Synthesis of $Mg(OH)_2$@Reduced graphene oxide nanocomposite and application for simultaneous micro solid phase extraction of uranium and thorium using micropipette tip syringe system

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Recently, nanoscale magnesium hydroxide ($Mg(OH)_2$) has aroused widespread attention because of low-cost, environmental friendly, recyclable, large specific surface area, and extraction ability. It has been shown that $Mg(OH)_2$ exhibits a hopeful prospect in removal of heavy metals, acid wastewater treatment, and decoloration of printing and dyeing wastewater [1].

Uranium and thorium are vital elements not only in industrial application but also in environmental and energy problems. However both of the metal ions are well-known to cause serious toxicological effects in human and their compounds are potential occupational carcinogens [2]. Based on the facts, highly selective and sensitive method for determination of uranium and thorium is blooming.

In this work, $Mg(OH)_2$@Reduced graphene oxide nanocomposite was synthesized using homogeneous precipitation and then consequent reduction with hydrazine hydrate and refluxing. This nanocomposite was characterized by using Fourier transform-infrared spectroscopy, X-ray diffraction and transmission electron microscopy. This nanocomposite exhibit good selectivity to uranium and thorium ions and applied for simultaneous micro solid phase extraction (µSPE) of these ions using micropipette tip syringe system. The effective parameters on µSPE were optimized using central composite design. The developed technique was applied to the determination of uranium and thorium in environmental water samples with satisfactory results.

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Novel *p*−*n* heterojunction of Ag/HAp/g-C_3N_4 photocatalyst: study the efficient photocatalystic performance for phenol degradation

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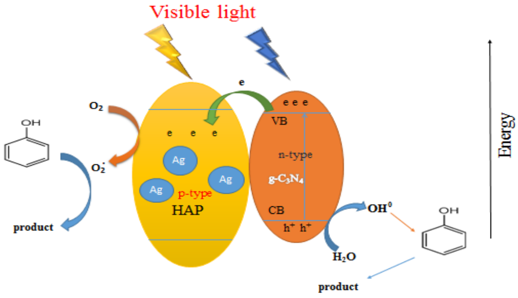
Abstract

3D heterojunction nano-structure of *p*-Ag/HAp/*n*-g-C_3N_4 photocatalyst was successfully synthesized by hydrothermally addition of *n*-type g-C_3N_4 on *p*-type HAp and in following addition of Ag^+ under visible light illumination procedure, which showed highest photocatalytic activity comparing with Ag/HAp and g-C_3N_4 components for visible-light degradation of phenol. The heterojunctions with facilitating the charge transfer along with increasing the lifetime of charge carriers, enhance the photocatalytic efficiency [1]. Phenol and its derivatives are known as hazardous environmental pollutants that are found in many industrial wastewater [2]. The structure and morphology of the synthesized *p*-Ag/HAp/*n*-g-C_3N_4 as a novel nano-heterojunction compound were studied by X−ray diffraction (XRD), fourier infrared spectroscopy (FTIR), elemental analysis of energy dispersion spectroscopy (EDS), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). The photocatalytic mechanism influenced by $O_2^{\bullet}$ and $OH^{\bullet}$ species that schematically has been shown in below. The obtained experimental results indicate the high photocatalytic performance of this new *p*-Ag/HAp/*n*-g-C_3N_4 nanocomposite for the removal of phenol contamination.



Proposed mechanism of phenol degradation by p-Ag/HAp/n-g-C_3N_4.

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Enhanced photocatalytic performance over new nano structure of HAp/g-C_3N_4: Methylene Blue photodegradation study

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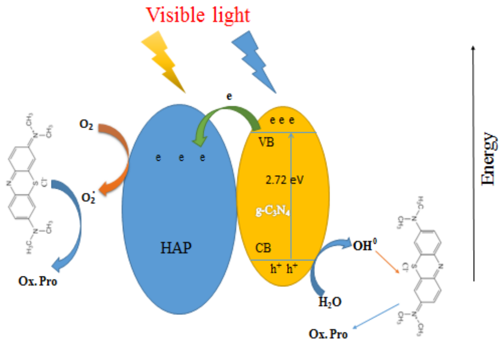
Abstract

In the present work, the new nanoparticles of HAp/g−C_3N_4 was synthesized by an easy sol−gel method. Visible light degradation of methylene blue (MB) on to HAp/g−C_3N_4 studied in aqueous solution at room temperature. For achievement to high photocatalytic efficiency, graphite carbon nitride (g−C_3N_4) as new heterojunction component along with hydroxyapatite (HAp) was selected. The heterojunction structures improve the catalytic activity with increasing the charge carrier of transferred ones between the components [1]. Influence of various operational parameters such as *p*H, composite dose, and degradation time for photocatalytic process were examined. New heterojunction structure of photocatalysts such as g−C_3N_4 composites were used for environmental remediation [2]. Moreover, the related mechanism of hole-electron pairs generation induced by HAp/g−C_3N_4 heterojunction (schematically illustrated below) were fully discussed. The structure of nanocomposite were studied by X-ray diffraction (XRD), FTIR spectroscopy, elemental analysis of energy dispersion spectroscopy (EDS), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). It can be concluded that the new synthesized nanocomposite of HAP/g−C_3N_4 show remarkable photocatalytic activity about degradation of MB pollutant.



Proposed mechanism of MB visible light degradation by HAp/g-C_3N_4 nanocomposite.

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Synthesis and Characterization of the new polyaniline-sulfonated/polyaniline nanocomposite

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Polyaniline (PANI) was another extensively studied conducting polymer which has high stability, good conductivity and reversible redox property. Sulfonated polyaniline (SPANI) has sulfonic groups on its backbones, so it is soluble in water [1]. SPANI has been used as the dopant for PANI and the resulting composite exhibited improved conductivity expansions [2, 3]. In this work novel nanocomposites comprising PANI/PMAS are prepared by the chemical oxidation of aniline in the presence of PMAS, and their physical properties characterized. The nanocomposites are found to possess novel properties, with conductivities higher than when an insulating or nonelectroactive material is used as the molecular dopant. UV-Visible spectroscopy and FTIR spectroscopy were used to investigate the analytical and functional groups present in the synthesized nanocomposites. The UV-vis spectrum of PANI/PMAS nanocomposite displayed the characteristic absorption peak of π-π* transition of the benzenoid ring at 348 nm. The oxidation state of PANI/PMAS nanocomposite was identified with FT-IR spectroscopy by comparing the two bands at 1580 (ring stretching in quinoid unit) and 1499 cm^{-1} (ring stretching in bezenoid unit).

