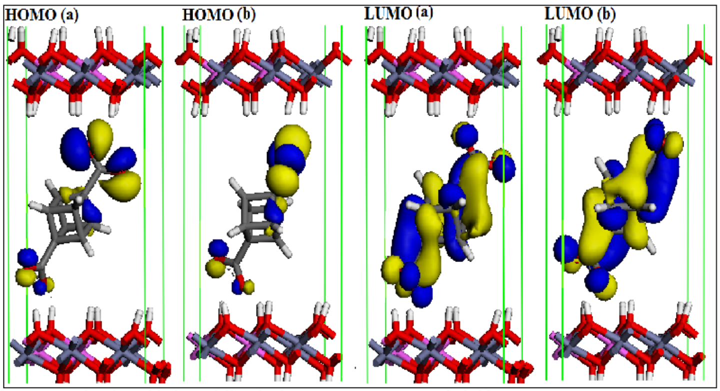

Fig. 2. Molecular orbital modeling in the LOA-LDHs as nanohybrid systems.

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Synthesis and characterization of some new phosphoramide and thiophosphoramide derivatives: crystal structure of $CHCl_2C(O)NHP(O)[NHCH_2CH_2CH_3]_2$

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A new phosphoric triamide structure, $CHCl_2C(O)NHP(O)[NHCH_2CH_2CH_3]_2$ (i), is investigated. The P atom is within an $[N_{CP}]P(O)[N]_2$ environment (N_{CP} is the nitrogen atom of the C(O)NHP(O) segment) with the bond angles at the P atom in the range of 103.46(9) to 118.51(9)°. The N_{CP}—H bond adopts a *syn* conformation with respect to the P═O group, whereas, the two other N—H units are in an *anti* conformation with respect to the P═O group. As it is expected and observed for analogous structures,[1] the P—N_{CP} bond length(of 1.6962(16) Å) islonger than the two other P—N bonds (1.6201(16) and 1.6257(18) Å). In the crystal structure, molecules are aggregated in a one-dimensional arrangement parallel to the plane (1–10) in the direction perpendicular to the (110) plane (Fig. 1). The spectroscopic features of the title structure as well as some phosphoramides($[2\text{-}Cl\text{-}C_6H_4O]P(O)[NHCH_2C_6H_4\text{-}4\text{-}Cl]_2$ (ii), $[2\text{-}Cl\text{-}C_6H_4O]P(O)[NHCH_2C_6H_4\text{-}4\text{-}CH_3]_2$ (iii), $[4\text{-}Cl\text{-}C_6H_4CH_2NH]_3P(O)$(iv))and thiophosphoramides($[4\text{-}Cl\text{-}C_6H_4CH_2NH]_3P(S)$ (v), $[4\text{-}CH_3\text{-}C_6H_4CH_2NH]_3P(S)$ (vi),$[CH_3O]_2P(S)[NHCH_2C_6H_4\text{-}4\text{-}CH_3]_2$ (vii)) are reported.

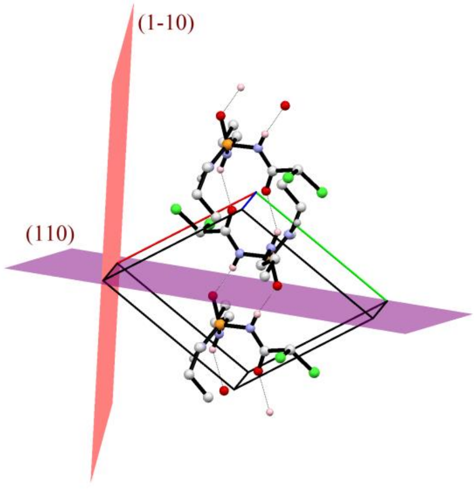

Fig. 1.A view of the crystal packing of $CHCl_2C(O)NHP(O)[NHCH_2CH_2CH_3]_2$is represented. The carbon-bound H atoms were omitted for the sake of clarity and the hydrogen bonds are shown as dotted lines.

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Synthesis and characterization of Mg-Al-layered double hydroxides intercalated with bis-tetrazole

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In this research work, Mg_3Al layered double hydroxide (LDH) intercalated with bis-tetrazole, was prepared from the reaction of solutions of Mg(II) and Al(III) nitrate salts with an alkaline solution of bis-tetrazole by using the coprecipitation method.[1,2] The successful preparation of a nanohybrid of bis-tetrazole with LDH was confirmed by powder X-ray diffraction, FTIR spectroscopy and thermal gravimetric analysis (TGA) and also CHN (elemental analysis). There are lots of works on intercalation of different componds within LDHs layers but almost all of those componds has negatively charged head groups such as nitrat , carboxylate , carbonate and other groups , but here we've worked on intercalation of bis-tetrazole wich has nagative charges on tetrazole rings not on head groups. And at the end we have investigated effects of bis-tetrazoles intercalation on its properties.[3] The interlayer structure, hydrogen bonding , and other porperties were shown by molecular stimulation , and A perfect agreement was achieved between stimulated and experimental results. The XRDs result shows no change in interlayer distances as can be seen from figure 1.

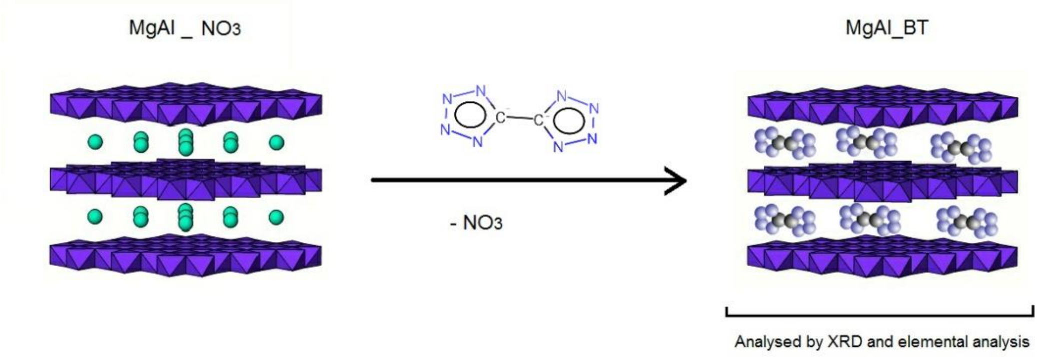

Figure 1. intercalation of bis-tetrazole into Mg_3Al layers

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Remove red coloring game 14 Fenton method and compared via removal by Fenton

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Wastewater treatment of industrial wastewater in the textile industry, with particular implications in the treatment process is One of the effective methods for removing paint using advanced oxidation process. The aim of this study was to compare the efficiency of dye removal by Fenton and Fenton is off 14 Red. After selecting the optimum concentration and the oxidizing catalyst and parameters, initial concentration and the color-generating efficiency and generating color removal rate was evaluated and then instead of using a catalyst Fenton other metals were used. In the same initial concentration of dye causing $50\ \mathrm{g/L}$ and pH =7 and the oxidizer 150 mg/L ,5 minutes and the volume of waste by 25 mL removal were investigated and the results showed that as well as the removal carried out..

Synthesis and characterization of a novel zinc magnetic metal–organic framework as drug carrier

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Metal–organic frameworks (MOFs) are a new class of crystallinematerials built up by metal ions (or metallic clusters) and variouspolyfunctional organic ligands through strong bonds. In the present work, asupramolecular MOF constructed by two-dimensional (2D) infinite coordination polymers, [Zn(BDC)(H2O)]n(1, BDC = 1,4-benzenedicarboxylate), was synthesized by the reactionof zinc acetate with H2BDC in dimethylformamide (DMF) under facile condition at ambient temperature and atmospheric pressure(as shown in Fig 1). This carrier with a magnetic core anda tunable MOF shell has beensuccessfully fabricated utilizing a versatile step-by-step assemblystrategy. The *in vitro*drug release study was carried out at different pH values and the release data indicated that both the pH and the type of the carboxylic acid unit played important roles in the drug release behaviors of the MOF .The structure of synthesized MOF was confirmed by SEM, TEM, CHN, and FTIR spectroscopy.

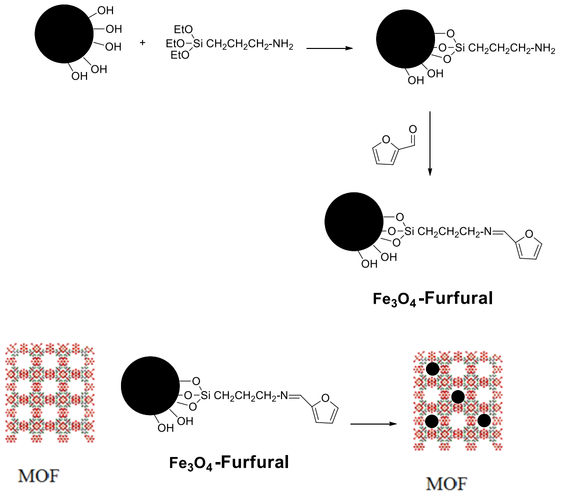

Fig. 1: Schematic illustration of synthesized magnetic MOF

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Synthesis of tetrahydro-chromenes with highly efficient catalyst of amidic pillar metal-organic frameworks

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Tetrahydrobenzo[b]pyrans have recently attracted considerable interest as an important class of heterocycles having a broad spectrum of biological properties, such as anticoagulant, diuretic, anticancer and antianaphylactic activities.[1] Metal-organic frameworks represent ideal candidates as heterogeneous catalysts by introducing catalytic sites intothem.[2]

The amine group of 2-amino-1,4-benzenedicarboxylic acid ligand in a novel twofold interpenetrated metal-organic framework (MOF), $\{[Zn(NH_2\text{-}BDC)(bpfb)].2DMF\}_n$**(1)** has been found to be a base catalyst active site. MOF **1** consists of both NH_2-BDC and the *N*,*N*′-bipyridine-type rigid linkers (N,N'-(1,4-phenylene)diisonicotinamide) with ZnN_2O_4 secondary-building units (SBUs)(Fig. 1). The MOF was characterized by FT-IRspectroscopy, powder X-ray diffraction, thermal gravimetric and single crystal X-ray diffraction. The amine-functionalyzed framework was used as an efficient heterogeneous base catalyst for synthesis of tetrahydro-chromenes(Fig. 2). Excellent conversions were obtained under mild conditions in the presence of 6 mol% catalyst. The MOF **1** catalyst could be reused several times without a significant degradation in catalytic activity.

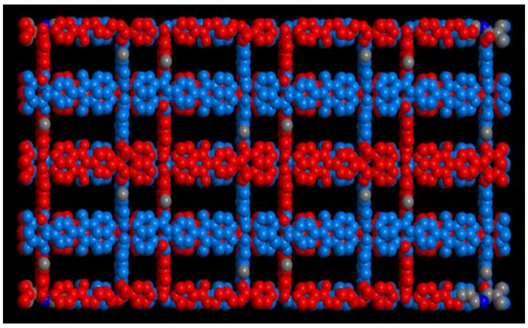

Fig. 1. Molecular-packing diagram of $\{[Zn(NH_2\text{-}BDC)(bpfb)].2DMF\}_n$**(1)** viewed along the *b*-axis.

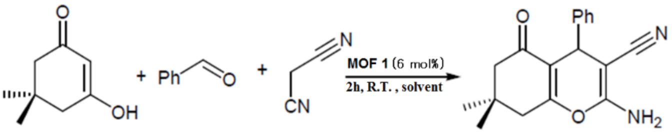

Fig. 2. The one-pot three component reaction of benzaldehyde, malononitrile and dimedonecatalyzed by MOF **1**.

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Synthesis of Mg/Al layered double hydroxide Intercalated with K_3 [$Cr(C_2O_4)_3$] complex

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The Mg/Al- NO_3 layered double hydroxide (LDH) with $[Cr(C_2O_4)_3]^{3-}$ anions in the interlayer space has been synthesized following two different routes; direct co-precipitation method, and anion exchange from a Mg/Al- NO_3 LDH. The prepared samples have been characterized by powder X-ray diffraction (PXRD) and Fourier transform infrared spectroscopy (FT-IR). The results obtained indicate that the most appropriate method is anion exchange, and the least appropriate method is direct co-precipitation, leading to a well crystallized LDH with interlayer spacing of 8.3 , 9.5 Å, respectively. The FT-IR study shows, most of the characteristic bands of the complex are also recorded in the FT-IR spectrum of sample Mg/Al-Cr-cp and Mg/Al-Cr-an, Which indicates the successful intercalation of $[Cr(C_2O_4)_3]^{3-}$ anions into the LDH.

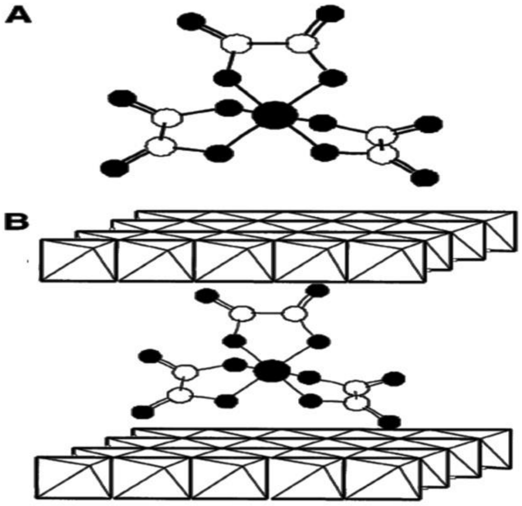

Fig1. Schematic diagram of Molecular free $[Cr(C_2O_4)_3]^{3-}$ anion and that intercalated between the sheets of the layered double hydroxide

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Sodium 30-tungstopentaphosphate: A green co-reducing agent in the bio-synthesis of antibacterial Ag nanoparticles in the presence of chaetomorpha linum seaweed

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In this research, we investigate and compare the results of the combination of a polyoxometalate, sodium 30-tungstopentaphosphate, with seaweeds in the synthesis of Ag nanoparticles. In other words, while both seaweeds and polyoxometalates are effective reducing and stabilizing agents by itself in preparation of metal nanoparticles, it is worthwhile to apply them in combination in order to compare their potentiality as whole for the more efficient synthesis of nanoparticles.

To this purpose, in this research, Ag nanoparticles synthesized *via* the reduction of aqueous $AgNO_3$ by the extract of Chaetomorpha linum. Interestingly, we found no report concerning the synthesis of Ag nanoparticles using Chaetomorpha linum in combination with sodium 30-tungstopentaphosphate as co-reductant. The obtained data revealed that this strategy led to the formation of Ag nanoparticles in a shorter reaction time, apparently due to synergism reductive ability of seaweed and sodium 30-tungstopentaphosphate,which do the reduction co-operatively. The TEM images showed that the nano silver particles are spherical with diameter of about 5–20 nm. The reflection peaks in X-ray diffraction (XRD) patterns indicated that silver is well crystallized. The Ultraviolet–visible (UV-Vis) absorption spectra of silver nanoparticles showed the characteristic absorption bands, with maximum at 420–430 nm. The antibacterial activities of the biosynthesized silver nanoparticles were investigated and the results showed that these nanoparticles displayed a good activity against bacterial cultures. This conclusion can potentially translate to the other metal nanoparticles and bacteria and may provide useful information for biochemists in nanomedicine.

Schiff base complex nanocatalyst

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Schiff base transition metal complexes have been widely used as homogenous or heterogeneous catalysts in various organic reactions.[1] Homogeneous catalysts exhibit higher catalytic activities than their heterogeneous counterparts because of their solubility in reaction media, which increases catalytic site accessibility for the substrate. These systems have several drawbacks such as the difficulty of catalyst recycling.[2] To overcome this problem, Many attempts have been done for immobilization of homogeneous catalysts on a solid supports. This is known as "heterogenization of homogeneous catalytic systems". These third generation catalysts not only preserve the activity and selectivity of homogeneous catalysts but also allow facile recovery and reuse of the catalyst akin to heterogeneous catalysts.[3,4] Heterogeneous base catalyzed organic synthesis is a promising field of research with potential application in pharmaceuticals and related fine chemical industries .[5,6]

In this work, we functionalized magnetite nanoparticles with amine groups and then incorporate a molybdenum Schiff base complex with anchoring method to obtain a heterogeneous molybdenum catalyst. The magnetic molybdenum nano-catalyst could be used as a heterogeneous catalyst with high catalytic activity in one-pot and green synthesis of 2-amino-4H-benzo[h]chromenes via three-component condensation reaction of different aromatic aldehydes, malononitrile and 1-naphthol under solvent free conditions. The attractive features of this process are short reaction times, easy isolation and excellent yields of the desired products.

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Synthesis, characterization and antibacterial activity of Mo (VI) and Cu(II) complexes with anthranilhydrazide Schiff base

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An important group of ligands in coordination chemistryis called Schiff baseinwhich have wide application in various fields of science. Metal complexes of these ligands attract a great attention due to their simple preparation, vast application, steric and electronic properties. Schiff base ligands can be easily coordinate many various metals to stabilize themat different oxidation states.[1,2] Many Schiff base and their complexes are considerablyinterest due to their biological activity such as antibacterial, antifungal, antitumor, antimalarial, antineoplastic and antiviral activities.[3] It has been suggested that in such compounds of the azomethine group is responsible for the biological activity.[4] During the later half of the century, a number of different classes of antibacterial agents have been discovered. At the present time, antibacterial sulfa drugs, nitrosulfa, cephalosporins, macrolides, nitrofuranes, penicillins, tetracyclines, oxaolidinones indicate antimicrobial activity.[5] It is demonstrated that more than 70% of bacterial infections are resistant to one or some antibiotics used for eradication the infection.It is necessary to search more effective antimicrobial agents and some Schiff bases have been known as promising antimicrobial agents.

In the present work, new Mo(VI) and Cu(II) complexes were prepared using tridentate Schiff base ligands that were derived from the condensation of anthranilhydrazide with naphthaldehyde and 2-Hydroxy4-methoxyacetophenon, respectively. These complexes were characterized by elemental analysis IR, ^{1}H and ^{13}C NMR, and UV-Vis spectroscopy. Moreover, the antibacterial activitiesof the complexes have been tested against some of Gram-positive and Gram-negative bacteria.

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Adsorption study of reactive dye by reduced graphene oxide/MgZnAlFe layered double-hydroxide nanocomposite: kinetic and isotherm

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In the present work, reduced graphene oxide and four cationic LDH (Mg-Zn-Al-Fe) nano composite has been developed by a facile one-step hydrothermal method. For the synthesis of this composite, the addition of salts was performed at the presence of precipitation agent (NaOH and Na_2CO_3) and graphene oxide simultaneously. At the hydrothermal condition, as well as composite formation, graphene oxide is reduced. [1] Then synthesized nanocatalyst was tested for Reactive red 43 removals under different reaction conditions and Batch adsorption experiments were carried out at room temperature (25 °C) for determination of the isotherms and kinetic models of the removal process. [2] The nanoparticles of adsorbent was characterized by X-ray powder diffraction (XRPD), thermal gravimetric analysis (TGA), Fourier transform infrared spectroscopy (FT-IR), specific surface area measurement. The size and morphology of nanoparticles were inspected by scanning electron microscopy (SEM). By comparing the adsorption capacity of Mg-Zn-Al-Fe LDH, this kind of nanocomposite can be more efficient candidate for removal of reactive dye from contaminated water.