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Experimental and Theoretical Investigations of Electronic Structure, Electrochemical Properties and Antibacterial Activity of $\beta{-}Ag_2MoO_4$

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In this investigation, a combined theoretical and experimental study on the electronic structure of (β-Ag_2MoO_4) nanocrystals has been employed.β-Ag_2MoO_4 sample were obtained by hydrothermal technique. Crystals were structurally characterized by XRD pattern and Rietveld refinement and the results showed the spinel-type cubic structure of β-Ag_2MoO_4 nanocrystals. The optical property of β-Ag_2MoO_4 was investigated by UV-Visible diffuse reflectance spectroscopy within the range of 250-850 nm and obtained an optical band gap value of 3.24 eV. TEM was used to study the morphological aspects of the prepared sample. In addition, the electronic band structure and density of state (DOS) of β-Ag_2MoO_4 were studied by *Quantum Espresso* package [1] based on density functional theory (DFT). The calculated band structure revealed an indirect band gap of approximately 3.41 eV. According to DOS results, the energy states of valence band are basically composed of Ag 4d ($4d_{z^2} + 4d_{x^2-y^2}$; $4d_{xz} + 4d_{yz} + 4d_{xy}$) orbitals and O 2p ($2p_x + 2p_y + 2p_z$) orbitals. However, the conduction band composition is predominantly constituted by hybridization between Mo 4d and O 2p orbitals.

Furthermore, electrochemical water splitting[2] and CO_2 reduction[3] were investigated. Antibacterial activity of β-Ag_2MoO_4 against *Escherichia coli* as a model Gram-negative bacteria was demonstrated. Finally, photocatalytic property of synthesized sample demonstrated good catalytic performance for degradation of methylene blue under UV–light.

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

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Abstract

In recent years, the Fischer–Tropsch synthesis (FTS) has received considerable attention from academic institutions and governments alike, due to environmental contamination, rapidly rising price of crude oil and subtractive oil reserves [1-3]. The FTS is a viable route for the production of clean fuels from biomass-derived syngas, natural gas, or coal. In this process, highly important factor is a catalyst, which is selected based on the key role in product distribution. The silica supported Cu catalyst synthesized by thermal decomposition of inorganic precursor was evaluated for Fischer–Tropsch synthesis (FTS); the structural properties and performance of the catalyst was compared to those of samples constructed via impregnation method. The results revealed that the synthesized catalyst have higher catalytic activity comparison to it prepared via the conventional impregnation method. Activity of the catalyst in FTS was investigated at 280-400 °C with H_2/CO ratio of 2 and specified that the fabricated catalysts are more active than impregnation reference sample.

Keywords: Inorganic precursor, Impregnation, Fischer-Tropsch synthesis, Synthesis route.

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Antioxidant activity, β-LG and HSA interactions of a novel tetradentate Schiff base Pd(II) complex

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The drug-protein interaction also has a prevailing contribution to drug temperament and effectiveness as the bound fraction of drug is a depository while the free fraction of drug exhibits pharmacological properties. therefore, It is essential to investigate the interactions between drugs and a carrier protein in order to specify the pharmacology and pharmacodynamics of drugs (1, 2). Pd(II) Schiff base complex by 3,4-diaminobenzophenone and diacetyl monoxime was synthesized. This complex was characterized by FT-IR, ^1H NMR, UV–Vis spectroscopies and molar conductance. This complex was studied for in vitro antioxidant activity as radical scavengers. Antioxidant activity of Pd complex was obtained $IC_{50} = 55$ mg L^{-1}. Protein interaction (Human serum albumin, HSA, and β-lactoglobulin, β-LG) were done. Our results show that this complex quenched the fluorescence of both protein by static mechanism and Pd complex with HSA showed a stronger binding ability than that of β-LG. Thermodynamic studies showed that Hydrogen bonds and Van der Waals forces in both examined systems were the main stabilizing forces in the development of drug-protein complex.
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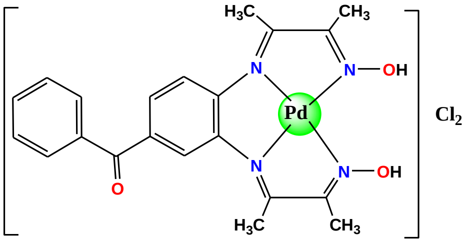
.**Key words**: Antioxidant, β-LG; HSA.



[PdSB]Cl$_2$

Fig. 1 Molecular structure of complex.

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Preparation and Characterization of New Carboxamide Ligand and its Metal Complexes

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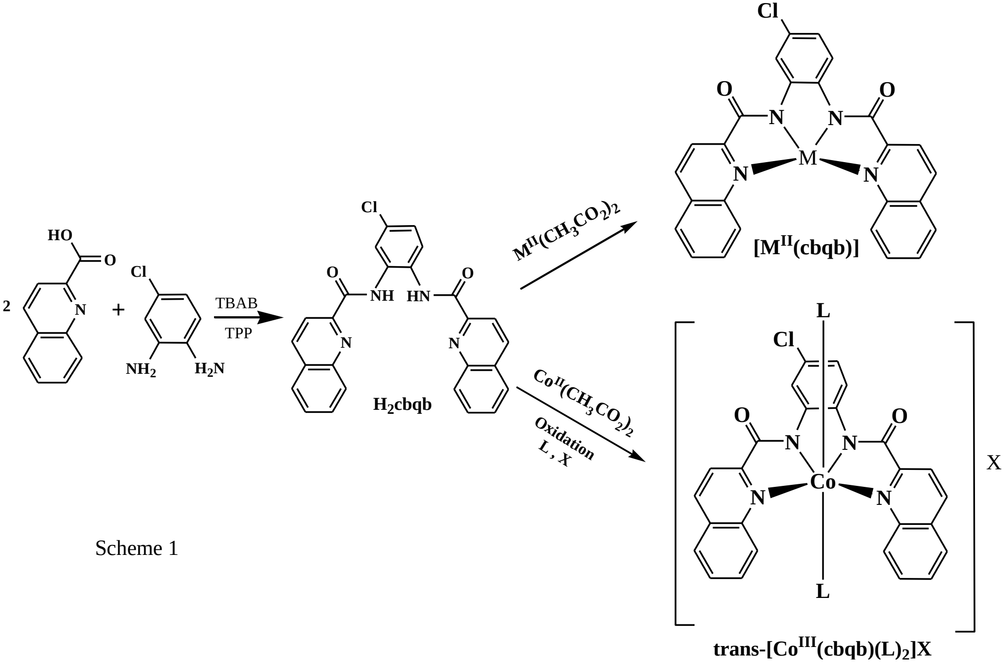
The design of new peptide ligands containing the carboxamide [-C(O)NH-] group has been continued in recent years and chemists have paid special attention to synthesis of carboxamide complexes of biological importance and production of therapeutic drugs [1]. The deprotonated amid is a strong σ-donor capable of stabilizing early as well as late metal ions in high oxidation states [2]. Green chemistry searches for alternative, environmentally friendly reaction media and strives to increase the reaction rate and efficiency. One of the key is the replacement of hazardous solvents with Ionic liquids [3].

As part of our aim in the transition metal chemistry of dianionic ligands, we describe the synthesis and spectroscopic characterization a new ligand [H_2cbqb = N,N′- bis(quinoline- 2–carboxamido) -4- chlorobenzene], [M^{II}cbqb] compounds, M^{II} = Ni, Co, Cu and a group of diaxially ligated complexes with $cbqb^{2-}$ as equatorial ligand [Co^{III}(cbqb)$(L)_2$]X, L = CN^-, N_3^- ,piperidine, morpholine, benzylamine, aniline, pyridine and X= ClO_4^- and $(n\text{-}Bu)_4N^+$.



Scheme 1

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Quantum chemical study of some candidate for molecular photo switches

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In general, a molecule that can be reversibly shifted between two or more stable states named molecular switching compound. The molecules may be shifted between the states in response to environmental stimuli, such as changes in pH, light, temperature, an electrical current, microenvironment, or in the presence of a compound. The oldest forms of synthetic molecular switches are pH indicators, which display distinct colors as a function of pH. Currently synthetic molecular switches are of interest in the field of nanotechnology for application in molecular computers. Molecular switches are also important to in biology because many biological functions are based on it. They are also one of the simplest examples of machines. Up to now, almost all of the organic molecules investigated for the second-order nonlinear optical materials contain electron-donating and withdrawing groups being linking through an intervening π-backbone has been calculated by the Restricted Density Functional Theory (DFT) methods with the basis set B3LYP/6-311G**[1-2]. The major purpose of this work is to calculate the molecular geometry of above compound and to theoretically study structural and electrical properties. Geometry optimization and calculation of the structural and electronic properties of (E)-N-(2-methyl-5-nitrobenzylidene)-3-chloropropan-1-amine compound have been carried out at DFT/B3LYP level of theory with 6-31G** basis set using Gaussian 03 program package [3]. All geometry parameters like bond lengths, bond angles, dipolmoment, energy of HOMO and LUMO levels, gap between the HOMO and LUMO levels, heat of formation and hyperpolarazibilty data were obtained.

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Synthesis, characterization and study of the relationship between the electronic property and corrosion inhibition activities of some compounds

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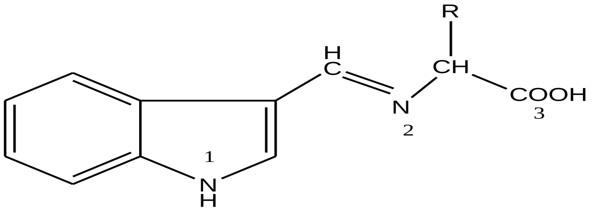
Quantum chemical calculations could provide valuable information about molecular properties such as geometry, stability, atomic charge distribution, determination of active sites of compounds and etc. In this study we were reported some theoretical data for three derivatives of 1H-indole-3-carboxaldehyde with Glycine, Alanine and Valine amino acids Figure 1. All of the calculations were performed using the hybrid density functional theory (DFT) method B3LYP, as implemented in *Gaussian 03*, and geometries were optimized at the B3LYP/6-31G(d,p) level. Single-point calculations at the B3LYP/6-311+G (2d,2p) level were performed on the optimized geometries to obtain more accurate energies[1,2]. Our calculations shows the coordination sites of these compounds are N(1), N(2) and O (3) atoms and R group has a major role on the charge density of these sits and molecular orbital levels of all compounds. We have reported herein a lot of correlations between the electronic property and the ion selectivity of these compounds.



R=H, CH_3, $CH(CH_3)_2$

Fig. 1. The structure of 1H-indole-3-carboxaldehyde derivatives

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Synthesis of binary nanoparticle of Ni-Zn from their inorganic complex as precursor and studies of its catalytic properties in the preparation of tetrahydrobenzo [*b*] pyran

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Abstract

Multi nuclear transition metal complexes have become a central theme of current research because of their potential properties. Synthesis and characterization of polynuclear iron, cobalt, nickel, copper and zinc complexes are reported by many researchers. [1-2]

In this report, first we synthesized a new precursor binuclear complex of Zn and Ni of formula [[Ni (phen)(L)(H2O)(μ-SCN)Zn(phen)(L')(OH_2)]**(1)** that phen=1-10 phenanthroline, L=Maleate, L'= 2-aminobenzoate and then we report facile synthesis of two-phase nanoparticle under thermal decomposition. This complex**(1)** has been characterized using FT-IR, UV–Vis, Conductivity and Cyclic voltammetry (CV) techniques. Characterization of nano compound from complex (1) was carried out by scanning electron microscopy (SEM), X-ray powder diffraction (XRD) and Fourier transform infrared (FT-IR) spectroscopy. The X-ray diffraction pattern at room temperature revealed, highly pure system Ni-Zn-O with monoclinic structure**.** Finally nanoparticle has been used as a catalyst in the preparation of tetrahydrobenzo [*b*] pyran. The FT-IR results showed that the ligands coordinate to metal center as a bidentate ligands by nitrogen and oxygen atoms.