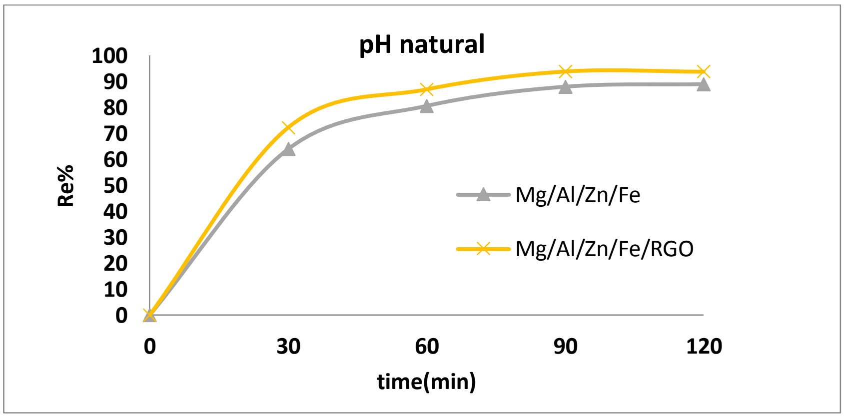

Fig. 1.

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New complex of zinc metal ion including pyridine-2,5-dicarboxylicacid N-oxid through proton transfer

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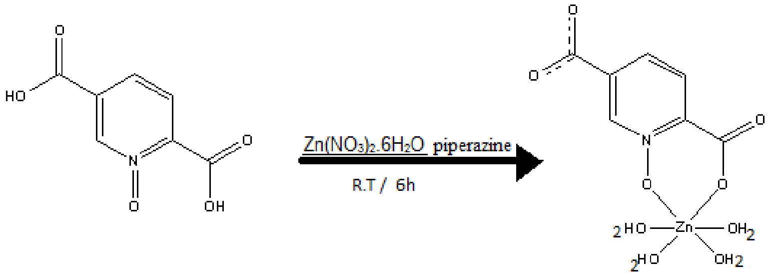
Supramolecular chemistry implies extended structures that are generated by means of non-covalent interactions, especially hydrogen bonding between discrete molecules. Hydrogen bond is able to control supramolecular structures because it is sufficiently strong and directional. Recently the combination of both coordination chemistry and hydrogen bonding has proved to be a particularly useful strategy for the self-assembly of complex structures and for controlling solid state chemistry. The area of solid state chemistry in terms of prediction of how molecules pack during crystallization by controlling all intermolecular forces that determine patterns in the crystal packing, refers to crystal engineering. In this context, here we described the syntheses of one proton transfer compound and its metallic complex of Zn(II) ion based on proton transfer mechanism which were characterized by elemental analyses, infrared spectroscopy, and melting point. The compounds chemical formulas are (H_2pipz)(pydco) and [Zn(pydco)(H_2O)$_4$] (pipz = piperazine; pydco = pyridine-2,5-dicarboxylicacid N-oxid).



Scheme 1. Preparative route of the complex

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Microwave Assisted Combustion Synthesis of CuO-ZnO-Al_2O_3 Nanocatalysts for Steam Methanol Reforming: Effect of Fuel/Nitrates Ratio

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Methanol's advantages such as no strong C-C bond, easy storage and transportation and transformation to hydrogen at low temperatures; cause to nominate as an attractive choice for production of hydrogen for automobiles. [1] Steam methanol reforming (SMR) is a promising and efficient process for transforming methanol to the hydrogen-rich product at low temperatures.[2] Therefore, in this paper CuO-ZnO-Al_2O_3 nanocatalysts as a common catalyst for SMR were synthesized by the microwave assisted combustion method. Glycerol was used as the fuel because of its cost, availability and environment friendly properties. Four nanocatalysts with different glycerol/ nitrates ratio were fabricated to investigate the best ratio. Various characterization analyses such as XRD, FESEM, BET and FTIR were utilized. Finally the synthesized nanocatalysts were tested in a laboratory apparatus to investigate their ability in the SMR process. It was concluded that the nanoctalyst with glycerol/ nitrates ratio equals 2 showed better performances due to its better characterization properties.

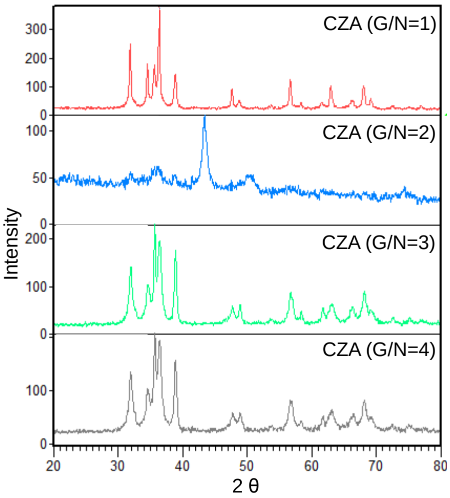

Fig. 1.XRD patterns of synthesized nanocatalysts.

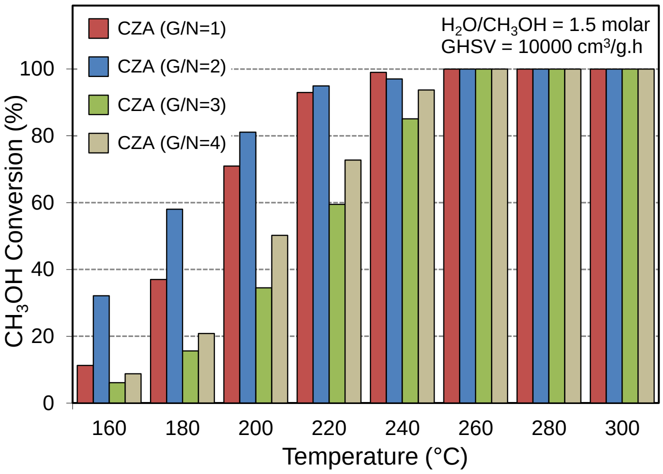

Fig. 2. Methanol conversion over CuO-ZnO-Al_2O_3 nanocatalysts

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Synthesis of nanoparticles of hydrogen sulfate ionic liquid immobilized on nanosilica and investigating its effect on Biginelli reaction

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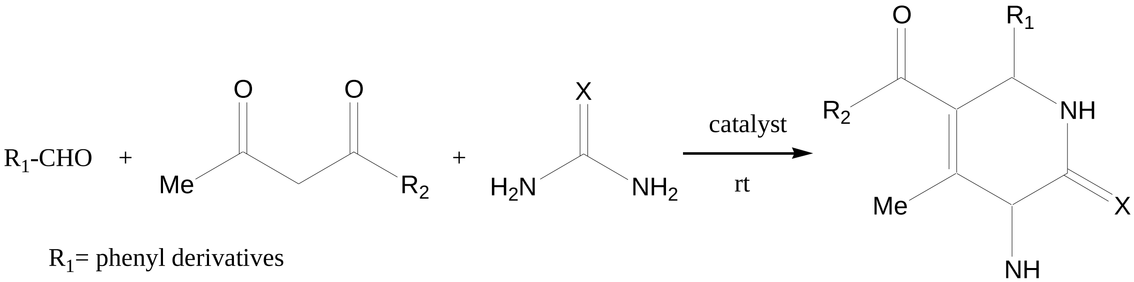
Imidazolium based hydrogen sulfate ionic liquid was prepared from the reaction of N-methylimidazole and (3-chloropropyl) trimethoxysilane. This ionic liquid was immobilized on silica covalently to give nanoparticles with the imidazolium hydrogen sulfate moiety remaining intact. The Biginelli reaction, 3,4-dihydropyrimidin- 2(1H)- thione, one-pot condensation of benzaldehyde derivatives, ethyl acetoacetate and urea/thiourea in presence of catalyst, was performed as a model reaction to examine the activity of this nanoparticle catalyst as proton source. Excellent performance was exhibited in the Biginelli reaction of various benzaldehyde derivatives in the presence of ethanol as solvent under mild heterogeneous conditions (room temperature and short reaction time) and also in solvent free conditions. Compared with the classical Biginelli reaction, easy workup, mild conditions, reusability of catalysis, good to excellent yield and short reaction time are privileges of this catalyst as efficient and green method. Products were identified using physical and spectroscopic data, which have a captivating assortment in natural, synthetic, pharmacological, therapeutic and bioorganic chemistry mainly due to their wide range of biological activities, and they are widely being studied because of their activities as calcium channel blockers, antihypertensive agents, alpha-la-antagonists and neuropeptide Y(NPY) antagonists.



R_1= phenyl derivatives
R_2= ethyl
X= O or S

Fig. 1. Biginelli reaction.

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Heteropolymolybdate- amino acid hybrid materials: Synthesis and characterization

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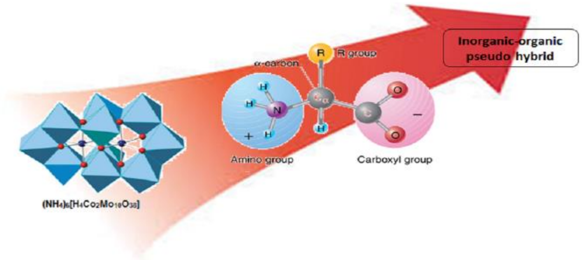
Polyoxometalates (POMs) as anionic early-transition-metal oxide clusters, bear many properties ranging from chemistry, catalysis and materials science to biology.[1] Owing to their great potential antitumor and antiviral activities, polyoxometalate complexes have become attractive to both inorganic chemists and biochemists.[2,3] However, POMs are often (potentially) toxic, making further trials as drugs unacceptable. One of the solutions to the toxicity problem is to modify the POMs by different organic ligands or enzymes. Cocrystallization with small organic molecules such as amino acids to modify the surface of these POM clusters may offer a rational way to not only fine-tune the properties of these compounds but also bring about novel synergistic effects. [4] During the course of our attempts to synthesize new POM-based hybrids organic-inorganic, we have obtained two novel heteropolymolybdates functionalized by amino acids including aspartic acid (L-Asp) and sodium glutamate (Na_2Glu). It has been showed that spectroscopic studies, especially FT-IR results, are accurate, more reachable, easier and cheaper methods for characterization of POMs and confirm different types of interactions between them and organic molecules.[5] This context describes the synthesis and characterization of $(NH_4)_6[H_4Co_2Mo_{10}O_{38}].(L.Asp)_2$ (1) and $(NH_4)_6[H_4Co_2Mo_{10}O_{38}].(Na_2Glu)_2$ (2) through elemental analysis, FT-IR spectroscopy and atomic absorption spectroscopy.



Scheme. 1. General procedure of synthesis

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Sonochemical syntheses of nano-sized dioxomolybdenum (VI) complexe;Aplication for catalysis

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Great opportunities and possibilities in the various fields of science and technology have lately been offered by nanotechnology. Generally speaking, nanoparticles have various properties in comparison to the similar material with larger particles. Indeed, the ratio of surface to volume of the nanoparticles is significantly increased with the decreasing the particle size.[1] It means that fraction of the molecule surface in the nanometer dimensions has considerably increased which in turn makes some properties of the particles improve such as heat, dissolution rate, catalytic activity, mass transfer.[2] During these years, almost more efforts have taken into the synthesis of nano scale particles of metals, oxides, sulfides and ceramic materials.[3] On the other hand, to date little attention was focused on nano-structures of supramolecular compounds. The use of ultrasonic irradiation for the preparation of nanomaterials is one of the most promising techniques to achieve such a goal.[4] In this present work, nano-structured Mo(VI) Schiff base complex have been synthesized under ultrasonic irradiation and used as catalyst with high catalytic activity in one-pot and green synthesis of 2-amino-4H-benzo[h]chromenes via three-component condensation reaction of different aromatic aldehydes, malononitrile and 1-naphthol under solvent free conditions. The attractive features of this process are short reaction times, easy isolation and excellent yields of the desired products and use of the concepts of green chemistry.

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Application of Response Surface Methodology for Catalytic Hydrogenation of Nitrobenzene to AnilineUsing NiSupported magnetic Fe_3O_4 nanoparticles

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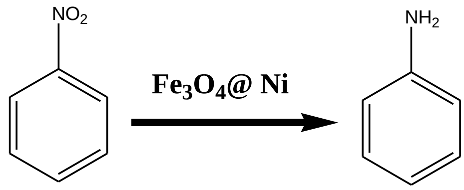
In this study, an efficient and highly selective heterogeneous catalyst was developed by immobilization of a nickel on Fe_3O_4 magnetite nanoparticle (MNP). Fe_3O_4 MNPs were prepared by co-precipitation (CP). Ni/Fe_3O_4catalyst with high loading of Ni (about 30%) were prepared through the wet impregnation method from nickel nitrate. Subsequent to this step, Response Surface Methodology (RSM) was used to study the cumulative effect of various parameters including, pressure, temperature, time and loading. In order to maximize the hydrogenation of nitrobenzene (NB) to aniline (AN) these latter parameters were optimized. Furthermore, catalytic activity was evaluated over a temperature range of 25–150°C, hydrogen pressure of 1-30 atm and reaction time of 30-180 min in a bench scale reactor. The optimized model predicted that the hydrogenation should be at a maximum level (approximately 100%) with the following conditions; reaction temperature of 130 °C, reaction time of 150 min and hydrogen pressure of 19.23 atm. The synthesized catalysts characterized by FT-IR, XRD, TEM, TPR and BET.



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Synthesis and Characterization of Modified Titanium Dioxide Nanoparticles and Their Effects on the Photocatalytic Degradation of Colors

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In this study, $ZrO_2/TiO_2/Nb_2O_5$ new photocatalyst which is named as ZTN, was synthesized from zirconium(IV) acetylacetonate, niobium(V) ethoxide and titanium(IV) ethoxide, at the Zr:Nb:Ti molar ratio of 1:1:2.5, in absolute Ethanol, through the sol-gel process at desired temperatures (400˚C, 600˚C ,800˚C). The prepared nanocamposits were characterized by XRD, FT-IR, EDAX, and SEM analyses. Among obtained catalysts, the catalyst calcined at 600˚C has the smallest particle size (80 nm) and least agglomeration. Also, XRD data showed that crystalite phase in structure was pure anatase. So synthesized ZrO_2/TiO_2 and Nb_2O_5/TiO_2 nanocomposites by the sol-gel method calcined at 600˚C were chosen in order to comparison photocatalytic activity between binary nanocomposites (ZT and NT) and triplet nanocomposites (ZTN). In the application study section, the photocatalytic activity of synthesized compounds was evaluated by degradation of methylen blue (as a pollutant model), under UV iradiation. Among the catalysts calcined at different temperatures, the samples calcined at 600˚C showed the most remarkable degradation of methylen blue, higher than not only the other calcined catalysts but also the pure TiO_2. The parameters such as catalyst loading, pH colored solution, initial concentration of colored solution, colored solution temperature, cross section of the reaction reactor, the reaction reactor distance to lamp and light intensity, were optimized for maximum degradation efficiency.

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Application of nanoparticles of hydrogen sulfate ionic liquid immobilized on nanosilica in Hantzsch reaction

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A new method for one-pot synthesis of Hantzsch 1,4-dihyropyridines was achieved by the reaction of an aromatic aldehyde (benzaldehyde derivatives), a β-dicarbonyl compound (ethyl acetoacetate) and ammonium acetate using a heterogeneous catalyst (imidazolium based hydrogen sulfate ionic liquid) in ethanol. An important advantage of this catalyst is the ease of separating it from the reaction mixture, as well as the fact that it could be recycled a number of times; mild conditions, excellent yield and short reaction time are other advantages of this catalyst as efficient and novel method. The present environmentally benign procedure for the synthesis of 1,4-dihydropyridines is suitable for library synthesis and it will find application in the synthesis of potent biologically active molecules. The excellent yield and extreme rapidity of the method is due to a concurrent effect of the catalyst. All reactions were monitored by TLC, and spectroscopic techniques such as ^{1}HNMR and FT-IR, have been used to identify the products.

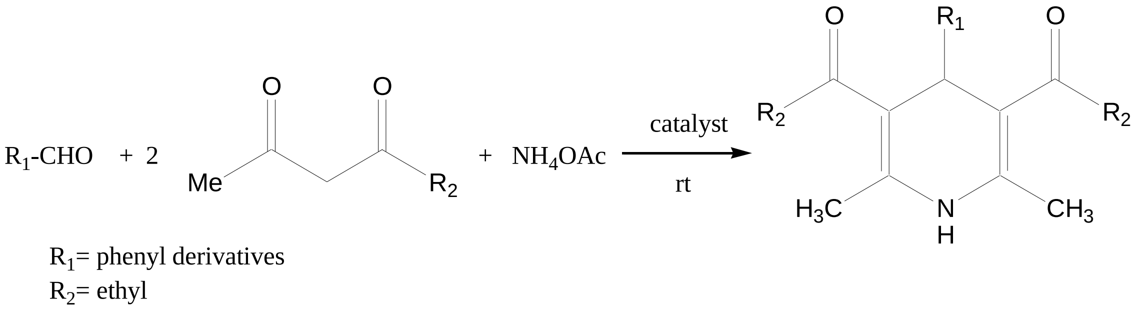

Fig. 1. Hantzsch reaction.

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Synthesis and Characterization of Palladacyclic Complex Containing Curcumin and Study of their Cytotoxicity Activities and DNA Binding - Bovine Serum Albumin Properties

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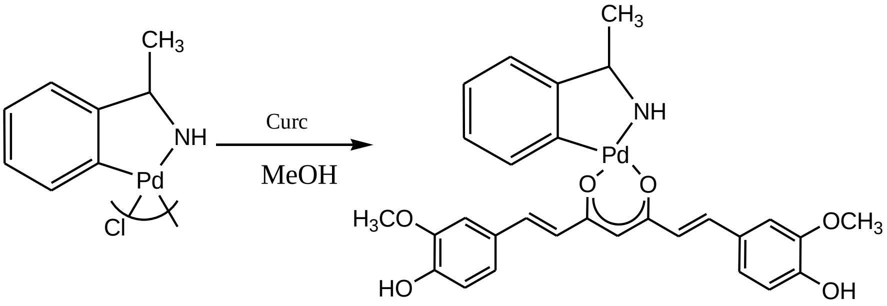
Curcumin (1,7-bis(4-hydroxy-3-methoxyphenyl)- 1,6-heptadiene-3,5-dione, diferuloyl methane, a naturally occurring pigment in Turmeric and its analogues, are exciting and multifaceted compounds, well known for their biological and pharmacological properties, they are such as antioxidants, antiinflammatories and have anticarcinogenic properties. Recently the study of the mechanism of their chemiopreventive activity has attracted increasing attention. [1,2] In the present work we report the synthesis of new hybrid complex based on dinuclear cyclopalladated benzyl amine and on curcuminoid fragment. The interactions of complex towards DNA and protein are investigated. The results suggested that the complex could interact with CT-DNA through the intercalation mode. Moreover, the reactivity towards BSA revealed that the micro environment and the secondary structure of BSA were changed in the presence of Pd(II) complex.