Key words: binuclear complex, Cyclic voltammetry, scanning electron microscopy

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Synthesis of Bis(N,N′ -di(5 -bromosalicylidene)-4,5-dimethyl -1,2 -phenylenediaminato) Zirconium(IV) Complexe And Study of Antibacterial Activity

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Schiff bases and their complexes are flexible compounds synthesized from the condensation of an amino compound with carbonyl compounds and extensively used for a broad range of biological activities including antibacterial, antifungal, antiviral, antimalarial, ant proliferative, anti-inflammatory, anticancer, anti-HIV properties [1]. The biological activity is usually increased by complexation therefore to understand the properties of both ligand and metal can lead to the synthesis of highly active compounds [2].

In this study the title complex zirconium (IV) has been successfully prepared by heating a 1:2 mole ratio of $[Zr(acac)_4]$ and the free ligand in absolute in methanol. It is mononuclear and eight-coordinate in the solid state. The new complexe have been characterized using FT-IR, ^{1}H NMR, ^{13}C{^{1}H} NMR spectroscopic techniques and elemental analyses (CHN).

Then, the synthesized Schiff base complexe and free ligand were screened for their biological activity against bacterial species, A Gram-positive bacteria (*Staphylococcus aureus*) and a Gram-negative bacteria (*Escherichia coli*) by the disk diffusion method. The antibacterial tests used 64 μg/mL concentrations of the test compounds dissolved in DMSO. Bacteria culture Petri dishes treated with the test compounds were incubated for 24 h at 37° C. The antibacterial activity were determined by evaluating the inhibition zone (mm), MIC and MBC. MIC is the lowest concentration of an antimicrobial compound that inhibits the noticeable growth of microorganisms at 37° C after overnight incubation. The MIC of the test compounds were assayed against bacterial strains through a broth dilution method, using test compound concentrations from 0.128 to 0.0005 mg/ml in DMSO. The in vitro biological screening experiments showed higher activities for the complexe compared to the free Schiff base.

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A Cobalt-Zinc heterometallic coordination polymer

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The connection of metal–organic coordination polymers based on transition metals and multifunctional bridging ligands has proven to be a promising field due to their intriguing topologies and potential functions in material chemistry [1,2]. Over the past decade, different classes of coordination polymers have been success fully designed and synthesized. Recently, bridging ligands containing N- or/and O-donor s, for example, polycarboxylate aromatic anions including benzene-1, 2-dicarboxylate, benzene-1,3-di carboxylate, benzene-1, 4-dicarboxylate, benzene-1,2,3-tri carboxylate, benzene-1, 2,4-tri carboxylate, benzene-1,3,5-tricarboxylate have been widely used for the syntheses of coordination polymers. In this research, A new metal-organic framework formulated as $[Co_{0.67}Zn_{0.83}(btc)(H_2O)_6]$ (1) was prepared and characterized by elemental analysis, and FT-IR spectroscopy. The single crystal analysis was used for determination of its structure. The structure was solved by direct methods with the Superflip program and refined by full-matrix least squares on F^2 using the program Jana 2006. All hydrogen atoms were discernible in difference Fourier maps and could be refined to reasonable geometry. The complex (1) is crystallized in the monoclinic crystal system with *I2* space group. Crystal data for complex (1): a= 6.4930 (1), b= 12.9426 (4), c= 16.1435 (5) [Å], $\beta = 89.951(2)$[°], Z= 6.

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Synthesis and characterization of nanocomplex (maleic)$_2$ Zn(μ-isophetalic)Ce(maleic)$_2$

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In the present research study, the reaction between 1 mmol cerium (III) nitrate with 4 mmol maleic acid, 1 mmol zinc nitrate salt and 1 mmol isophthaltic acid. The reaction was carried out during 48 hours of reflux at 50° C temperature. The same reaction also was conducted in the ultrasonic environment for comparison purposes (complex 2). The resulting product was identified and studied using UV-Vis and FT-IR methods. Infrared analysis of the intended complex in the carbonyl (C = O) of Maleic acid with a sharp peak was seen in the 1691 cm^{-1} area. A band was also seen in the 1601 cm^{-1} area that corresponds to the C = C bonds of the loop. Also, 1596 cm^{-1} and 1419 cm^{-1} regions belonged to the loop. Figure 1 shows the sharp peak in 729 and 621 cm^{-1} regions, which belonged to metal oxides. Electronic spectrum (UV-Vis) complex was recorded at room temperature. In the ultraviolet region, the absorption bands appeared in 215, 224, 287 and 249 nm belonged to the transitions between $\pi \rightarrow \pi^*$ ligand and the intended $n \rightarrow \pi^*$ ligand. Also, there was no $d \rightarrow d$ transition in the vis region due to the spin arrangement. Further, the results of UV-Vis and FT-IR were consistent with the results recorded using the ultrasonic method. The morphology of complexes synthesized by sonochemistry characterized by scanning electron microscopy (SEM). Images show that, the particles size of complex was prepared by sonochemical method about 80 nm.

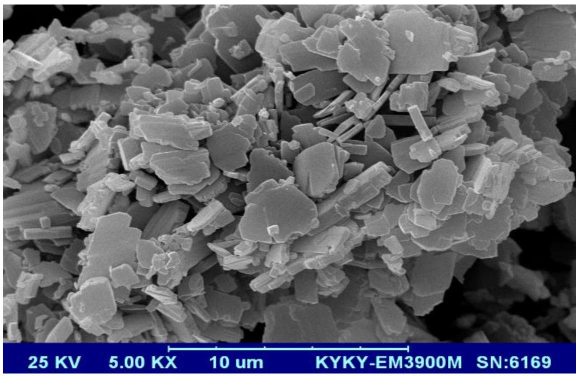

Figure1. SEM of nanocomplex

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Synthesis and characterization of nanoparticle ($CeCuO_3$) using precursor { [Ce (2amb)$_2$(H_2O)(μ-iso phtal)Cu (2- amb)$_2$(H_2O) }

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In this investigation, we report facile synthesis of transition metal oxide ($CeCuO_3$) as nanoparticles. The process contained two steps: first preparation of complex {[Ce (2amb)$_2$(H_2O)(μ-iso phtal)Cu (2-amb)$_2$(H_2O) }**(1)** where 2-Amino=2-Amino banzuic asid and Isophtal= Isophtalic acid. Then the precursors were calcination. In first step, complex **(1)** synthesized using a mix of ethanolic solution of $Ce(NO_3)_3$(1mmol), and 2-Amino (4mmol) and $CuCl_2$(1mmol) , iso phtal(1 mmol). Then desired product was collected by suction filtration and characterized using Fourier transform infrared (FT-IR), Ultra Violet-Visible (UV-vis) spectroscopy and cyclic voltammetry (CV) method for electrochemical studies. The next step to prepare nanoparticles, amount of compound **(1)** was placed in a furnace with a temperature of 800. After calcination of title compound, this sample studied using XRD (X-ray Diffraction) and SEM (Scanning Electron Microscopy) techniques. Particle size for several diffraction and average crystallite size were measured from the XRD data based on Debye- Scherrer¼equation. The X-ray diffraction patterns at room temperature revealed that, highly pure and crystallized Ce-Cu nanoparticles as $CeCuO_3$ formula with Hexagonal phases in 800°C, with an average particle size of about less than 100nm for both nano-oxide. SEM figure show that the particles have same morphology with a uniform porous surface [1].

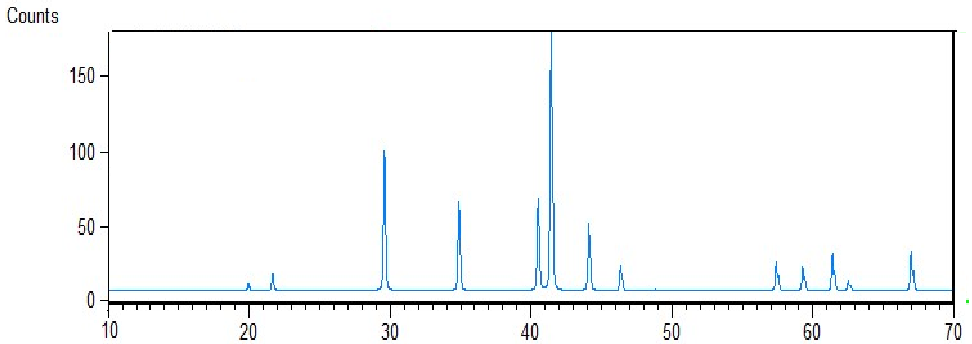

Figure1.XRD of nanoparticle $CeCuO_3$

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The effects of solvent and ultrasonic irradiation in synthesis of novel supramolecular compound

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coordination compounds are very interesting because of their interesting properties such as: sensing, catalysis, separation, gas storage, lasers, transistors [1-3]. One cadmium(II) zero-dimensional supra molecule compound $[Cd(L)_2(I)_2]$ **(1)**, {L= 2-picolyl amin} has been synthesized by branch tube and sonochemical irradiation methods. In order to study the effects of solvent and time of reaction on the formation of $[Cd(L)_2(I)_2]$ **(1)** supra molecule compound, some experiments were designed and four samples of **1** were synthesized by sonochemical process. Less time of reaction resulted in the formation of smaller particles with mix morphologies. These micro and nano crystals were characterized by IR spectroscopy, X-ray powder diffraction (XRD) and Scanning Electron Microscopy (SEM).

Keywords: *Morphology, Sonochemical process., branch tube method.*

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Two new VOL(acac) and ZnL(OAC) Schiff base complexes containing ionic Schiff base ligand: synthesis and characterization

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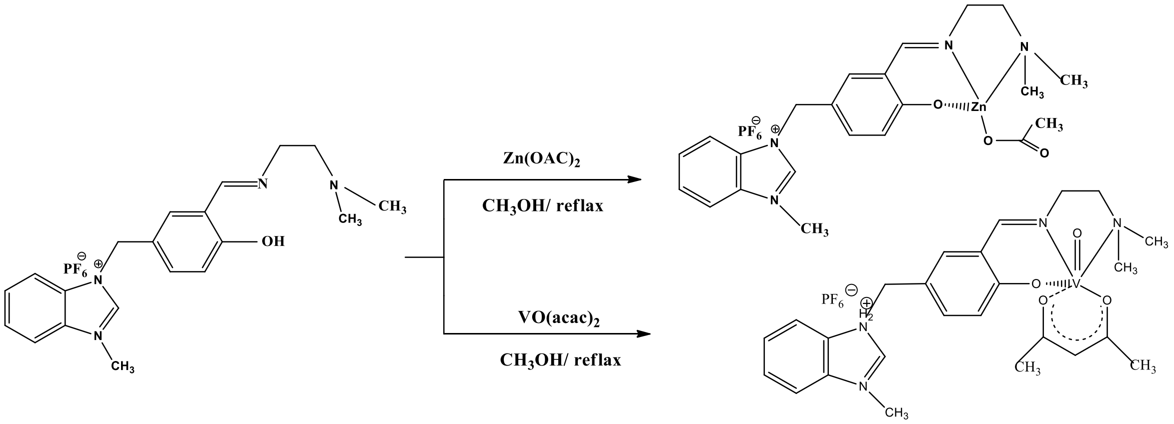
Azomethine compounds (mostly known as Schiff bases chelating ligands) played central role in metal coordination chemistry [1]. They bind to almost all of the metal ions to give complexes with suitable properties for theoretical studies and/or practical applications [2]. Moreover, water-soluble ligands and their metal complexes containing ionic fragment can be important because of their potential applications in biology. The synthesis of these kinds of complexes are very rare in literature. Thus in this study we report the synthesis and characterization of two new ionic metal complexes of VO^{2+} and Zn^{2+} containing the Schiff base ligand of 5-methyl 1-methy benzimidazolium salicylimine ethylene N, N- dimethyl amine-chloride. By reaction of the N-methyl benzimidazole and chloromethyl silicylaldehyde and next by KPF_6, the benzimidazolium methyl silicylaldehyde hexafluorophosphate was synthesized. It was reacted by N, N-dimethyl ethylene diamine to synthesis of three dentate Schiff base ligand (L). The reaction of L with $VO(acac)_2$ and $ZnCl_2$ resulted to synthesis of the VOL(acac) and ZnL(OAC). The Schiff base ligand and related complexes were characterized *via* different analytical and spectral methods (CHN, FT-IR, UV-vis, ^{1}H-NMR and ^{13}C-NMR).