Scheme 1. Representation of the cleavage reaction of the dimeric cyclopalladated complex by Curcumin

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Preparation of Organic-Inorganic Nanocomposites Based on Monmorillonite Clay

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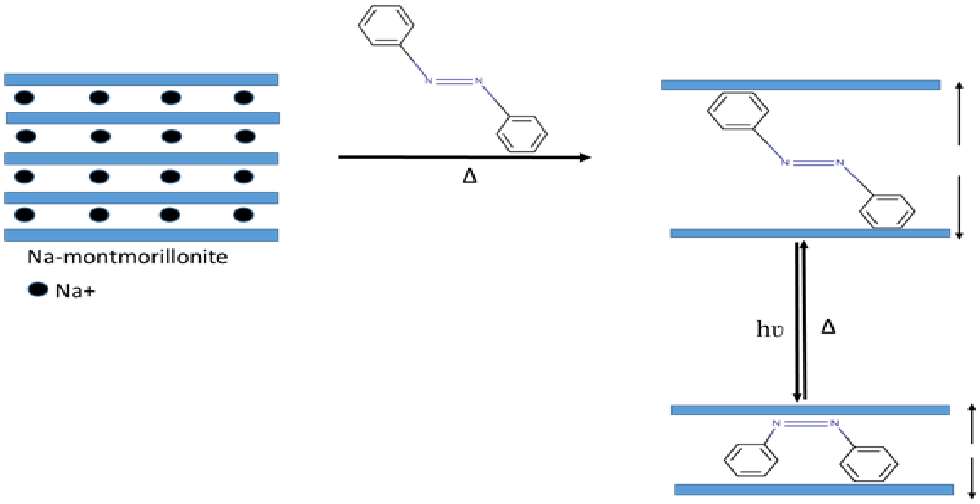
Azobenzenes are well known photochromic dyes capable of trans–cis isomerization. The photochromic reactions of these compounds in the interlayer space of Na-montmorillonite have been extensively investigated and the photochromic behavior has been found to be different from that observed in solutions or other solid matrixes. [1,2]

In this work, we synthesized a series of variable alkyl chain length modified azobenzene derivatives (AZ*) in order to intercalate of modified azo dyes into the interlayer space of montmorillonite due to its high surface area and high cation exchange capacity. The intercalation conducted by the conventional ion exchange method. The successful preparation of nanocomposite was confirmed by powder X-ray diffraction and thermal gravimetric analysis (TGA). The increase in the basal spacing of montmorillonite 9.67 Å to 14.71 Å shows that modified azobenzen dye were successfully incorporated into the interlayer space. Thermogravimetric analyses confirm that the thermal stability of the modified azobenze dye (AZ*) is greater than that of the pure form before intercalation. Also, investigated of photochemical behaviors of AZ*-montmorillonite showed that the modified azo dye isomerized effectively in the interlayer space of montmorillonite.



Scheme 1. intercalation of azobenzen dye.

References

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Hydrothermal Synthesis of CuS-TiO_2 Composite Nano-photocatalyst used in Degradation of Azo Dyes

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During recent years, the semiconductor photocatalytic process to remove persistent organic compounds and microorganisms in water attracts much attention because of its potential as a low-cost and environmental friendly treatment technology.[1] With the aim of obtaining photocatalysts which are active in visible region, CuS(10%)/TiO_2 nanocomposites were synthesized by a simple hydrothermal method.[2] Synthesis of nanocatalysts was done using coppernitratetetrihydrate, thiourea and TiO_2-P25 as precursors. The as-synthesized samples were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Brunauer-Emmert-Teller (BET) surface areas and ultraviolet-visible diffuse reflection spectroscopy (UV-vis DRS). XRD results confirmed formation of hexagonal CuS and anatase TiO_2 phase. The photocatalytic activity of as-prepared CuS(10%)/$TiO_2$was investigated based on the decolorization of Acid Orange 7 (AO7) as model compound in an aqueous medium under visible light irradiation. According to the performance results the values of decolorization efficiency via adsorption onto CuS(10%)/TiO_2 in dark (0.29%)and photolysis by visible light (6.89%) were insignificant compared to photocatalysis, which was (44.85%) using initial dye concentration of 5 mg/L and catalyst dosage 1g/L indicating the good performance of the as-synthesized nano-photocatalysts.

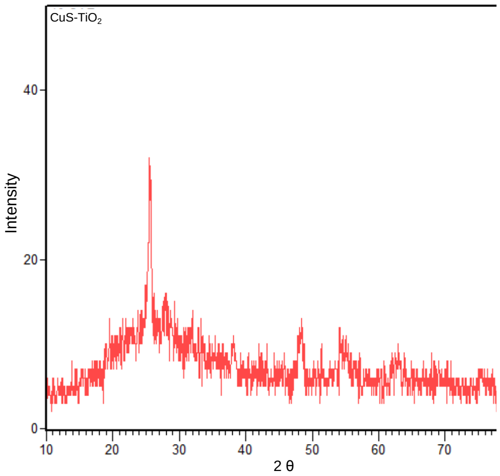

Fig. 1.XRD pattern of CuS(10%)/TiO_2nanostructures.

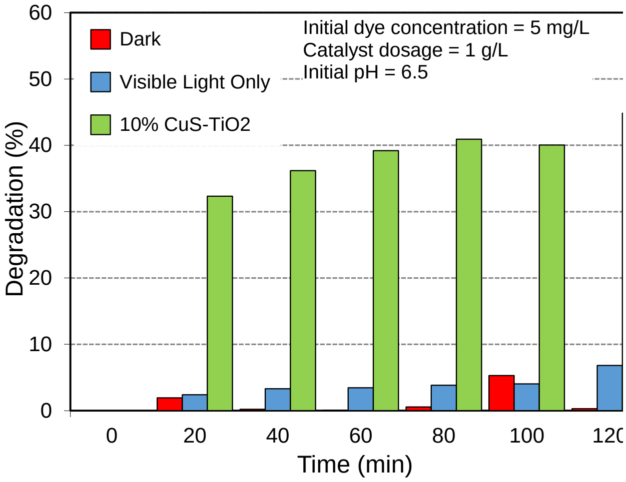

Fig. 2. Comparison of the processes in the degradation of AO7. Initial dye concentration = 5 mg/L, catalyst dosage = 1 g/L, initial pH = 6.5.

References

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Effect of CdS Addition on Photocatalytic Properties of TiO_2 Used in Water Treatment

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For the sake of enhancing the charge separation and extending the absorption response of TiO_2 into visible region in the photocatalytic degradation of azo dye, Acid Orange 7 as model compound in an aqueous medium, the composite of two inorganic semiconductors CdS and TiO_2 was synthesized. [1]CdS(10%)/TiO_2 nanocomposites were prepared by a simple hydrothermal method[2]. The nanocatalysts have been synthesized using cadmium nitrate tetrahydrate, thiourea and TiO_2-P25 as precursors. The as-synthesized samples were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and Brunauer-Emmert-Teller (BET) surface areas. According to the XRD results cubic CdS and anatase TiO_2 phases were identified. The photocatalytic activity of as-prepared CdS(10%)/TiO_2 and TiO_2were investigated based on the decolorization of AO7 under visible light irradiation. The decolorization efficiency was found to be 100% and 85.15% for CdS(10%)/$TiO_2$and TiO_2, respectively after 120 min of illumination and using initial dye concentration of 5 mg/L and catalyst dosage of 1g/L. According to the performance results, the values of decolorization efficiency via adsorption onto CdS(10%)/TiO_2 in dark (0.29%) and photolysis by visible light (6.89%) were insignificant compared to photocatalysis. The results indicated that the composite of CdS and TiO_2 with appropriate oxidation reduction energy levels enhanced the photocatalytic degradation of AO7 in comparison to TiO_2 alone.

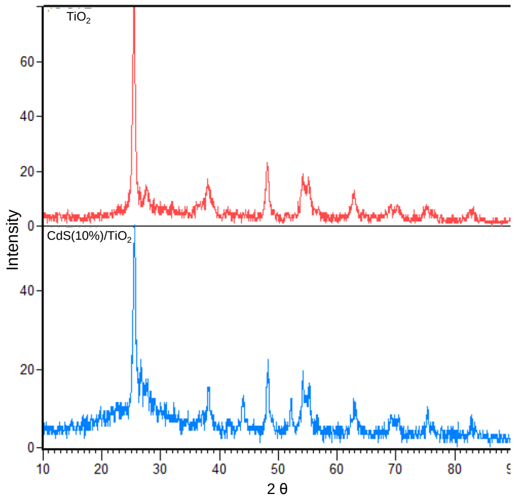

Fig. 1.XRD pattern of TiO_2 and CdS(10%)/TiO_2 nanostructures.

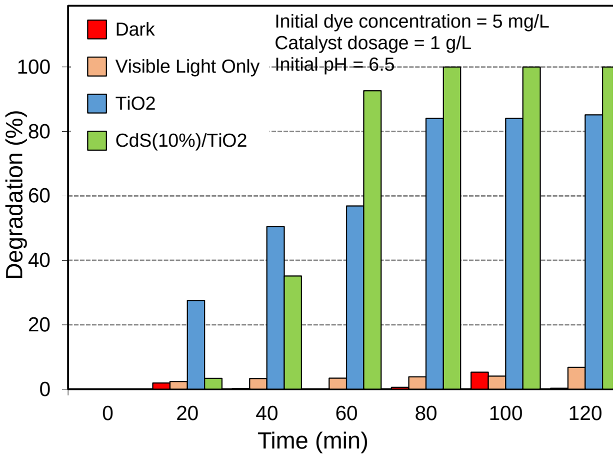

Fig. 2. Comparison of the processes in the degradation of AO7. Initial dye concentration = 5 mg/L, catalyst dosage = 1 g/L, initial pH = 6.5.

References

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Effect of Ultrasound Irradiation on Sonochemical Synthesis of $CuO/ZnO/Al_2O_3/ZrO_2$ Nanocatalyst for Hydrogen Production via Steam Methanol Reforming

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The depletion of fossil fuel sources and increasing power demand make hydrogen as an attractive substitute energy source. Problems in safety, storage and refuelling have hindered for the full utilization of hydrogen as an alternative fuel. Steam reforming of methanol (SRM) which produces in-situ hydrogen is one of the best outages. [1] Copper based catalysts are the most investigated catalysts for SRM due to their higher activity and selectivity to hydrogen. The common preparation method for synthesis of nanocatalyst of SRM synthesis is the co-precipitation method however one of the major drawbacks of this method is the disability to control the size of the precipitating particles and their subsequent aggregation. Therefore, hybrid methods in which de-agglomeration of the synthesized nanomaterial control the size of particles should be considered. Ultrasound assisted co-precipitation synthesis method resulted in nanocatalyst with more uniform morphology compared to conventional method and yields smaller particles with better dispersion and higher surface area.[2] $CuO/ZnO/ZrO_2/Al_2O_3$ nanocatalyst was synthesized by ultrasound-assisted co-precipitation method and the conventional co-precipitation. The fabricated nanocatalyst was characterized by XRD, FESEM, BET, and FTIR analyses. XRD results showed that, using ultrasound energy would decrease CuO crystal size and therefore improve its dispersion. At high levels of power, control of morphology was better and the structure was uniform and agglomerate free. BET surface area was higher for catalyst synthesis with ultrasound assisted co-precipitation. In presence of ultrasound, reactor tests exhibited more reactive in hydrogen production due to well-defined structural properties.

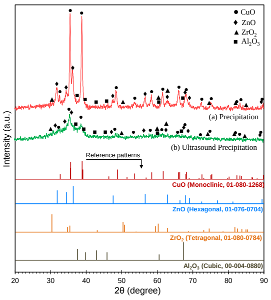

Fig. 1.XRD patterns of synthesized nanocatalysts

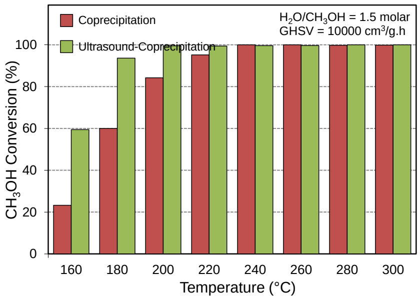

Fig. 2. Methanol conversion over synthesized nanocatalysts

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Effect of Synthesis Method on Catalytic Properties and Performance of $Ce_{0.8}Zr_{0.2}O_2/Al_2O_3$ Nanocatalyst toward CO Oxidation

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Using ceria is conventional in CO oxidation process because of oxygen storage capacity and its lattice oxygen. Zirconia improves the oxygen storage capacity. 1 Inaddition; alumina increases the effective surface of catalyst. Homogeneous $Ce_{0.8}Zr_{0.2}O_2/Al_2O_3$ composite nanosized catalyst has been prepared on the Al_2O_3 surface, using a modified citrate complexation synthesis method. For modification of the citrate complexation, three different methods have been used in this paper; impregnation, microwave combustion and ultrasound assisted impregnation. For characterization of nanocatalysts, XRD and SEM tests have been done. To evaluate performance of nanocatalysts in CO oxidation process, gas chromatography with Plot U column, FID and TCD indicators has been used. According to the results, microwave combustion has decreased the crystalline size, enhanced the dispersionand consequently improved the activity of catalyst. Due to the sudden exit of combustion gases during the catalyst formation, the porous structure is obtained, that has improved access to the depth of catalyst. 2 As a result, the conversion is increased in comparison to impregnation. Ultrasound is not a good choice. The citric acid is a trifid ligand which uses in citrate complexation method. Ammonia solution has been added to the solution in order to increase pH from 1 to 7, just to keep ultrasound's probe safe during the irradiation. Ammonia can react with citric acid and undoes the citric acid effect. As a result, ultrasound cannot be a good modification for citrate complexation method. Consequently,microwave combustion is the best choice between these three methods.

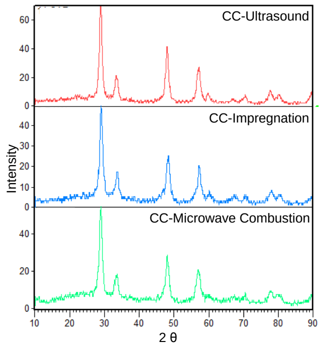

Fig. 1.XRD pattern of synthesized nanocatalysts

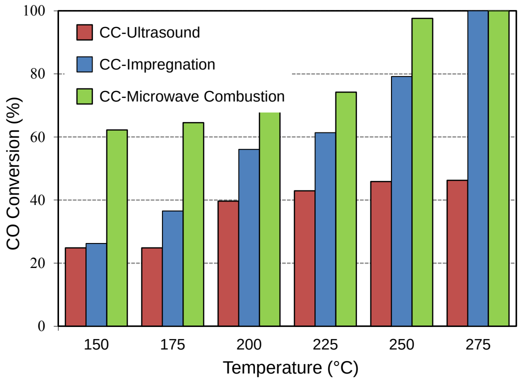

Fig. 2. Catalytic performance of synthesized nanocatalysts toward Low Temperature CO Oxidation

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Influence of Ultrasound Irradiation on Coprecipitation Synthesis of $Ce_{0.8}Zr_{0.2}O_2/Al_2O_3$ Nanocatalyst Used in Low Temperature CO Oxidation

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The oxidation of CO to CO_2 is a very important reaction from environmental control point of view. Although, this reaction is traditionally carried out on supported noble metals, it has been well known for many years that transition metals are also very good catalyst. [1] In this research, $Ce_{0.8}Zr_{0.2}O_2/Al_2O_3$ composite nanocatalyst for carbon mono oxide oxidation synthesized with coprecipitation method. Then comprised with ultrasound assisted coprecipitation in order to see the ultrasound irradiation effect on coprecipitation method. For characterization of nanocatalysts, XRD and SEM tests havebeen used. Finally, to evaluate the performance of nanocatalysts in CO oxidation process, a gas chromatography with plot-U column, FID and TCD detectors has been used. Regards to the XRD analysis and reactor test, ultrasound irradiation has decreased the crystalline size, enhanced the dispersion and consequently improved the activity of catalyst. [2] Ultrasound irradiation during coprecipitation could decrease the light off temperature, from about 250 to 150ºC. To test the stability of this nanocatalyst in different feed compositions, various CO concentrations (1% (for fuel cells), 2 % and 4 %) have been chosen.As the CO concentration increased from 1 to 4 %, the reduction of conversion has been observed, the reason of this reduction can be obtained from lower CO–oxygen interactions as a result of higher CO accumulation on the nanocatalyst active sites.

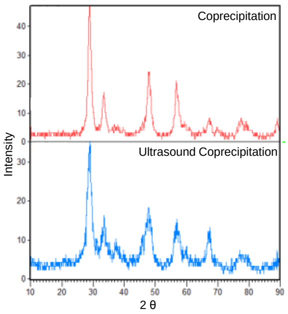

Fig. 1. XRD pattern of synthesized nanocatalysts $Ce_{0.8}Zr_{0.2}O_2/Al_2O_3$via Coprecipitation and ultrasound assisted Coprecipitation.

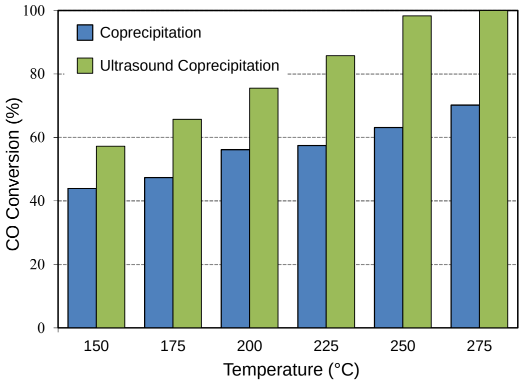

Fig. 2. Catalytic performance of composite nanocatalysts $Ce_{0.8}Zr_{0.2}O_2/Al_2O_3$toward CO oxidation

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Coprecipitation Synthesis of ZrO_2-Doped $CuO/ZnO/Al_2O_3$ Nanocatalyst Used in Steam Reforming of Methanol

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Environmental problems are one of the world biggest concerns, so it is imperative to develop new and clean sources of energy. A promising environmentally technology is the production of electrical power with fuel cells. Among the different fuels that are capable for production of on-board hydrogen for fuel cells, methanol is considered as the best option. Copper-base catalysts have high activity and selectivity to the desired products, but they have lower thermal stability and to improve the performance of these catalysts can be work on different promoters. [1] The $CuO/ZnO/Al_2O_3$ catalysts for production of hydrogen via methanol steam reforming were prepared by co-precipitation method due to its high Cu loading and dispersion. So many promoters were used for this process, in which zirconium oxide is one of the best promoters that was studied on Cu-based catalysts having a large impact on the dispersion and the stability of the catalysts. [2] Prepared catalysts were characterized by XRD, FESEM, BET and FTIR analysis. XRD analysis showed that the addition of zirconia to nanocatalyst made copper crystallites smaller. The FESEM results indicated that zirconia enhanced the surface homogeneity of the samples and made particles with smaller size. Catalytic performance tests proved the good practicability and high stability of synthesized catalysts. When the ZrO_2 promoter was added to the $CuO/ZnO/Al_2O_3$ catalyst, its methanol conversion and H_2 selectivity have been improved greatly.

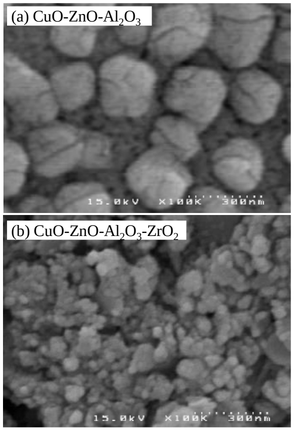

Fig. 1. FESEM images of synthesized nanocatalysts

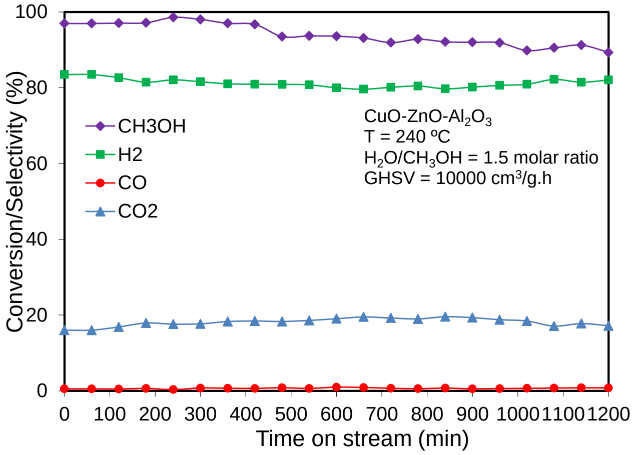

Fig. 2. Time on stream performance of $CuO-ZnO-Al_2O_3$

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Immobilization of Cu (II)-Salen Schiffbase complex on the surface of MWCNTs as a new nanocatalyst for the synthesis of 1-amidoalkyl-2-naphthol derivatives

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Reusable heterogeneous catalysts have attracted a great deal of interest from laboratory and industrial points of view. Since most of the catalysts are expensive and contaminate the environment, the development of efficient methods for recovery and reuse of the catalysts is a very important aspect from an economical point of view. One way to overcome this problem is to immobilize the homogeneous catalysts on solid supports. The major advantages of solid-supported catalysts are the facile recovery from the reaction mixture and possibility of reusing them. Furthermore, supporting of the catalysts efficiently increases the surface area and subsequently the reactivity of the catalysts.[1]

Metal complexation has been a recent choice for functionalization of CNTs and fabrication of CNTs/inorganic hybrid materials.[2] The main objective of this paper, is to immobilize a Cu(II)-Salen Schiff base complex on the surface of MWCNTs by (3-aminopropyl) trimethoxysilane as a Si-linker and spacer. The catalytic application of Cu(II)-Salen Schiff base complex on the surface of MWCNTs as a new nanocatalyst for the one-pot three-component condensation reaction of various aromatic aldehydes, amides and b-naphtholwas studied through the preparation of 1-amidoalkyl-2-naphthols at room temperature under solvent free condition. In the present study, some products were produced and reported for the first time.[3]

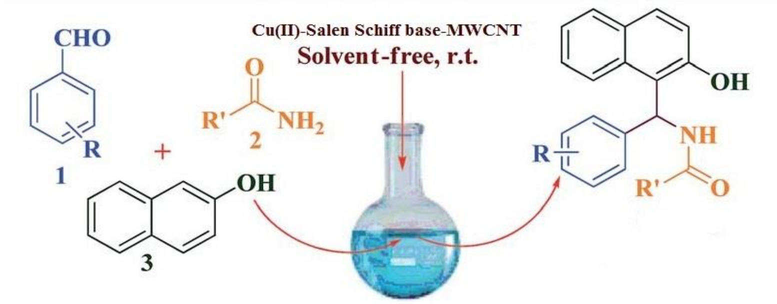

Fig. 1. The synthesis of 1-amidoalkyl-2-naphthol derivatives in the presence of Cu(II)-Salen Schiff base complex on the surface of MWCNTs

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Synthesis and characterization of phosphotungtic acid supported on $LaFeO_3$ nanocomposite

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Nano-sized and pure single-phase perovskite-type $LaFeO_3$ powders were synthesized via thermal decomposition of $La[Fe(CN)_6].5H_2O$ complex and characterized with different methods. This nanosized perovskite-type oxide with an average particle size of 35 nm was used as a precursor for synthesis of a new nanocomposite. These pure phase $LaFeO_3$ nanoparticles were first time surface modified effectively by means of silylating agents tetraethyl orthosilicate (TEOS) and 3-Aminopropyl triethoxysilane (APTES). Then phosphotungstic acid (HPW) supported on silica-coated $LaFeO_3$ nanoparticles. The nanocomposite ($LaFeO_3$@SiO_2-$PrNH_2$-PW) was characterized with FT IR, PXRD, energy-dispersive X-ray spectroscopy (EDX) and Field Emission Scanning Electron Microscopy (FE SEM) and Surface Area Analysis (BET BJH). The FT-IR, XRD , EDS and VSM results confirm that the synthesized nanocomposite is pure and singlephase with a weak ferromagnetic behavior. The FE SEM image shows that morphology of the nanoparticles are quasispherical and the surface morphology of nanopartcles is quite porous with smaller subunits. The surface area results obtained for nanocomposite by the N_2 adsorption isotherms was 9.44 m^2/g with total pore volume of 3.326 cc/g and Average pore diameter of 1.305 nm.

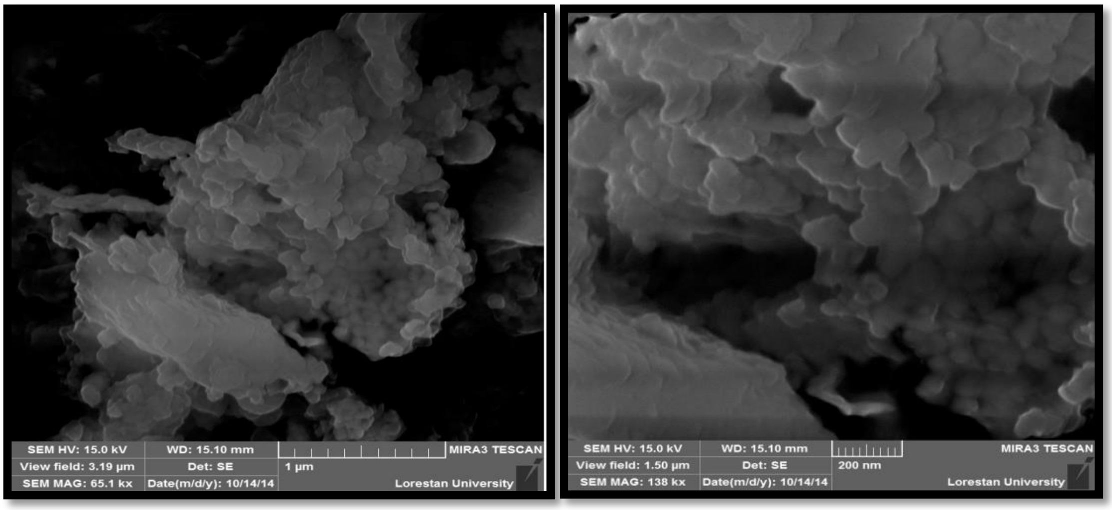

Fig. 1. FE SEM images of $LaFeO_3$@SiO_2-$PrNH_2$-PW

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$H_3PW_{12}O_{40}$ supported on magnetic nanostructure $BiFeO_3.Fe_3O_4$: preparation and characterization

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A single-phase perovskite-type $BiFeO_3$ was synthesized by thermal decomposition of Heteronuclear $Bi[Fe(CN)_6].5H_2O$ complex at 600˚ C for two hours. For synthesis of a magnetic nanocomposite, magnetic Fe_3O_4 and pure phase $BiFe_3O_4$ were used. This pure phase $BiFeO_3.Fe_3O_4$ magnetic nanoparticles were characterized with FT IR and PXRD. Then the nanoparticles were first time surface modified effectively by means of silylating agents tetraethyl orthosilicate (TEOS) and 3-Aminopropyl triethoxysilane (APTES). Modified nanocomposite, were efficiently introduced into phosphotungstic acid to synthesis of ($BiFeO_3$. $Fe_3O_4@SiO_2$-$PrNH_2$-PW) nanocomposite. The synthesized nanocomposite were characterized with FT IR, PXRD, energy-dispersive X-ray spectroscopy (EDX) and Field Emission Scanning Electron Microscopy (FE SEM). The FT-IR, XRD , EDS and VSM results confirm that the synthesized nanocomposite is pure and single phase with a weak ferromagnetic behavior. The FE SEM image shows that morphology of the nanoparticles are quasispherical with an average size of 35 nm.

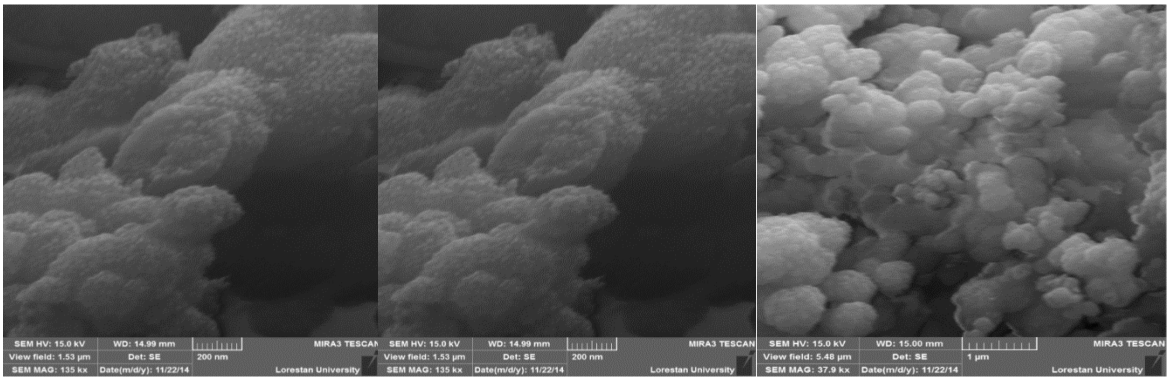

Fig. 1. FE SEM images of $BiFeO_3.Fe_3O_4@SiO_2$-$PrNH_2$-PW

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Synthesis and Physiochemical Properties of Nanostructured SAPO-34 Molecular Sieve Using Different Contents of Seed

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Among the different types of templates, DEA can produce SAPO-34 with high purity and crystallinity and TEAOH has shown excellent physiochemical properties because of its appropriate particle size distribution. However, its relatively high cost can be a serious obstacle for commercial production.[1] Consequently, the application of seed in the synthesis of nanostructure SAPO-34 molecular sievecan result inphysiochemical properties improvement, while reducing the preparation costs.Hydrothermal treatment was applied to prepare each of the SAPO-34 molecular sieves. The catalytic performance of the samples can be studied in the MTO reaction. The successful preparation of nanostructure SAPO-34 molecular sieve was confirmed by powder X-ray diffraction, FTIR spectroscopy, Brunauer–Emmett–Teller analysis (BET) and X-ray spectroscopy (EDX). Seeded SAPO-34 (seed=10%) show the higher crystallinity and BET surface areasthan seeded SAPO-34 (seed=5%) because of its smaller particle size and smooth surface area. The FESEM results indicated that samples prepared by a large amount of seed decreased particle size from microstructure to nanostructure because of its effect on the rate of crystal growth. The external surface area provided by the seeds played a vital role in accelerating the nucleation rate by offering specific sites for the formation of nuclei. The reduction of particle size can result in diffusion enhancement of both reactants and products into the nano-crystals simply because of the large number of pores which can beimproved as result of the physiochemical properties.

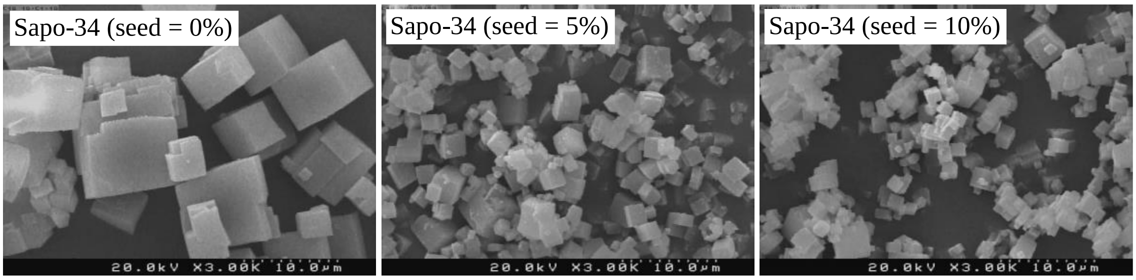

Fig. 1. FESEM images of nanostructured SAPO-34 molecular sieve synthesized with different Contents of Seed

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Investigation of Template Content Reduction with the Aid of Seed Application in the Nanostructured SAPO-34 Synthesis

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The use of organic template in synthesis of molecular sieves has obvious disadvantages like being poisonous and expensive. From this point of view, the template-free synthesis method in the presence of seed in order to generating controllable sized crystals seems to be more idea [1]. For this reason, the effect of different amounts of templates together with seed on the physicochemical properties of SAPO-34 molecular sieves was investigated. The catalysts were prepared via hydrothermal method and characterized with XRD, FESEM, EDX, BET and FTIR techniques. The catalytic performance of the samples can be studied in the MTO reaction. The X-ray diffraction patterns and Brunauer–Emmett–Teller analysis (BET) exhibited the decrease in the crystallinity and surface areas with DEA/Al_2O_3 ratio reduction. The complete removal of template results in formation of a single impurity phase. Templates have essential role in the molecular sieves structure that cannot completely be removed from the SAPO-34 molecular sieves. However at low DEA/Al_2O_3 ratio, proper amount of seed and operational condition can produce SAPO-34 molecular sieves with highest purity and smaller particle size.

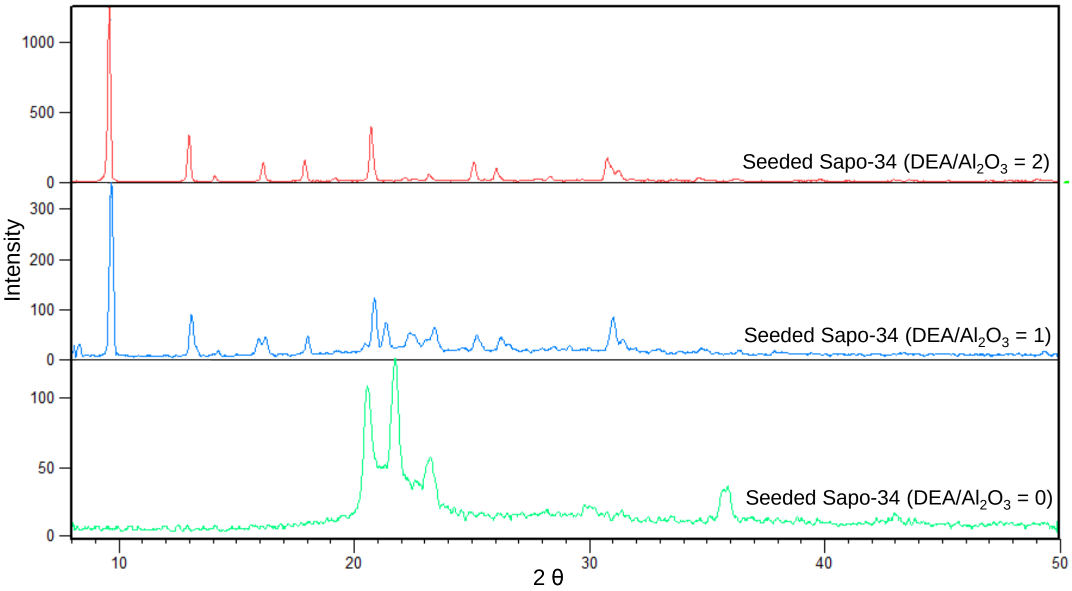

Fig. 1. XRD patterns of nanostructured SAPO-34 synthesized with different Contents of templates

References

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Synthesis and Characterization of Cadmium-Doped TiO_2 Used in Photocatalytic Degradation of Acid Orange 7 Dye

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Doping the metal and nonmetal components on the photocatalyst is a promising way to enhance the photocatalytic activity and some other determinant properties.[1] Doping can prevent the recombination of charge carriers as a major barrier of photocatalysis.[2] In the present work the cadmium ions doped in the nanostructure of well-known TiO_2 photocatalyst, forming Cd-doped TiO_2 photocatalyst. The nanostructured photocatalyst was synthesized through a hydrothermal assisted sol-gel method in the different precursor molar ratios of Cd/Ti=0, 0.5, 0.1, 0.15. The morphological properties investigated via analyses such as FESEM, BET surface area and FTIR. The successful synthesis was affirmed using X-ray diffraction so that a distinct peak of anatase phase was recognized for titania (shown at Fig.1). The degradation ability was evaluated using UV-Vis spectroscopy. The photocatalytic activity of the catalyst was evaluated via acid orange7 as an azo dye, under visible light. As shown at Fig.2 the performance test was carried out for 20 min of darkness adsorption test followed with exposure to visible light of a tungsten lamp for 120 min. The test resulted a fine enhancement at dye degradation ability for the Titania photocatalytic after the cadmium addition. After 120 min of degradation under visible light, the Cd/Ti=0.15 catalyst has represented 74.27 percent of degradation conversion. The photocatalyst with the ratio of Cd/Ti=0.15 was exhibited the most degradation ability during the performance test. The 20min of darkness test showed the adsorption ability of the catalyst and resulted a distinct increase at adsorption after cadmium loading.

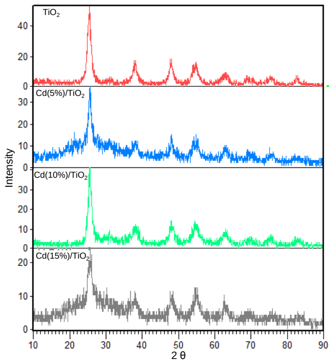

Fig. 1. X-ray diffraction analysis of various photocatalysts.

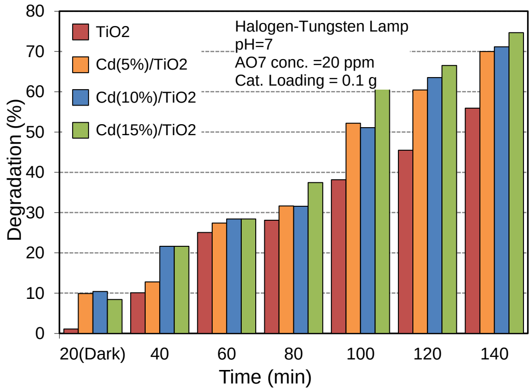

Fig. 2. The performance test evaluated under visible light up to 140 min for AO7 degradation.

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Synthesis and Characterization of TiO2-ZrO2 Nanophotocatalyst for Degradation of Acid Orange 7 Dye

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Among advanced oxidation processes, the photocatalytic degradation of contaminants has been recognized in the energy efficient category of wastewater treatment processes. [1] Many photocatalysts has been evaluated through the history of photo catalysis. ZrO_2 and TiO_2 are well-known photocatalysts exhibiting fine efficiency in processes such as degradation of contaminants. [2] In the present work it is focused on the composite photocatalyst synthesized in various compositions of TiO_2 and ZrO_2 for the aim of using under a wide range of UV-Visible spectra of mercury vapour light bulb. The catalysts synthesized through precipitation method and the titania was added to the zirkonia enhancing the photo-activity of the catalyst. The photocatalysts characterized through morphological and performance analyses such as X-ray diffraction, FESEM, FTIR, BET, UV-Vis Spectroscopy. However the azo dyes are the pollutants widely assessed by researchers to evaluate the photocatalyst activity under light emission. Acid orange 7 azo dye had been selected as an important contaminant with the aim of degradation ability assessment. Fig.1 introduces the FESEM analysis of the catalyst surface demonstrating the nonmetric size of the catalysts. Fig.2 illustrates the degradation test, exhibiting a fine enhancement at the degradation ability of catalyst after addition of TiO_2 to the ZrO_2. The test demonstrates a distinct adsorption for the 50-50 percent composite of two nanocatalysts.