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Formaldehyde adsorption on Ni doped single-walled carbon nanotube; a DFT study

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The structural and electronic properties of Ni doped single-walled carbon nanotubes indicate benefits as new composites that qualify a wide variety of applications as nanostorage devices, nanosensors and nanoplatform in biosensors. Formaldehyde (FO) is the most toxic gas which is being considered as a serious interior pollutant. It wildly employs in decorative materials and some productive while causes respiratory irritation, watery eyes, pulmonary edema, dermatitis and asthma [1]. Due to weak van der Waals interaction of gases with CNT, they are not able to detect a large variety of molecules, such as poisonous gases (e.g. CO), H_2, H_2O molecules and biomolecules [2]. In this work, within density functional theory (DFT) framework, adsorption of formaldehyde by Ni-loaded on SWCNT surface is studied as a novel chemical sensor for detecting the FO gas. The adsorption processes of the FO molecule on pristine and Ni loaded single-walled nanotube are investigated by using density functional theory (DFT), implementing the Gaussian 09 software. It was found that the FO molecule was interacted with the Ni/SWCNT, and as shown in Fig1 the most stable adsorption configuration was that in which the O atom would prefer to be attached to the Ni atom of Ni/SWCNT with electronic charge transfer from FO to the nanotube. The adsorption energy for the most stable configuration of adsorbed FO on Ni/SWCNT was -1.45 eV. Moreover, the strong binding energies and short binding distances were consistent with the larger charge transfer between the FO molecule and the Ni/SWCNT system. This phenomenon dramatically would increase the electrical conductivity of the nanotube which suggests the potential sensor of Ni/SWCNT for the FO gaseous molecule detection.

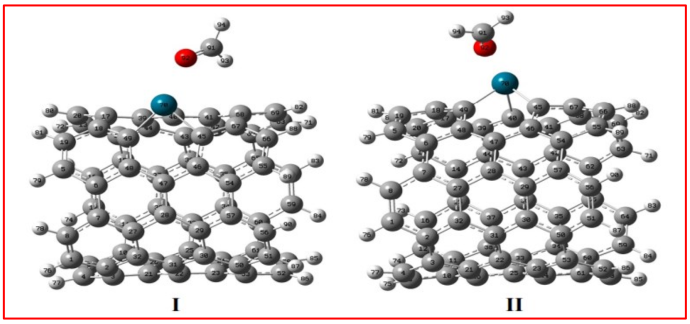

Figure 1. Optimized structures of a FO molecule adsorbed on the Ni/SWCNT: the FO-Ni/SWCNT systems labeled by panels I and II with the O-Ni/SWCNT and P-Ni/SWCNT position, respectively.

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Magnetic sodium alginate: An efficient Nanocatalyst for the one-pot synthesis of substituted imidazoles and benzimidazoles

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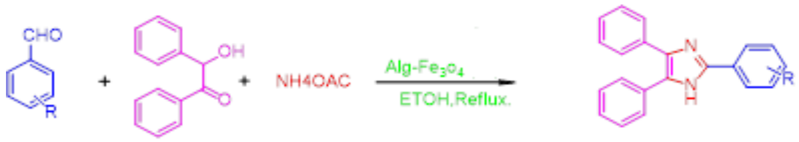
Magnetic sodium alginate was shown to be a highly active and efficient recyclable catalyst for three-component synthesis of imidazole derivatives from benzoin, different aldehydes and ammonium acetate under mild reaction conditions in short reaction times and good to excellent yields in EtOH. Also, benzimidazole derivatives were efficiently prepared from *o*-phenylenediamine and different aldehydes in the presence of magnetic sodium alginate . Moreover, the catalyst was also recovered and reused at least four times without significant decrease in its reactivity. The magnetic sodium alginate catalyst was characterizred by fourier transformer infrared (FTIR) spectroscopy, powder X-ray diffraction (XRD) and nitrogen adsorption–desorption isotherms (NADI) techniques as well as scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Compared to the classical methodologies, this method illustrated the advantages including low loading of the catalyst, short reaction times, high to excellent yields, easy separation and purification of the products, and reusability of the catalyst.

Imidazole and benzimidazole molecules are important substructures in a number of molecules which exhibit an array of biologic and pharmacological activities. The imidazole ring system is an important constituent of numerous natural products and medicinally important compounds, such as Cimetidin, which acts as antiulcerative agent. Omeprazole a proton pump inhibitor, and the benzodiazepine antagonist flumazeni. A platelet coagulation drug in animal and human beings, trifenagre, is a 2, 4, 5 trisubstituted aryl-1H-imidazole derivative.



Magnetic sodium alginate catalyzed one-pot three-componet synthesis of imidazoles from benzoin, different aldehydes with NH4OAc under Optimized conditions

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Structural Characterization of $LaMnO_{3+\delta}$ Nano-Perovskite

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Nanosized $LaMnO_{3+\delta}$ with particles size ~ 20 nm has been synthesized via citrate method [1]. The sample was characterized by XRD, BET, SEM and TEM analysis. The structural characterization of $LaMnO_{3+\delta}$ by X-ray diffraction, X'pert package and Fullprof program provides evidence for a rhombohedral structure with 4% excess oxygen. The main defect type, especially known for $LaMnO_3$, is based on cation vacancies defined by an oxygen excess. A high concentration of cation vacancies leads to a small anion conductivity [2]. The nonstoichiometry can increase the catalytic activity, but only in structures where Mn is defective. The unit cell parameters decrease with increasing of Mn^{4+} content. This effect can be correlated with an ionic radius smaller of Mn^{4+} (0.54 Å) into radius Mn^{3+} (0.64 Å) in the structure (Table 1). The cation vacancy improves the stability of $LaMnO_{3.12}$ because the B-site ion is oxidated from unstable Mn^{3+} ($t_{2g}^3 e_g^1$) to the more stable Mn^{4+} (t_{2g}^3). It has been possible to evidence that $LaMnO_{3.12}$ shows great catalytic activity, because of its small particle size, high surface area and also because its defect structure, are favourable for development of active sites [3].