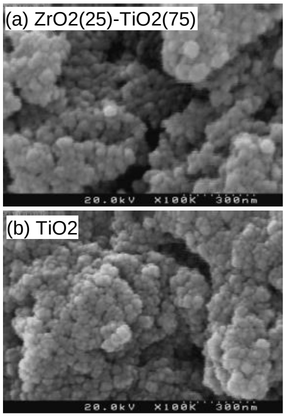

Fig. 1. FESEM images of the photocatalysts.

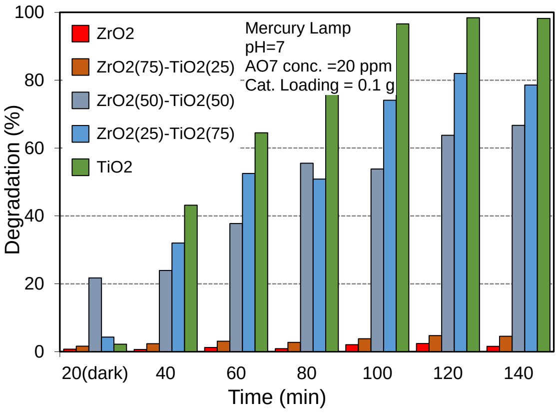

Fig. 2. The AO7 degradation test of the photocatalysts.

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Synthesis and characterization of new compounds of boron-bridged [1] ferrocenophane

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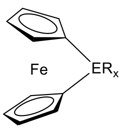
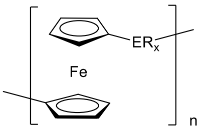
Ferrocenophanes are derivatives of ferrocene, which containa one to three atom-bridge, connecting the cyclopentadienide ligandsof ferrocene.The first **[1]** ferrocenophane, the silicon-bridged species**1** was synthesized and characterized in 1975 by Osborne.[1] Subsequently, the range of [1]ferrocenophanes has been extended to those bridged with heavier main group elements of the second period and below such as group 14 (Ge, Sn), group 15 (P, As), group 16 (S, Se), and group 4 elements (Ti, Zr, Hf).[2]**[1]**ferrocenophanes**1** represent unusual examples of strained species of this type in which the introduction of a single bridging element between the cyclopentadienide ligands of ferrocene leads to a strained, ring-tilted structure.[2]These molecules are important due to their facile ring-opening reactions, including ring-opening polymerization (ROP) to obtain poly-(ferrocenes) **2**.The first example of a [1]ferrocenophane containing a boron bridge was the compound**3**,which was reported by Braunschweig and manners in 1997.[3]Now we report here on the synthesis of new compound ofboron-bridged [1]Ferrocenophane **4**, which was obtained by the reaction of1,1′-dilithioferrocenewith dibromoborylferrocene($FcBBr_2$, Fc=ferrocene) under argon atmosphere. The new compound of ferrocenylbora[1]-ferrocenophanes**4** was characterized by ^1H, ^{13}C- and ^{11}B-NMR-spectroscopy.



1 ER$_x$ = SiPh$_2$



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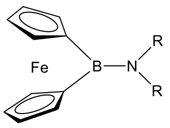

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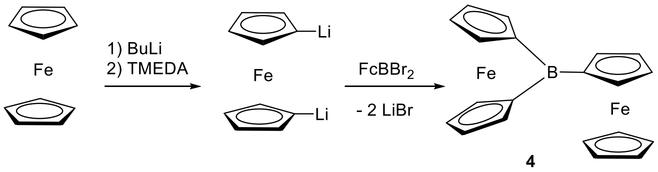

Figure 1: Synthesis of new ferrocenylbora[1]-ferrocenophanes**4**.

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Sonochemically Preparation and Characterization of Pd/Al_2O_3-Clinoptilolite-CeO_2 Nanocatalyst Used in Treatment of Polluted Air

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In recent years, many studies have been focused on catalytic oxidation of VOCs. Different methods for catalyst preparation and their effects on catalyst activity are investigated. [1-3] In this research Pd/Al_2O_3-clinoptilolite-CeO_2 nanocatalyst was successfully synthesized via ultrasound assisted wet impregnation method to be utilized for total oxidation of toluene. Chemical analysis, XRD, FESEM, EDX, BET and FTIR techniques are used to determine physicochemical properties of synthesized samples. Chemical analysis confirms the presence of all the elements in natural and treated clinoptilolite. XRD patterns prove the formation of ceria as a crystalline phase with the average crystallite size of 19.5 nm. FESEM images show the nanometric size of catalyst particles. EDX analysis indicates homogeneous dispersion of elements. BET surface area presented large surface for nanocatalysts. The results confirm the positive effect of ultrasound irradiation on surface morphology and elemental dispersion. Catalytic performance tests indicated high removal efficiency of nanocatalyst in oxidation reaction. High conversion at low temperatures (200-225˚C) and thermal stability are suitable reasons for this claim.

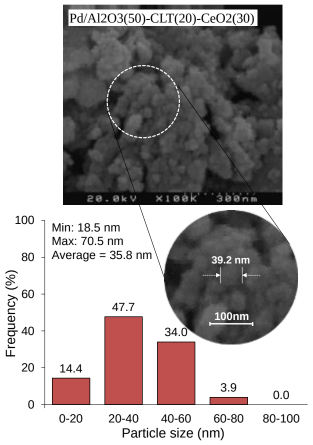

Fig. 1.FESEM images of synthesized nanocatalysts.

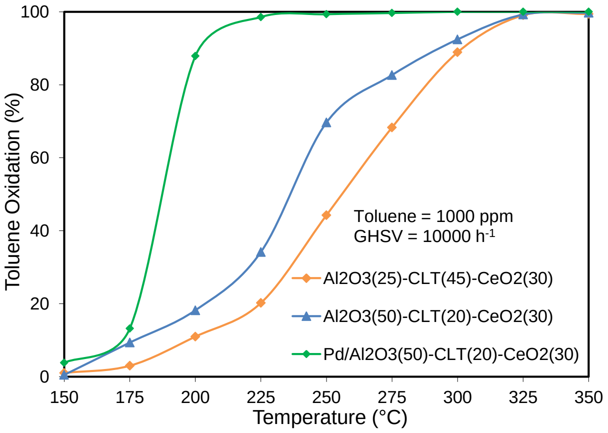

Fig. 2. Catalytic performance of synthesized nanocatalysts.

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Comparative Preparation of Pd/Clinoptilolite and Pd/Al_2O_3 Nanocatalysts Used in Total Oxidation of Toluene

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Catalytic oxidation of volatile organic compounds as air pollutants is an interesting subject for experimental studies. [1,2] In this research, Pd/clinoptilolite and Pd/Al_2O_3 nanocatalysts prepared to use for oxidation of toluene in air as an organic compounds in air. The effect of alumina and clinoptilolite on catalyst properties and activity was compared. Chemical analysis, XRD, FESEM, EDX, BET and FTIR techniques are used to determine physicochemical properties of synthesized samples. XRD patterns and FTIR confirm formation of all species of catalysts. FESEM images show the morphology and nanometric size of catalysts. Figure 1 shows smaller particles of Pd/Al_2O_3.EDX analysis proves homogeneous dispersion of elements on samples. BET analysis indicates alumina has high surface area that causes Pd/Al_2O_3has more surface area than Pd/clinoptilolite. Smaller particle size of Pd/Al_2O_3 and high surface area makes more catalyst activity and oxidation reaction does in low temperatures. Figure 2 shows this result.

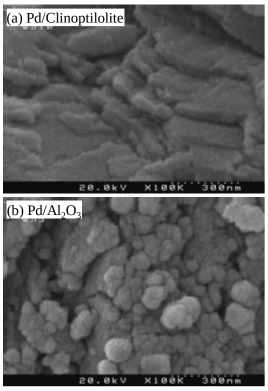

Fig. 1.FESEM images of synthesized nanocatalysts.

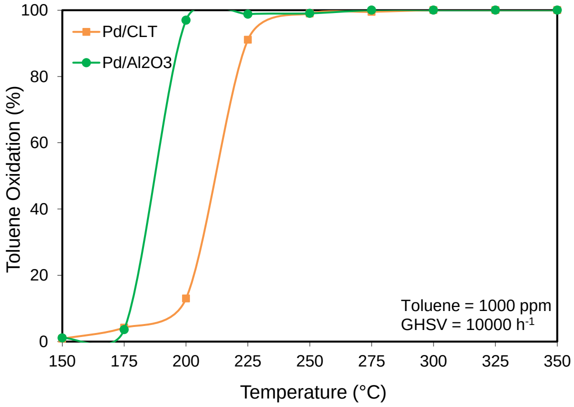

Fig. 2. Catalytic performance of synthesized nanocatalysts.

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Morphological and structural study of sol-gel ceramic silica/zirconia nanocomposite layers

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In order to increase in uniformityand reducing the crack and porosity in ceramic layersafter sintering,ceramic nanocomposite layershave been developed. In this study, ceramic silica/zirconia nanocomposite layersweredepositedon metallic substrate by sol-gel (dipping) method. The effect of sintering temperature on layer characteristics was also studied.The morphology and structures of the layers were evaluated by scanning electron microscope (SEM), and X-ray diffraction (XRD) and Fourier transformed infra-red spectroscopy (FTIR), respectively. The results showed that the deposited layers were dense and consisted of nano-scale microstructure with a grain size in the range of 70-170 nm of silica and zirconia whichwas increased with increasing sintering temperature from 500 to 700 ^{o}C. The layers had an amorphous nature and dense appearance.

Formation and characteristics of ceramic silica/titania nanocomposite coatings by sol-gel method

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In this study, ceramic silica/titania nanocomposite coatings were deposited on metallic substrates by sol-gel method. The sols were prepared using metal alkoxides. The gel was formed by the use of acid catalyst. The formed layers wereheat- treated at 450°C. The morphology of the layers was studied by scanning electron microscopy (SEM). The structural features of the coatings were evaluated by X-ray diffraction (XRD) and Fourier transformed infrared spectroscopy (FTIR). The results showed thatthe grain size of composite was in the range of 50-200 nmwith a sphericalmorphology. The XRD result showed that SiO_2 and ZrO_2 phases were existed in structure of layers with an amorphous nature.

Synthesis and characterization of Pd(II) complexes of two carboxamide ligands, (H_2bqbenzo) and (Hqcq), derived from aminoquinoline

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The carboxamides are a group of chemical compound containing C-(O)-NH, and have various application such as antibacterial, antitumor, and are also used as catalysts. Synthesis of carboxamides in environmentally friendly reaction media is very attractive to synthetic chemists. The favorable characteristics of ionic liquids (ILs) make them promising reagents for carrying out reactions according the principles of green chemistry. ILs are environmentally friendly or "greener" alternatives to organic solvents because of their very low vapor pressure and are non-explosive and thermally stable over a wide temperature range. They can be employed as solvents for a wide range of chemical processes, and their application as novel media may provide convenient solutions to both the solvent emission and catalyst reuse problem.

Carboxamide ligands have been part of the growing research in the field of coordination chemistry of transition metal complexes. The solvent used in the classical method of synthesis of these compounds is pyridine, a solvent which is extremely toxic. We have developed a new method of synthesis using ionic liquids as the reaction media and have prepared H_2bqbenzo and Hqcq under optimum conditions. The Pd(II) complexes of bqbenzo^{2-} and qcq^{-} with the formula:

(**1**) [Pd(bqbenzo)]   (**2**) [Pd (qcq)(OAc)]

have also been synthesized and characterized by elemental analysis and different spectroscopic methods.

The structures of [Pd(bqbenzo)] (**1**) and [Pd(qcq)(OAc)] (**2**) have been determined by X-ray crystallography. The di-anionic bqbenzo^{2-} in (**1**) acts as a tetradentate ligand and [Pd(bqbenzo)] has a distorted square-planer geometry. The mono-ionic qcq^{-} is a tridentate unsymmetrical ligand occupying three equatorial positions. Acetate ion act as mono dentate ligand in [Pd(qcq)(OAc)] completing the square-planer structure.

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Spectroscopy and structural determination of Co(III)schiff base complexes, intraction of complexes with Nano clay.

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Cobalt Schiff base complexes have been studied extensively. They are investigated as models for the Cobalamine (B12) coenzymes[1] classified as an oxygen carrier.[2] Sodium Montmorillonite (MMT) is the most commonly used clay owing to its natural abundance, high aspect ratio and high cationic exchange capacity (about 80–120 meq/100 g).[3] The $[Co(acacen)(PBu_3)(H_2O)]ClO_4$, $[Co (acacen)(PEt_3)(H_2O)]ClO_4$ and $[Co(acacen)(PPh_3)(H_2O)]ClO_4$ complexes were synthesis and characterization by FT-IR , UV-Vis and HNMR spectroscopy and elemental analysis technique. The coordination geometry of the synthesis complexes were determinate by Xray crystallography. Cobalt complexes have six coordination Pseudo-octahedral geometry. The synthesis complexes were incorporated on to the montmorillonite K10 Nano clay via simple ion exchange reaction .the structure and morphology of the obtained Nano hybrid were identified by FT-IR, XRD, SEM, TEM, TG technique. Base on the XRD results of the new Nano hybrid material the Schiff base complexes were intercalated in the interlayer space of clay. SEM and TEM micrographs of the clay complex shows that the resulting hybrid nanomaterial has layer structure.

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Modification induced by La Incorporation on Nanostructured Cr/SAPO-34 Catalyst Used for Oxidative Dehydrogenation of Ethane with CO_2

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The development of efficient catalysts for selective functionalization of alkanes is one of the primary goals aimed by the petrochemical industry. 1 In this context, extensive works have investigated catalytic oxidation process, especially for ethylene production, using the CO2-assisted dehydrogenation of ethane route. In this work, dehydrogenation of ethane to ethylene in the presence of CO2 has been carried out over chromium oxide catalysts sonochemically supported on parent SAPO-34 and LaAPSO-34 nanocomposite with the aim of understanding the effects of La incorporation on the physicochemical properties and catalytic performance. Like SAPO-34, LaAPSO-34 nanocomposite with nominal Si/Al ratio of 0.2 in the gel was successfully synthesized via one-pot hydrothermal method. Based on the characterization results, La incorporation into the framework of SAPO-34 (0.2) not only increases the surface area but also neutralizes mostly strong acid sites, resulted in higher dispersion of Cr species and more effective surface acidity. This reflects in higher content of redox Cr species stabilized in comparison with parent SAPO-34 (0.2), which accounts for superior catalytic performance and stability of Cr/LaAPSO-34 (0.2). By employing SAPO-34 supports, a reasonable catalytic performance was observed. Moreover, doping SAPO-34 (0.2) by lanthanum metal completed crystallinity of SAPO-34. It was found that chromium nanocatalyst supported on the La-modified SAPO-34 (0.2) effectively dehydrogenated ethane to ethylene in the presence of CO2 at 700°C even after 10 h on-stream operation, giving 42.3 and 97% ethylene yield and selectivity, respectively. Less sensitivity to deactivation during the course of running the reaction evidently indicated the synergism effect of lanthanum exictance and ultrasound irradiation on alleviating the catalyst deactivation in ethane dehydrogenation with CO2.

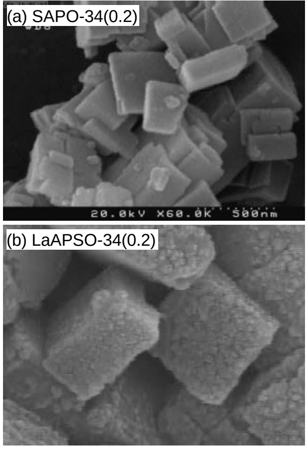

Fig. 1. FESEM images of (a) SAPO-34 and (b) LaAPSO-34.

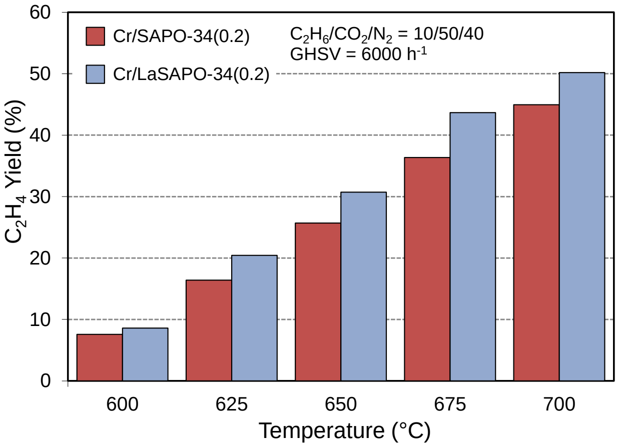

Fig. 2. Effect of La incorporation and temperature on C_2H_4 yield.

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CO_2-Assisted Dehydrogenation of Ethane over Nanostructured Cr/SAPO-34 Catalysts: Effect of Si/Al Ratio on Catalytic Properties and Performance

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Ethane oxidative dehydrogenation is a promising alternative method to produce ethylene from ethane, minimizing the main environmental and economic restrictions associated with the currently applied technology. [1] In this regard, a series of SAPO-34(x) supported chromium oxide catalysts varying in Si content were prepared by the ultrasound assisted incipient wetness method, characterized with XRD, FESEM, BET, EDX, TPD-NH_3 and FTIR and tested in dehydrogenation of ethane with CO_2. SAPO-34 supports with nominal Si/Al ratios of 0.1, 0.3 and 0.4 in the gel were successfully synthesized via hydrothermal method. The variation of silicon content indicates that crystallinity, surface area and effective acidity of samples increased with Si/Al ratio up to 0.3. However, a decreasing trend was observed with further increase of the silicon content. It was found that there is the optimum silicon content in SAPO-34 (0.3) support for the best catalytic activity, attributable to perfect crystallinity, higher surface area and appropriate surface acidity. Based on the EDX and FTIR analysis of Cr/SAPO-34 samples, employing SAPO-34 (0.3) as support resulted in higher dispersion of Cr species and more effective surface acidity. This reflects in higher content of redox Cr species stabilized in comparison with rest, which accounts for superior catalytic performance and stability of Cr/SAPSO-34 (0.3). The results of catalytic performance tests showed that chromium nanocatalyst supported on the SAPO-34 (0.3) effectively dehydrogenated ethane to ethylene in the presence of CO_2 at 700°C, giving 40.4 and 91% ethylene yield and selectivity, respectively.