Table 1. Rietveld refinement results and surface area of the $LaMnO_{3.12}$ sample

Space group	R-3c
a(Å)	5.481
b(Å)	5.481
c(Å)	13.293
V(Å^3)	345.01
S_{BET} (m^2/g)	14.45

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Synthesis, characterization, antimicrobial and theoretical investigation of some new zinc halide complexes

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Schiff base ligands are nitrogen analogue of aldehydes or ketones in which the carbonyl groups (C=O) have been replaced by an imine or azomethine groups. Schiff base compounds are widely used as pigments and dyes, catalysts, intermediates in organic synthesis and as polymer stabilizers .Schiff base compounds have also been shown to exhibit a broad range of biological activities including antifungal, antibacterial, antimalarial, anti-proliferative, anti-inflammatory, antiviral, and antipyretic properties. The imine group present in Schiff base compounds has critical role in their biological activities [1-3]. In this work we report synthesis and characterization of some new zinc halide complexes formulated as $ZnLX_2$ (X= Cl^-, Br^-, I^- and L= Schiff base ligand). The Schiff base ligand was prepared by a condensation of chlorobenzaldehyde and 2-aminoethylethylenedianie in 2:1 molar ration in ethanol for 3h at room temperature. The zinc complexes were synthesized by direct reaction of the ligand and zinc salt in 1:1 molar ratio in ethanol. Furthermore the ligand and its complexes have been screened for their antibacterial and antifungal activities and the data reveal that the complexes have higher activity than the free ligand. Finally, optimized structures, molecular parameters and vibrational frequencies were calculated at the B3LYP/LANL2DZ level of theory.

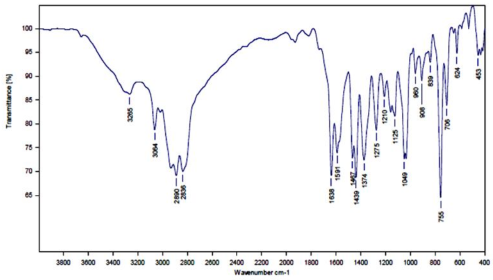

Figure 1- The FT/IR of ligand

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Silver nanoparticles synthesized using dried and aqueous Teucrium polium extract

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Today, silver is produced in the form of particles smaller than 100 nm, called silver Nano particles or Nano silver. These particles exhibit unusual physicochemical property and biological activities. Through extensive research activities, the use of Nano silver, especially in the health field, has expanded vastly [1]. Silver is extensively used in Nano systems and employed in various biomedical purposes. Silver nanoparticles have excellent medical and nonmedical properties and applications when compared with other metal nanoparticles. The green approach of nanoparticles synthesis possesses reduced or no toxicity and number of plants and herbal extracts has been reported to be involved in such synthesis. Plant extracts contain number of secondary metabolite which plays a critical role during the nanoparticle synthesis by acting as reducing or capping agents. Studies have shown that silver nanoparticles are highly stable and toxic to bacteria, fungus, and viruses [2].

The shapes of nanoparticles depend on their interaction with stabilizers and the inductors around them and also their preparation method. It is also known that reaction rate is influenced by the shape of synthesized silver nanoparticles [1]. In this study we prepared the aqueous extract of Teucrium polium flowers in two physical states: liquid extract and (freeze) dried extract, in the next step, after green synthesizing silver Nano particles using both types of extracts, we compared the size and the shape of both produced silver nanoparticles. SEM figures are taken below:

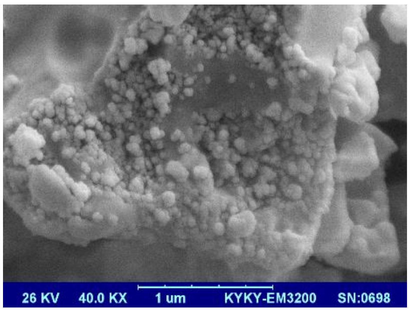

Fig. 1. SEM picture of silver nanoparticles synthesized by liquid extract of T. Polium

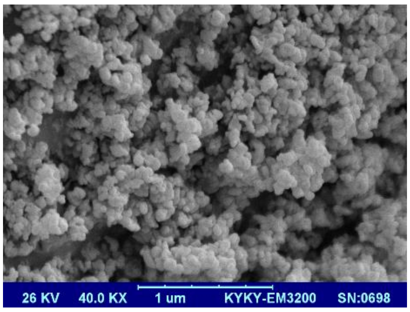

Fig. 2. SEM picture of silver nanoparticles synthesized by freeze dried extract of T. Polium

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Preparation and identification of Lanthanum oxide and its application as catalyst

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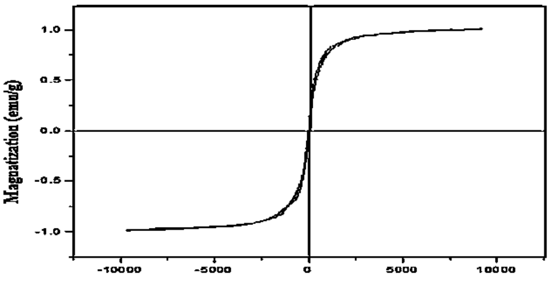
Application of nanoparticles are used in many different fields, such as transportation, cosmetics, pharmaceuticals, airplanes. Many nano-particles of lanthanum, such as LaF3, La $(CO_3)_3$, and La_2O_3, have been synthesized [1]. Lanthanum compounds are widely used in carbon bulbs and projectors. Lanthanum oxide using to make optical fiber and various alloy. Catalyst is a substance that increases speed of a chemical reaction. The goal of chemists is to produce high-activity catalytic activity, complete selectivity. The heterocyclic compounds are a major contributor to the major pharmaceutical, veterinary, and chemical compounds [2]. Heterocyclic compounds are found in many fossil fuels, which has been a source of concern for environmental pollution. In this project first we synthesized La_2O_3 nano-particles and characterized using FT-IR, XRD, SEM and VSM techniques. Then nano-particle applied as catalyst for synthesize of Quinoxalin.