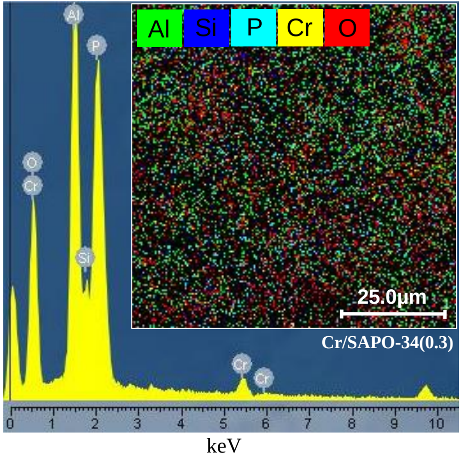

Fig. 1. EDX analysis of Cr/SAPO-34(0.3)

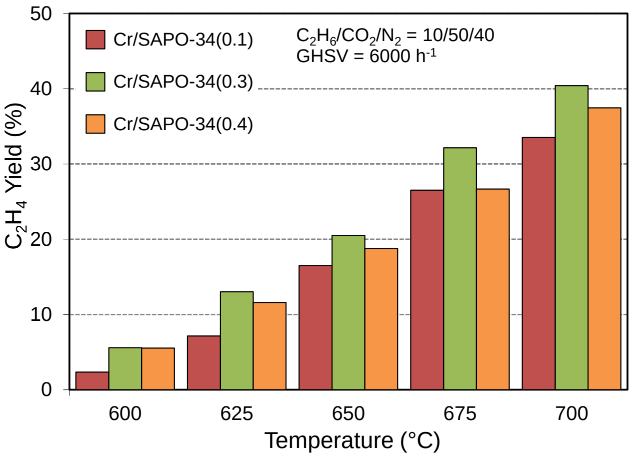

Fig. 2. Effect of Si/Al ratio and temperature on C_2H_4 yield.

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Catalytic performance of Nanostructured Pd/HCl Treated Clinoptilolite Catalysts for CO Oxidation: Effect of Pd Loading

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The increasing demand for clean and efficient energyhas resulted in an increased global willingness to embrace the proposed hydrogen economy as a potential long termsolution to the growing energy crisis. CO oxidation is one of the ways that can be used to purify the hydrogen stream for fuel cells.[2] A series of nanostructured Pd/HCl treated clinoptilolite catalysts with different loadings of Pd (0, 1 and 5 wt.%) were prepared by impregnation of treated clinoptilolite in $PdCl_2$ solution and tested for oxidation of CO. To prepare the modified clinoptilolite samples, the acid leaching (12 M HCl) were applied to the zeolitic tuff. The synthesized nanocatalysts were characterized by XRD, FESEM, BET and FTIR analysis. FESEM images showed that nanocatalysts have nanometric particles. Specific surface analysis revealed that the synthesized nanocatalysts had large enough surface area. However, increasing the Pd loading decreases the surface area. Catalytic performance tests of synthesized samples were performed in temperature range of 50–350 °C and gas hourly space velocity (GHSV) of the 15000 ml/gcat.h. The feed consisted of 2% CO in air balance. The results showed that the activity of the supported Pd catalysts was much higher than that of treated clinoptilolite. It was found that Pd(1 wt.%)/HCl treated clinoptilolite exhibited the best activity over the course of reaction. This could be well explained on the basis of more accessibility and higher surface area. Complete oxidation was obtained at 250 °C over catalysts containing Pd.

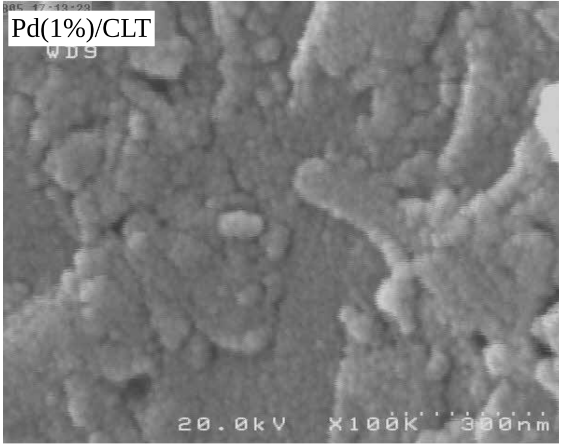

Fig. 1. FESEM image of Pd(1 wt.%)/Clinoptilolite.

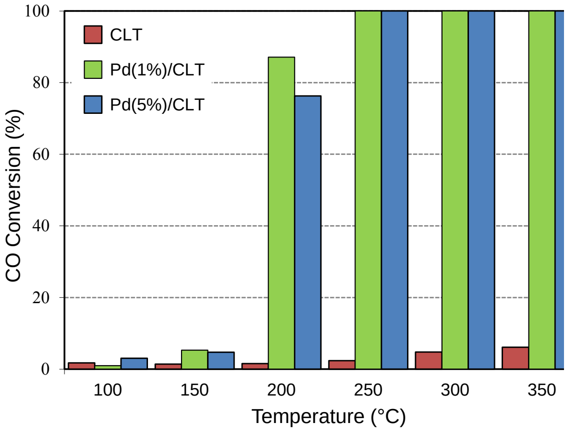

Fig. 2. Effect of Pd loading on CO conversion over synthesized Pd-based nanocatalysts at different temperatures.

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Effect of Dual Metals Content on Catalytic Properties and Performance of Sonochemically Synthesized Mn_xCu_{10-x}/Clinoptilolite Nanocatalyst Used in Low Temperature Oxidative Destruction of Toluene

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Volatile organic compounds (VOCs) are widely produced by direct and indirect sources of air pollution.From an environmental point of view, control of VOC emission due to negative effect on health of human and animals is very necessary. [1-3] In this research, a series of nanostructured Mn_xCu_{10-x}/Clinoptilolite catalysts were synthesized for the aim of destruction of toluene from polluted air. The clinoptilolite as support of nanocatalysts was modified by ion-exchange and acid treatment. Then, the nanocatalysts with different ratios of Cu/Mn were sonochemically synthesized and catalytic performances were studied for toluene oxidation. The nanocatalysts were characterized by XRD, FESEM and EDX analyses. XRD data confirmed the formation of CuO as nano-crystalline phase. FESEM images showed nanometric size of surface particles on support. EDX dot mapping indicated homogenous dispersion of active metals on the catalyst surfacerevealing remarkable positive effect of ultrasound irradiation on the surface morphology and elemental dispersion. The performance results showed that highly active nanocatalysts were synthesized and the nanocatalyst performance test demonstrated the best performance test for the $Mn_{(7\%)}Cu_{(3\%)}$/Clinoptilolite catalyst. Accordingly, as the Mn /Cu ratio increases, the lower temperature activity was achieved by the performance testresults. The stability test of catalyst demonstrated that the removal efficiency has remained constant for long time.

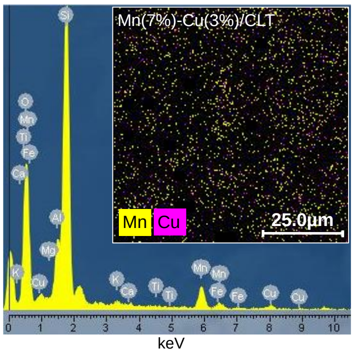

Fig. 1. EDX analysis of the synthesized nanocatalyst.

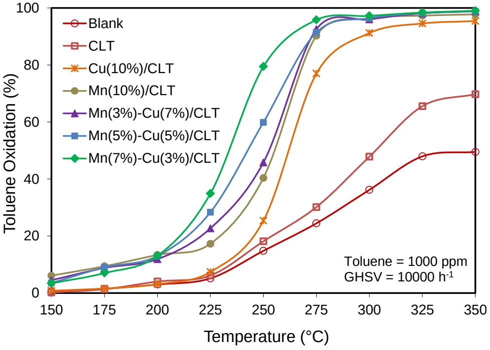

Fig. 2. Effect of dual metals content on toluene oxidation.

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Synthesis of nanocopper chromite with co-precipitation method in the absence and presence of surfactant

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In this work, we used co-precipitation method for preparing nanoparticles of copper chromite ($CuCr_2O_4$) and investigated the effect of Polyethylene glycol 400 (PEG 400) as surfactant on size and morphology of nanoparticles.First the precursor ($Cu(OH).NH_4Cr_2O_4$) prepared fromthe reaction of basic solution of $Cu(NO_3)_2.5H_2O$ and $(NH_4)_2Cr_2O_7$), after that the precursors were calcinated at 600ºC. [1-3] In order to investigate the effect surfactant on size and morphology of nanoparticles, PEG 400 was used. Some precursors were prepared in the presence of 1% and 2% solution of PEG 400. nanoparticles characterized by X-ray diffraction, scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX) and IR analysis. The XRD patterns indicated that the synthesized nanomaterial swhich consisted of Spinel $CuCr_2O_4$ and CuO are without any impurity. The EDX analysis of all nano-copper chromites exhibit assignments of Cu, Cr and O. The microstructure of the nanopaiticles showed that the size of nanoparticles is in the range of 25– 50nm in the absence of surfactant, but big aggregation was seen because of small size of nanoparticles (Fig.1). When surfactant was used the morphology of nanoparticles were completely improved and almost no aggregation was seen, but the sizes become large. The size of nanoparticles here is in the range of 150-250 nm (Fig.2).

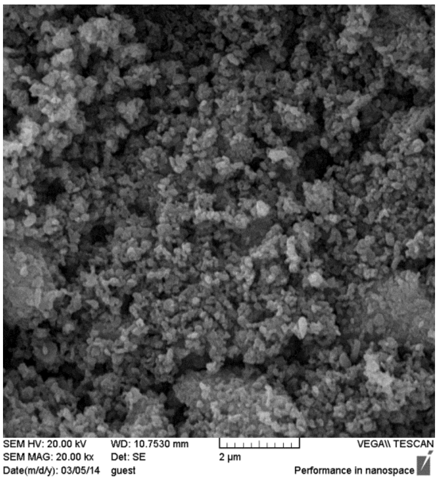

Fig1. SEM of nanoparticles in the absence of PEG 400

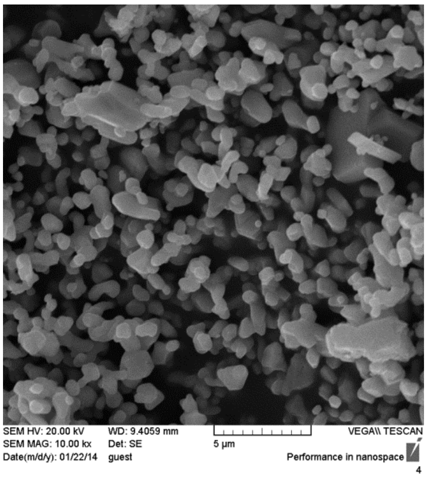

Fig2. SEM of nanoparticles in the presence of PEG 400

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Synthesis, characterization and application of new Cu(I) complex of α-keto stabilizedphosphorous ylide toward Suzuki reaction

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Phosphorus ylides are a member of very interesting ligands in organometallic chemistry[1] and metallic complexes of these compounds are also useful in organic synthesis and have been used as precursor in catalytic reactions[2]. Recently, the use of copper complexes in the cross-coupling reactions has been studied [3]. The origin of Suzuki coupling procedures involves the use of palladium phosphine complexes as catalysts, but due to the economy aspects, the use of cheaper metalssuch as copper complexes as well as palladium homologous combined with a ligand (phosphorous ylide) is an alternative choice for this coupling reaction. Herein, we report the synthesis, characterization and application of new Cu(I) complex $[Cu(\mu\text{-}Cl)\{Ph_2P(CH_2)_2PPh_2C(H)C(O)Ph\text{-}m\text{-}Br\}]_2$ toward the Suzuki cross-coupling reaction. Reaction of α-keto stabilized phosphorous ylides $Ph_2P(CH_2)_2PPh_2C(H)C(O)Ph\text{-}m\text{-}Br$ with CuCl in 1:1 ratios leads to binuclear products of the type $\{CuCl(ylide)\}_2$. Characterization of the complex by IR, ^1H, ^{31}P and ^{13}C NMR spectroscopy confirmed coordination of the ylide to the metal through the carbon atom (**Fig. 1**). The complex was found to exhibit good catalytic activity in the Cu-catalyzed Suzuki cross-coupling reactions inan air atmosphere at medium catalyst loading in NMP as a solvent for coupling of various aryl halides with phenyl boronic acid.

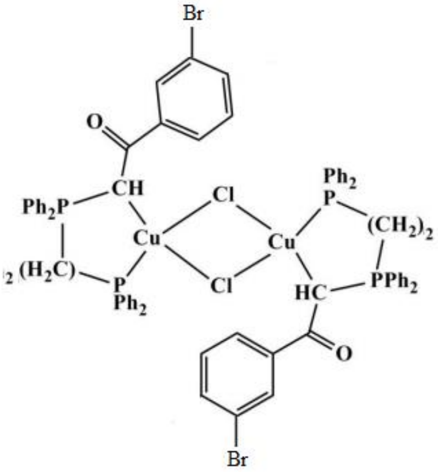

Fig. 1. The Cu(I) complex bearing phosphorous ylide .

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Preparation of pH-sensitive Organic-Inorganic Nano-composites through In-situ Copolymerization of Modified Nano-silica with Methacrylic Acid

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Although oral route is one of the most popular approaches for drug administration, for some drugs the oral route shows many shortcomings. For example, these drugs are degraded in the stomach acidic medium. To overcome these problems, controlled release systems have been showing significant potential application. One class of materials that widely used in drug delivery systems is pH-sensitive materials. [1,2]

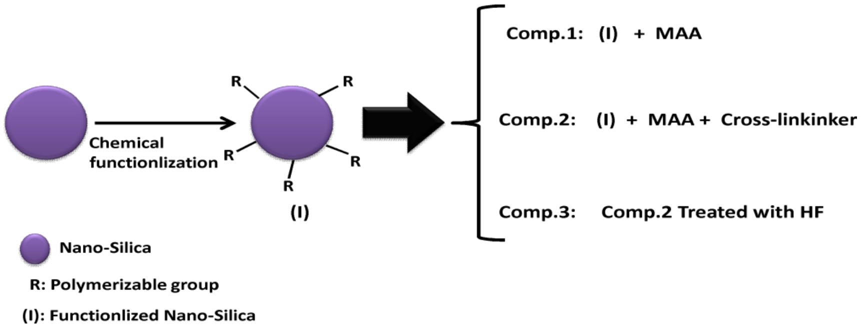
In this work, 3 types of pH-sensitive drug carriers based on modified nano-silica were synthesized (scheme 1). First, the nano-silica particles were synthesized and then chemically modified (polymerizable groups were attached onto the nano-silica surfaces).

To prepare comp.1: A pre-determined amount of modified nano-silica and MAA were copolymerized.

To prepare comp.2: In addition to modified nano-silica and MAA, a crosslinking agent (N,N′-Methylenebis(acrylamide)) was added.

To prepare comp.3: The comp.2 was treated with HF in order to remove nano-silica particles.

The prepared pH-sensitive nano-composites were characterized by FT-IR, SEM, TGA. Furthermore, the in vitro studies performed in both SGF and SIF media at 37±1 °C. Naproxen as a non-steroidal and anti-inflammatory drug was used as a model drug. The results show that the nano-composites have higher thermal stability. In all samples, drug releases proceed more efficiently at higher pH (SCF) than acidic medium (SGF). This can be attributed to the presence of polar groups in the nano-composites.



Scheme1. The schematic illustration of nano-composites preparation

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Effect of Irradiation Time on Ultrasound Assisted Impregnation of Nanostructured Sulphated Zr-MCM-41 Catalyst used in Esterification of Oleic Acid

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Technology, P.O.Box 51335-1996, Sahand New Town, Tabriz, Iran.
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Biodiesel also called fatty acid methyl ester is a clean-burning, renewable fuel produced from vegetable oils and recycled cooking oil. It is not only biodegradable but also free of sulfur, making it a cleaner burning fuel than petroleum diesel with reduced emission of SO_x and CO. Among solid acid catalysts that have been investigated as potential replacements for mineral acids, sulfated Zr-MCM-41 have been known to give high activity and selectivity in the esterification reactions. In this case, mesoporous Zr-MCM-41 was synthesized using cetyltrimethylammonium bromide as template under hydrothermal conditions. For sulfation of this catalyst, an ultrasound-assisted impregnation method with sulfuric acid was applied. After the thermal activation at this temperature, some sulfate ions are strongly retained onto the superficial zirconia, thus generating acidic catalysts which are able to produce the esterification of oleic acid with methanol at 60°C in 5 h. The experimental results reveal that the unique way to obtain stable catalysts without leaching of sulfate species to the liquid medium of reaction is using ultrasonic irradiation. Only with 1.5 g of this stable catalyst a conversion close to 93% was attained. The effect of irradiation power have been studied by changing time of the sonication (15, 30, 45 min) during the synthesis which led to different physiochemical properties of the nanocatalyst. The XRD, FTIR and BET analyses exhibited that performance of investigated nanocatalysts in esterification of oleic acid by ultrasound-assisted synthesized nanocatalysts have higher biodiesel conversion in comparison to non-sonicated catalyst.

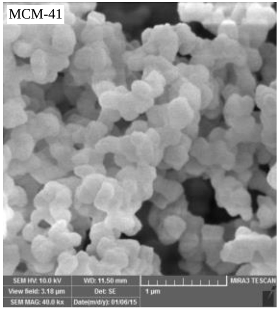

Fig. 1. FESEM images of synthesized MCM-41 nanocatalysts

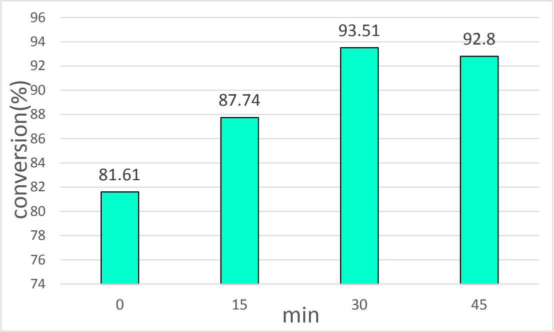

Fig. 2. effect of time irradiation in biodiesel conversion

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Effect of Ultrasonic Power on Synthesis of Sulfated Zr-MCM-41 Nanocatalyst Used in Biodiesel Production

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Biodiesel, a biofuel that can replace directly petroleum-derived diesel without engine modifications, has gained much attention because of its environmental and technological advantages. Furthermore, among solid acid catalysts that have been investigated as potential replacements for mineral acids, sulfated Zr-MCM-41 has been known to give high activity and selectivity in the esterification reactions. Stable sulfated Zr-MCM-41 has been prepared by an ultrasound-assisted impregnation hybrid method with zirconium doped mesoporous MCM-41 silica and sulfuric acid calcined at 750°C. After the thermal activation at this temperature, some sulfate ions are strongly retained onto the superficial zirconia, thus generating acidic catalysts which are able to produce the esterification of oleic acid with methanol at 60°C in 5h. The experimental results reveal that the unique way to obtain stable catalysts without leaching of sulfate species to the liquid medium of reaction, is using ultrasonic irradiation. Only with 1.5 g of this stable catalyst a conversion close to 96% was attained. The effect of irradiation power have been studied by changing power of the sonication (30, 60, 90 W) during the synthesis which led to different physiochemical properties of the nanocatalyst. The XRD, FTIR and BET analyses exhibited that the performance of investigated nanocatalysts in esterification of oleic acid by ultrasound-assisted synthesized nanocatalysts has higher oleic acid conversion in comparison to non-sonicated catalyst.

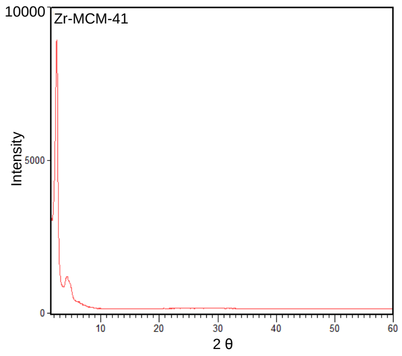

Fig. 1. XRD pattern of Zr-MCM-41.

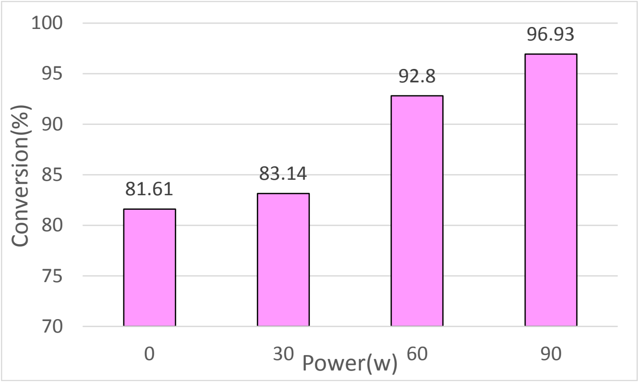

Fig. 2. Effect of power irradiation in biodiesel conversion

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Synthesis and characterization of ZnO nanoparticles obtained by calcination of [Zn(Br_2salabza)] complex.

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The chemistry of Schiff base ligands formed by the condensation of primary amines and carbonyl containing compound has been the focus of attention due to their role as effective corrosion inhibitors,[1] or their extensive application in the synthesis of metal complexes that are exploited in catalysis,[2] or exhibit interesting biological activities.[3] These metal complexes are in some cases used as the precursors of metal oxide nanoparticles.[4] In this study,4-bromo-2-(((2-((E)-(5-bromo-2-hydroxybenzylidene) amino)benzyl) -imino)methyl)phenol (H_2Br_2Salabza) was first used as a Schiff base ligand for the synthesis of [Zn(Br_2 -salabza)] (**Scheme 1**). This complex was then used for the preparation of ZnO nanoparticles by calcination method at suitable temperature. The obtained nanoparticles were characterized by using FT-IR and UV-Vis spectroscopy, X-ray diffraction analysis (XRD), and field emission scanning microscopy (FE-SEM).

Thermal decomposition $\longrightarrow$

$$\mathbf{H_2Br_2salabza + Zn(ACo)\ \ [Zn(Br_2salabza)] \longrightarrow ZnO\ (NPs)}$$

Scheme 1. Synthesis of [Zn(Br_2salabza)] and ZnO nanoparticles

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CO Oxidation over Ultrasound-Assisted Synthesized Ag/SiO_2 Nanocatalyst

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Nowadays, theproblem of environmental pollution caused by greenhouse gases and other pollutants has become a national and international problem. The carbon monoxide is a colorless, odourless, highlytoxic gas having density close to the density of the air. Moreover,it has natural and artificial sources. Due to the side reactions, the catalyst of this reaction must be active.Between different elements, silver has good activity at low temperature and silica (SiO_2) has a good surface area. Until now, different synthesis methods such as impregnation, co-precipitation, sol-gel and combustion have been carried out. Using ultrasound is one of the most modern methods for the catalysts synthesis that causes a better distribution of the active phase on support. In this study, the effect of ultrasound on the performance of Ag(6%)/SiO_2 was investigated. To evaluate the characteristics of the catalyst XRD, BET and FESEM analyses were used. Finally, the performance of the samples for oxidation of carbon monoxide in the process was analysed by a laboratory system.Temperature range of 100-275°Cwas obtained for this reaction.

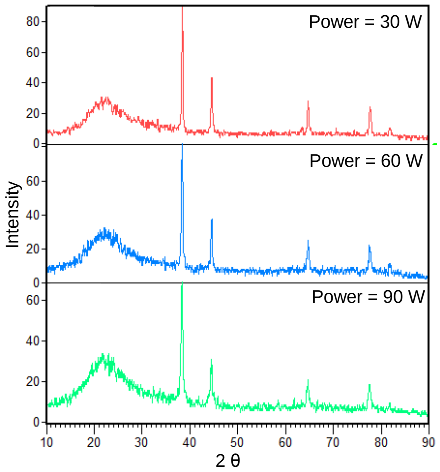

Fig. 1..XRD patterns of Ag(6%/SiO_2) with different power.

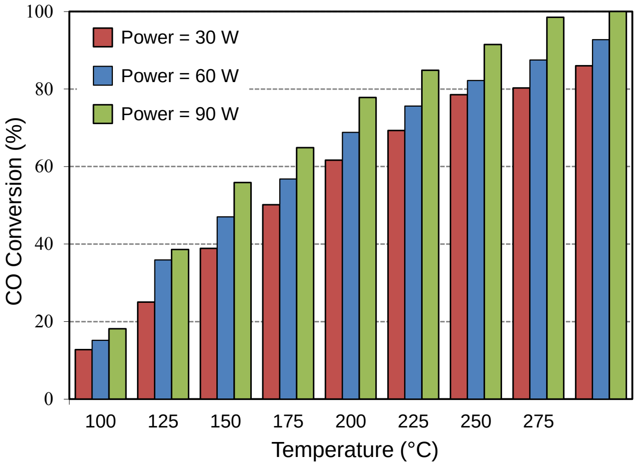

Fig. 2. Effect of Power on CO conversion over Ag(6%/SiO_2) .

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Effect of Various Ag-Content on Synthesis and Catalytic Performance of Ag/SiO_2 Nanocatalyst Used in low temperature CO Oxidation

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Carbon monoxides one of hazardous pollutants. Several methods have been suggested and used to remove this contaminant. The catalysts of this process are normally divided into five categories. Catalysts based on gold, ruthenium, platinum, palladium and other noble metal oxide. One of them is silver, which is cheaper than other metals and has a good activity in oxidation of components like methane, ethylene and NOx compounds. On the other hand Silica (SiO_2) has a high specific surface as a support in this process. In this study the effect of different amounts of silver metal loading on the silica (SiO_2) were studied. The sonochemical method was used for the synthesis of these catalysts; this method will give homogeneous distribution of the silver particles on the base. To evaluate the characteristics of the catalyst XRD, BET and FESEM analysis were used. Finally, the performance of the samples for oxidation of carbon monoxide in the process was analyzed by a laboratory system, gas chromatography with Plot U column, FID and TCD indicators. XRD analysis shows the peak intensity increase with the increase of silver content. Reactor test results showed the catalyst oxidation in the temperature range100-275°C.

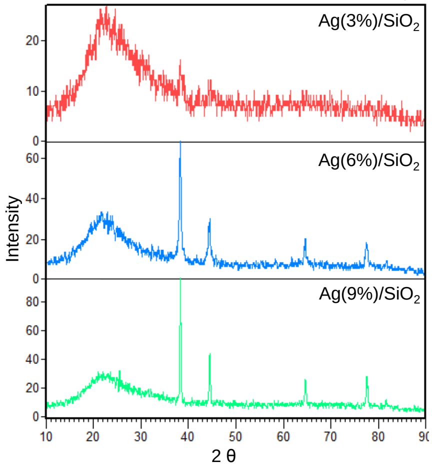

Fig. 1. XRD patterns of Ag(X%/SiO_2).

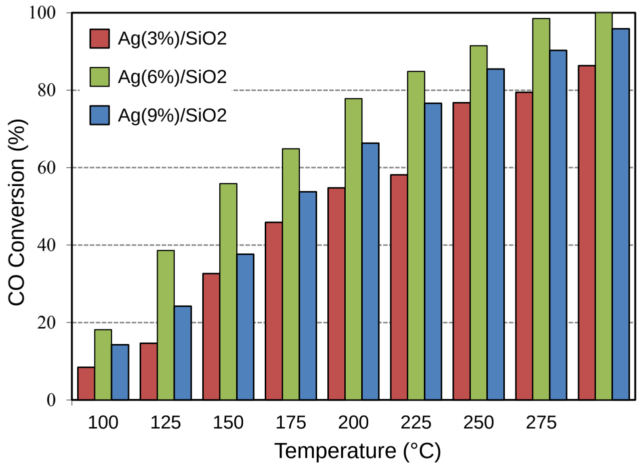

Fig. 2. Effect of Ag loading on CO conversion over Ag(X%/SiO_2)

References

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The Synthesis & Determination of Molecular Structure of Palladium(II) bisdipropylphosphate complex compound

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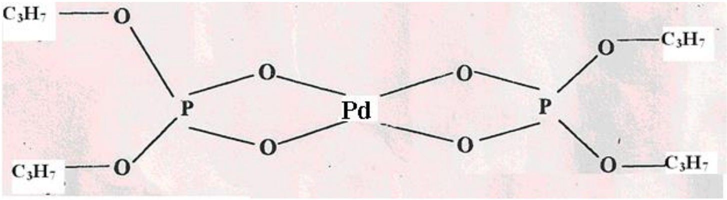
The main aim of this research, is introducing the alkyl phosphate complex compounds. This research, is on the basis of hydrolysis of trialkylphosphate salts. In this research, Palladium(II) bisdipropylphosphate complex compound prepared by direct combination of the alcoholic solution of Palladium(II)Nitrate salt with T.P.P(Tri Propyl Phosphate) as ligand and then it’s electronic spectrum was obtained in 210-892 nm. The electronic spectrum of this complex exhibits 3 main absorbance in that range(v_1, v_2, v_3). v_1, v_2 are related to d-d transitions. The first absorbance is in 13941 cm^{-1},the second is in 24427 cm^{-1} and finally the third is in 33335 cm^{-1} with high intensity which is related to charge transfer in the complex. Since the DPP(Di n-Propyl Phosphate ligand)acts as an bidentate ligand, we expect that an almond-faced deviation is done upon the molecule. [1-3] As a result of this deviation and the appeared shoulder upon the v1 band resulted of that, we encounter with a symmetry decreased phenomenon and the real symmetry of this coordination compound should be D_2h instead of D_4h. [3-5] Consequently, Palladium(II) bisdipropyl -phosphate complex has a planar structure and because of the formation of coordinative bond in the molecule plane with an almond-faced stretching encounter with a conversion in it’s point group from D_4h to D_2h and therefore, we can consider this molecular structure for this complex compound:

Pd(DPP)2



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Synthesis and characterization of novel copper complexes of bismercapto ligand

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The azoles and their derivatives have gained much attention in recent years due to their potential biological applications such as antimicrobial and anticancer activities.[1,2] Besides, their biological applications 1,2,4-triazoles and their derivatives serve as good corrosion inhibitors for copper and other metals and their alloys.[3,4] In this study , 1,4-bis((1H-1,2,4-triazol-3-yl)thio) butane was prepared via 3-mercato-1,2,4-triazole and 1,4-bromopropane in the presence of the triethyl amine as a base followed the method of refrece 5.[5] Finally , the copper salts was poured into the solution of corresponding ligand and stirred for 4h in 35°C. The green residue after evaporating the solution was dried on the desicator under the vaccum pressure. The mentioned complex have been characterized with FT-IR spectroscopy, electronic spectroscopy and cyclic voltametry , and CHN analysis.

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Copper(II) complexes of new bisindole ligand: synthesis, characterization, spectroscopic and electrochemical studies

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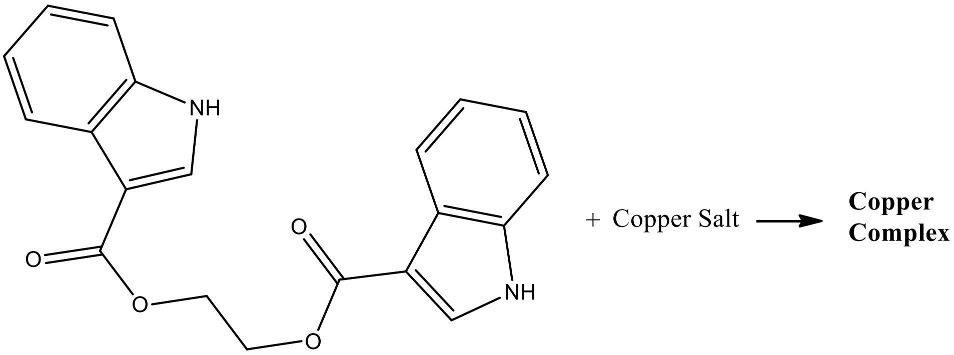
Indole acetic acid is containing proton in the aromatic ring and on carboxylic acid group, so provides different possibility of connection for produce al ot of ligand and multi dimensional polymer depends on consumer base.[1-3] In this project , the purpose ligand was prepared in direct method in dry THF solution via Indole3-acetic acid and 1,2 dibromo ethane and KOH as base followed the method of refrence 4. After the removing ligand of other solid residue via extracting by diethyl ether , the methanol solution of copper salt ($CuCl_2$, $Cu(NO_3)_2$) was droped into ligand solution and refluxed for 2h. The result dark green crystal for $CuCl_2$ and green residue for $Cu(NO_3)_2$ was characterized with FT-IR spectroscopy, electronic spectroscopy , H NMR analysis and CHN analysis.



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A Characteristic Survey upon the Organolead(IV) Carboxylates along with 4-Pipridinecarboxylic Acid

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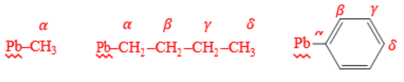
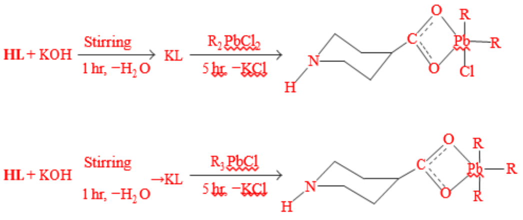
Organolead (IV) carboxylates with the general formula R_2 Pb(Cl)L [R = Me (1), n-Bu (2), Ph (3)] and R_3 PbL [R = Me (4), Ph (5)] have been synthesized by the reaction of 4-pipridinecarboxylic acid (HL) with KOH and R_2PbCl_2 (R = Me, n-Bu, Ph)/R_3 PbCl (R = Me, Ph) in methanol under stirring conditions. The metal ligand binding site, structure, and stability of complexes have been verified by FT-IR, (^{1} H, ^{13} C) NMR. The FT-IR data indicate the bidentate chelating mode of the carboxylate ligand which is also confirmed by semi empirical study. The complexes exhibited comparatively higher hemolytic activity as compared to free ligand. Organolead complexes are matter of great interest due to their structural diversities and wide range of applications in various fields. The signals in ^{1}H NMR spectroscopy were assigned by their distinct multiplicity patterns, resonance intensities, coupling constants. The number of protons found by integration of peaks in the spectra agreed well with those calculated from the expected composition.The absence of signal for carboxylic (–COOH) proton at 11.69 ppm of the free ligand in the spectra of complexes verified the coordination through deprotonated carboxylate anions. [1]



Scheme 1

Table 1: (C–Pb–C) angles (°) based on NMR parameters.

Comp. number	$^{2}J(^{207}$Pb,^{1}H) (Hz)	Angle, θ
1	91.2	136.4
4	53.3	109.9



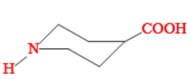
HL	R	Comp. number
	Me n-Bu Ph	**1** **2** **3**
	Me Ph	**4** **5**

Figure 1

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Inorganic complex precursor route for preparation of high-temperature Fischer-Tropsch synthesis Cu-Co nanocatalysts

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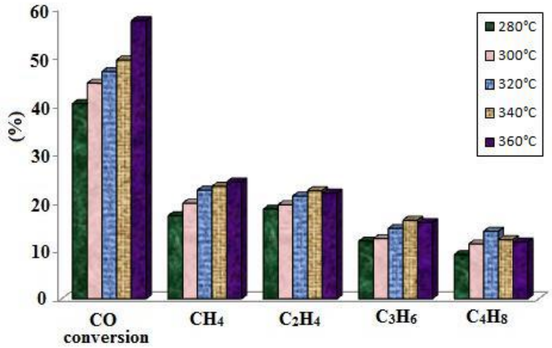
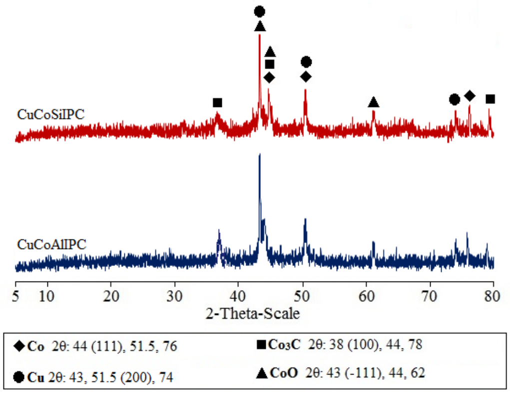
(javadfr@pgs.usb.ac.ir)

Fischer-Tropsch synthesis (FTS), i.e. the conversion of syngas (H_2+CO) to hydrocarbons, has been used since the early 20th century to produce liquid fuels and chemicals from coal, natural gas and other C-based materials. Generally, catalyst for the FTS consist of metals such as manganese, nickel, cobalt, iron and ruthenium impregnated on supports ranging from metal oxids to zeolites. Research and development of a high performance catalyst is one of the key technologies for FTS. Consequently, choosing a suitable catalyst is very important. [1,2]
In this study, the effect of preparation method on structural properties and activity of Cu-Co catalysts in the Fischer-Tropsch synthesis has been explored. Impregnation, co-precipitation and a novel method, thermal decomposition of inorganic precursor complex procedures were applied for generation of the Cu-promoted alumina- or silica-supported cobalt catalysts. The precursors and the catalysts that were obtained from calcination of them were characterized by powder X-ray diffraction, thermal gravimetric analysis, Brunauer-Emmett-Teller specific surface area measurements, scanning electron microscopy and Fourier transform infrared spectroscopy. The catalytic performance in Fischer-Tropsch synthesis was investigated upon all calcined catalysts in the temperature interval from 280 to 360°C. The Cu-Co/SiO_2 catalyst prepared by thermal decomposition of $[Cu(H_2O)_6][Co(dipic)_2].2H_2O/SiO_2$ as a precursor performed optimally for the conversion of synthesis gas to light olefins. The outcomes revealed that this novel procedure was more advantageous than impregnation and co-precipitation methods for the preparation of effective and durable cobalt catalysts for Fischer-Tropsch synthesis.





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Synthesis, characterization, DFT calculation and antibacterial activities of new nickel complexes containing novel thiourea derivatives

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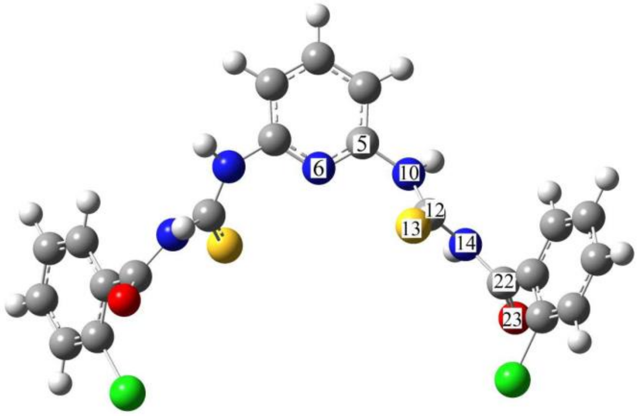
On the basis of the pharmacological studies of the compounds containing carbonyl and thiocarbonyl groups such as urea, thiourea and their related analogues, it is proposed that the thiourea derivatives and their transition metal complexes represent a wide diversity of biological functions including antibacterial, antifungal, anti-diabetic, antitubercular, anti-human immunodeficiency virus (anti-HIV), anti-Hepatitis C virus (anti-HCV), antitumor, antithyroid, anthelmintic, rodenticidal, insecticidal, herbicidal, and plant-growth regulator properties. [1]

In this study, three new thiourea ligands derived from the condensation of aroyl- and aryl-isothiocyanate derivatives with 2,6-diaminopyridine, named 1,1'-(pyridine-2,6-diyl)bis(3-(benzoyl)thiourea) (L1), 1,1'-(pyridine-2,6-diyl)bis(3-(2-chlorobenzoyl)thiourea) (L2) and 1,1'-(pyridine-2,6-diyl)bis(3-(4-chlorophenyl)thiourea) (L3) and their nickel complexes were synthesized and characterized by elemental analysis, FTIR and ^{1}H NMR and UV-visible spectroscopies. Proposed structures for free thiourea ligands and their nickel complexes were corroborated by applying geometry optimization and conformational analysis. The antibacterial properties of these compounds were investigated in vitro against standard Gram-positive and Gram-negative bacterial strains. The experiments showed that nickel complexes had the superior antibacterial activities than novel thiourea derivatives against all Gram-positive and Gram-negative bacterial strains.



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Carbon supported Au and Au-Cr catalysts for ethanol and iso propanol in fuel cell

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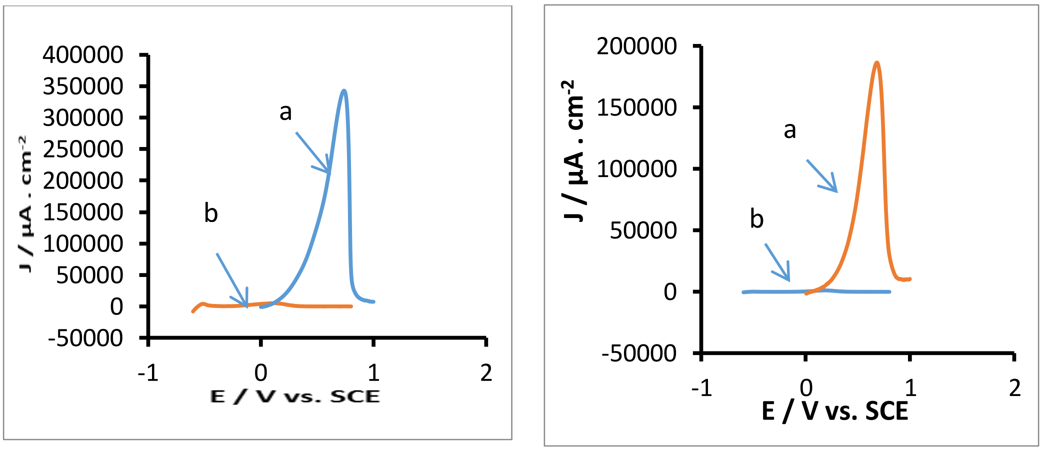
Fuel cell, especially low temperature fuel cells are clean energy devices that are expected to help address the energy and environmental problems that have become prevalent in our society. In this study carbon supported Au and Au-Cr alloys (Au: Cr atomic ratios of 0.8:0.2) were synthesized by electrochemical methods. Physical and electrochemical properties of the C/Au and C/Au/Cr catalyst were evaluated using SEM, cyclic voltammetry (CV) chronoamperomertry (CA), and LSV. Among all the Au-basted catalysts tested, C/$Au_{0.8}$-$Cr_{0.2}$ showed the highest ethanol and isopropanol oxidation activity in terms lowest onset potential and highest current density mass activity and specific activity at(0.8)V vs. SCE [Activity of ethanol and iso propanol electro oxidation is tested in alkaline medium(NaOH0.3 M) at room temperature using CV , LSV, and CA] .

The maximum power density with C/$Au_{0.8}$-$Cr_{0.2}$ catalyst Was (23×10^4 μA.cm^{-2}) at room temperature which is higher than with C/Au.



A

B

LSVgrams(A) of a) C/Au/Cr modified electrode in Presence of ethanol (5M) and b) bare Pt electrode in same condition.

LSVgrams (B) of a) C/Au/Cr modified electrode in presence of iso-propanol (5 M) and b) bare Pt electrode in same condition

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Effect of Cu Addition on Catalytic properties and Activity of Nanostructured Pd/Ceria-Clinoptilolite Catalyst Used for CO abatement from Waste Gas Stream

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Among the currently available CO removing methods, selective CO oxidation appears to be the simplest and most economic method. To date, the catalysts extensively studied in the selective CO oxidation have focused on supported noble metal catalysts.[1] In the present work, the modification effect of CuO on the catalytic properties and activity of nanostructured Pd(1wt.%)/HCl treated clinoptilolite-Ceria(30 wt.%) catalyst in CO oxidation from waste gas stream was investigated. Nanostructured Pd(1%)/CeO_2(30%)-Clinoptilolite and Pd(1%)-CuO(5%)/CeO_2(30%)-Clinoptilolite catalysts were prepared by sequentinal wet impregnation method and characterized by XRD, FESEM, BET and FTIR analysis. To chemical treatment of clinoptilolite, HCl (12 M) was used. The synthesized nanocatalysts were characterized by XRD, FESEM, BET and FTIR analysis. XRD patterns presented that acid treatment relatively destroyed clinoptilolite structure and some amorphous structure was formed. The formation of crystalline ceria was also confirmed. Copper loading significantly changed the samples morphology to the nanoscale, improving the structure of composites and distribution of noble metals. BET surface analysis showed that Cu addition to the Pd-based catalyst has no significant effect on the surface area. Catalytic performance tests of synthesized samples were performed in temperature range of 100–360 °C and gas hourly space velocity (GHSV) of the 15000 ml/gcat.h. The feed consisted of 2% CO in air balance. The results revealed that the addition of copper to Pd/CeO_2-Clinoptilolite catalyst improved the catalytic activity for CO oxidation. Complete oxidation was obtained at 200 °C over Pd-Cu/CeO_2-Clinoptilolite catalyst.

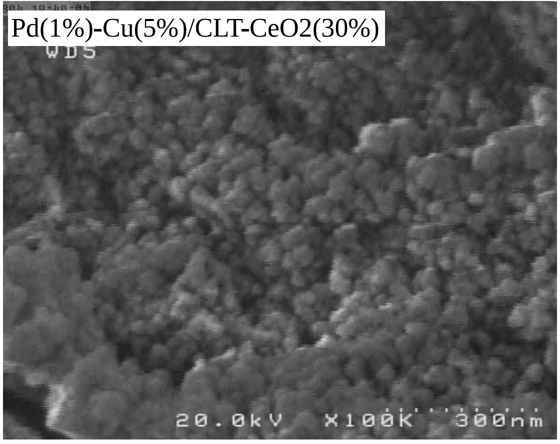

Fig. 1. FESEM image of Pd-Cu/CeO_2-Clinoptilolite.

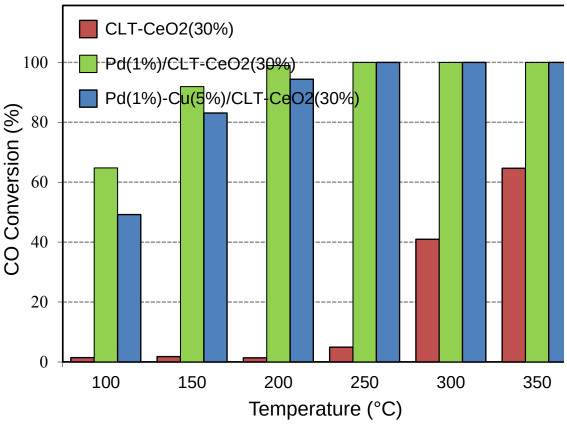

Fig. 2. Effect of Cu addition and temperature on CO conversion.

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Ultrasound-Assisted Synthesis of Nano Pillared Metal-Organic Framework with an extremely long and linear *N*-donor ligand

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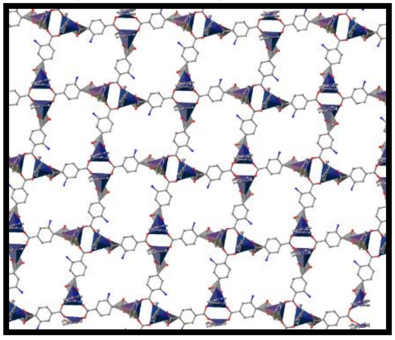
Nanoporous metal–organic frameworks (MOFs) are one type of novel crystalline materials constructed from clusters of metal ions which are connected by organic linkers.[1] During the last decade, the rational design and syntheses of novel metal-organic frameworks with multi-dimensional networks, which involves self-assembly of organic multitopic ligands with appropriate functional groups and metallic centers, with potentially useful application as gas storage, separations, catalysis, air purification, molecular sensing and removal toxic chemicals have made considerable progress in the field of coordination chemistry and crystal engineering.[2] In this poster, a simple synthetic sonochemical preparation procedure for the fabrication of nano-structures of a Cd (II)-based MOF Cd (NH_2-BDC)(4-bpmbp).DMF (1) with N-donor ligand as a pillar is presented. Structure of compound (1) was studied by different methods, such as X-ray crystallography, powder X-ray diffraction and IR spectroscopy. NH_2-BDC refer to 2-Amino benzoic acid and 4-bpmbp refer to ((N^4E,$N^{4'}$E)-N^4,$N^{4'}$-bis(pyridine-4-ylmethyene)-[1,1'-biphenyl]-4,4'-diamine) that is a nitrogen donor ligand as pillar in this framework.



A 1D view of the crystal structure of compound 1 along the *a* axis

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Synthesis and Characterization of Pd(1%)/CeO$_2$(10%)/HCl-Treated-Clinoptilolite Nanocomposite

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Zeolites are crystalline aluminosilicates renowned as promising support to stabilize transition metals with great potentials for the various aims. Clinoptilolite is a natural zeolite utilized extensively in the environmental and industrial applications. [1] It has the capacity to be modified by treatment methods such as acid leaching, ion exchange and hydrothermal treatment. [2] Three different clinoptilolite supported Pd(1%)/CeO$_2$(10%) composites were prepared by impregnation of synthesized ceria and HCl-treated zeolite; simultaneous impregnation of clinoptilolite and cerium; and impregnation of Ce^{3+} exchanged zeolite with the PdCl$_2$ solution. The structural and textural properties of these composites were characterized by N$_2$ adsorption/desorption, SEM, TEM and EDX analysis. The quantitative analysis showed that the specific surface area of the composites with synthetic CeO$_2$ using redox method was higher than the others. Nanostructured Pd/Ceria-HCl-treated-clinoptilolite composites with the highest surface area was analyzed with SEM, EDAX and TEM to show the morphological properties. The SEM images confirmed the nanoscale morphological structures brought about by acid activation and incorporation of cerium oxide in zeolite cavities. EDX analysis showed that composition of desirable component exists in the synthesized composites along with fine dispersion of metal phase on the composite. TEM image of sample (first method) also revealed the nanocomposite structure. Based on the characterization results, HCl treatment and incorporation of synthetic cerium oxide via redox method changed significantly the samples morphology to the nano scale, improving the structure of composites and distribution of noble metals to be used in the various applications.

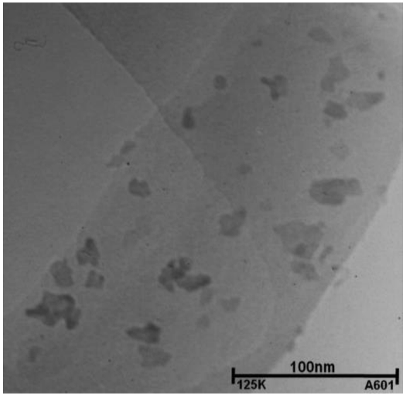
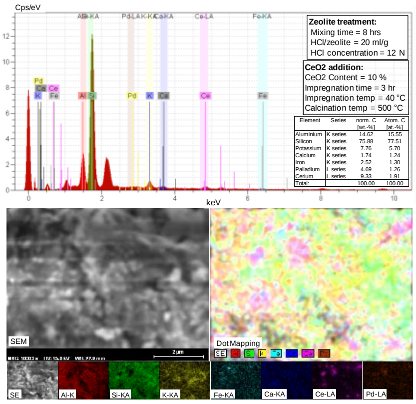


Fig. 1. TEM image of Pd(1wt%)/CeO$_2$(10%)/HCl-treated-clinoptilolite nanocomposite.



Zeolite treatment:
Mixing time = 8 hrs
HCl/zeolite = 20 ml/g
HCl concentration = 12 N

CeO2 addition:
CeO2 Content = 10 %
Impregnation time = 3 hr
Impregnation temp = 40 °C
Calcination temp = 500 °C

Element	Series	norm. C [wt.-%]	Atom. C [at.-%]
Aluminium	K series	14.62	15.55
Silicon	K series	75.88	77.51
Potassium	K series	7.76	5.70
Calcium	K series	1.74	1.24
Iron	K series	2.52	1.30
Palladium	L series	4.69	1.26
Cerium	L series	9.33	1.91
Total:		100.00	100.00

Fig. 2. DAX images of Pd(1wt%)/CeO$_2$(10%)/HCl-treated-clinoptilolite nanocomposite.

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Synthesis and Electrochemical study of Copper(II) Complex of an Aminophenol Ligand as a Model for Galactose Oxidase Metalloenzyme Active Site and its application in Aerial Alcohol Oxidation

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Galactose oxidase (GOase) is a metalloenzyme containing single copper at the active site, consists of donors from the side-chains of amino acids such as histidine and tyrosine holding it. This enzyme catalyzes the oxidation of primary alcohols through the formation of an active form (Cu^{2+}-Tyr$^{\bullet}$) include tyrosyl radical.[1,2] In the present work, we have synthesized and characterized a copper(II) complex of 6,6'-(propane-1,3-diylbis(azanediyl))bis(2,4-di-tert-butylphenol) due to its structural similarity to galactose oxidase active site. The electrochemical oxidation of [Cu(L^{DAP})X] complexes (X= OAc, Cl) show that the oxidation process is ligand-centered due to the oxidation of phenolate to the phenoxyl radicals. The [Cu(L^{DAP})X] complex also undergoes an electrochemical metal-centered reduction. The difference in oxidation and reduction peaks considered as stability of the mentioned complex which has been estimated in the presence of various coordinating ligands such as acetate and chloride. Also a highly efficientand eco-friendly oxidation of alcohol to aldehyde with air as oxidant and [Cu(L^{DAP})X] complex as catalyst was performed.

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Preparation of support for propane dehydrogenation catalyst in bench scale

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Dehydrogenation is one of the most important methodsfor olefins production. Synthesis of these substances has special importance in order to increase of request and biological effects. Most of the dehydrogenation reactions perform Pt or Cr over the gamma alumina supports.[1,2] In this research, the preparation of gamma alumina supportthat is used for propane dehydrogenation (PDH) processes, was done in bench scale under optimized conditions. Oil drop method and sol-gel technique were employedto produce gamma alumina particles. Effective parameters comprising pH, temperature, concentration of reactants, aging time in base solutions were optimized. The process starts with preparation of the aqueous sol of gelatinous boehmite then particles dropped into a suitable oiland consequently were firmed in ammonia solutions with certain concentrations . There after, it was dried in 100-130 ^{o}C and finally were calcinedat150-750 ^{o}C. The short reaction time, perfect physicochemical characters of product in aging by basic solutions at least time, using of oil with perfect chemical and biological specifications conducted to the production of gamma alumina support with crush strength of 80-140N. The XRD results validated that the synthesized spherical particles possess crystallinity of γ-alumina phase. Also the N_2 adsorption-desorption isotherm and BJH pore size distribution of particles elucidated the existence of mesoporous characteristic.The final γ-alumina particles had the following specifications; diameter of 2 mm , pore volumeof 0.55-0.7 cm/g, surface area between 160-250 m^2/g and mean pore diameter of80-200 A^o.

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Preparation of support for LAB (Linear Alkyl Benzene) processcatalyst in bench scale

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Gamma alumina has been regarded as one of the most important supports for application in catalytic processes used in refining, petrochemical and gas industries. This support is preferred high surface area, suitable thermal stability and high crush strength either in moving or fluidized bed reactors. Technologically, the preparation of these supports has potential to be developed and optimized.[1, 2] In this research, bench scale synthesis of gamma alumina supports used in LAB (Linear Alkyl Benzene) processes was investigated and the production conditions were optimized. Oil drop method and sol-gel technique were employed to produce gamma alumina particles. Effective parameters such as pH, temperature, concentration of reactants and aging time in base solutions were optimized. The process, which starts with aqueous sol of gelatinous boehmite, involves droplet formation,gelation in suitable oil, conditioning in ammonia solutions with perfect concentrations and drying and calcining in optimized temperature. The XRD and XRF results revealed that the synthesized spherical particles possess crystallinity of γ-alumina phase. Also, the N_2 adsorption-desorption isotherm and BJH pore size distribution of particles elucidated the existence of mesoporous characteristics.The final γ-alumina particles were 1.8-2 mm with crush strength of 12-35 N, pore volume of 0.58-0.8 cm/g, surface area between 125-200 m^2/g and mean pore diameter ranging 80-200A^o.

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Numerical Analysis of municipal solid waste LeachateTabriz using biological products EMRO and final purification using MBR

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Rapid population growth, industrial development, increasing consumerism and technological progress in human societies has led to a proliferation of urban waste. Communities and disposal of such cases in most countries, especially developing countries, technology is not so advanced, but the municipal waste management Tabriz to try to understand the basic steps to improve and progress and by creating landfill engineering and biological treatment plant to improve environmental issues the MBR process is faster in Tabriz. The aim of this study was to investigate the effect of slope COD reduction by biological products is EMRO.

This research using biological products EMRO has been done to reduce BOD and COD. Leachate containing high levels of inorganic and organic materials and heavy metals harmful to the environment. This is a fundamental research-based practical experience in laboratory scale and pilot plant was created using landfill leachate was conducted in the fall of 1393 on. The experimental concentrations of sampling and sampling intervals and a 1/1000 and 10/1000 as-is. The samples tested leachate from landfill leachate ponds collect and store harvested and leachate flow rate between 0.2 - 0.4 liters per second to 200 cubic meters of aerated lagoons paired entered in throughput. In this study, leachate analysis software Design Expert analysis of the leachate removal and removal of trade by product EMRO is studied.

The COD and BOD 16000 raw 33200 ppm after the addition of 1/1000 EMRO 17000 and 34000 BOD and COD reached the leachate were faced with an increase in both. With the addition of the 15000 and 30800 Rsydh and 10/1000 both factors that reduce BOD and COD were 2000 and 3200 mg Results show a negative effect on the reduction of COD slope leachate treatment system is the use of the product EMRO to use.

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