Hysteresis curve of lanthanum oxide nanoparticles

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Preparation and identification of nanoparticles of lanthanum oxide and its application as antibacterial

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Preparation of nanoparticles is by chemical means different processes, such as: Chemical vapor deposition, Coexistence, Sonochemistry, Sol-gel, Hydrothermal. An important advantage of these methods is the possibility of achieving a high degree of chemical homogeneity [1]. From the past, nanoparticles have been discussed in two sections, metallic and non-metallic. Bacteria are a group of microscopic organisms that surround a fairly thick outer covering. They have simple structures and belong to prokaryotic cells. Metal oxide nanoparticles exhibit different antibacterial properties based on surface to volume ratio. Gram-positive bacteria exhibit more resistance than gram-negative bacteria against metal nanoparticles, which can be related to the structure of the cell wall. Staphylococcus aureus is one of the most important pathogenic bacteria in hospital infections. Staphylococcus aureus is a major pathogen for humans and is responsible for food poisoning and non-intestinal infections such as skin infection, ulcers, and abdominal abscesses [2]. Escherichia coli has a fecal origin due to its digestive tract and can be easily spread through humans and animals. In this study, we prepared La_2O_3 nanoparticle. This compound has been charaterized using FT-IR, XRD, SEM and VSM techniques. The antibacterial properties of the this compound have also been investigated.

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Novel barium coordination polymer based on 1,3,5-benzenetricarboxylic acid ligand

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Abstract

The design and synthesis of metal-organic frameworks (MOFs) are of great interest not only for their potential applications in sorption, photochemical areas, magnetism and catalysis but also for their intriguing variety of architectures and fascinating new topologies [1,2]. So far, a large number of mixed-ligand MOFs with 1D, 2D, and 3D structures have been rationally designed and physically characterized [3]. In this paper, a new Ba(II) 3D metal-organic framework namely $[Ba_3(H_2btc)_6(H_2O)_{11}]. 3H_2O$ (1) has been synthesized with reaction between barium nitrate and 1,3,5-benzenetricarboxylic acid. The complex has been characterized by IR spectroscopy and X-ray diffraction. The complex (1) is crystallized in the orthorhombic crystal system with $P2_1\,2_1\,2_1$ space group. Crystal data for complex (1): a= 13.4436(4), b= 21.8558(6), c= 22.3824(7), $\alpha = \beta = \gamma = 90[°]$, Z= 4.

Keywords: Coordination polymer, Crystal structure, Metal-Organic framework, Barium complex, 1,3,5-benzenetricarboxylic acid

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Preparation and characterization of Cu^{+2}-BTC MOF as an Electrodic Material for supercapacitors

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Electrochemical capacitors store electrical energy either in the electrochemical double layer (EDL) formed by the electrolyte ions on the surface of the electrode, or faradaically by redox reactions involving the surface regions of electrode materials [1]. The important distinction between the two charge-storing mechanisms is that in the former no electrons are passed between the solution and the electrode, whereas the latter involves interfacial electron transfer between the solution and the electrode, giving rise to pseudocapacitance.

One class of materials that far surpasses even the porosity of activated carbons is metal–organic frameworks (MOFs) [2]. In this study, we prepared Cu^{+2}-BTC MOF in aqueous solution. The crystal structure of prepared material and MOF formation were certified by XRD and FT-IR. The capacitive behavior of prepared Cu^{+2}-BTC MOF was investigated using cyclic voltammetry, charge-discharge curves and electrochemical impedance spectroscopy in aqueous solution of 1.0 M Na_2SO_4. Finally, to enhance its electrical conductivity, some nanocomposites containing prepared MOF and different amounts of graphene oxide were prepared and their electrochemical capacitances were investigated and compared to pristine MOF.

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The Levothyroxine Effects On The Catalytic Activity And Structural Stability Of Bovine Liver Catalase

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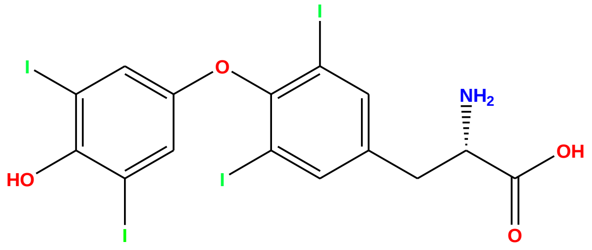
Levothyroxine (LEV, Fig. 1), is a manufactured form of the thyroid hormone, thyroxine. It is used to treat hypothyroidism, a condition where the thyroid gland does not produce enough thyroid hormone [1, 2]. To explore the possible side effects of LEV on the antioxidant defense system of the liver, we analyzed the conformational and functional changes of bovine liver catalase (BLC) in the presence of LEV, using different spectroscopic and molecular docking techniques. Fluorescence studies revealed that LEV quenches intrinsic emission of BLC via static quenching process. Thermodynamic data suggested that hydrophobic interactions play a major role in the binding reaction of LEV on BLC. Structural studies indicated that the binding LEV to the enzyme is responsible for the changes of the percentage of secondary structures' elements especially α-helix. Despite remarkable structural changes of BLC due to hydrophobic interactions with ligands, its function was not influenced considerably. The molecular docking results are in well agreement with the experimental data confirming that there exists one binding site for LEV on BLC at the distance of Forster theory.

Keywords: Catalase, Enzymatic activity, Fuorescence, Molecular docking



Levothyroxine

Fig. 1 Molecular structure of levothyroxine.

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Heavy Metal Adsorption by a Novel Chitosan-Schiff Base Nanocomposites Kinetics and Isotherms

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Lead is a highly toxic environmental pollutant; thus, there is an urgent need to develop new materials for its simultaneous detection and removal from water (1-3). In this study 2-Amino hydroxypyridine derivatives functionalized-chitosan adsorbent was synthesized. The adsorbent was characterized by fourier transform infrared spectroscopy (FT-IR), scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDX), dynamic light scattering (DLS), vibrating sample magnetometer (VSM) and X-ray Diffraction (XRD). The adsorption capability of modified chitosan was investigated by the removal of Pb(II) from aqueous solutions. The adsorption and regeneration studies were performed by batch techniques. The effects of pH, contact time, and initial metal concentration were studied. Metal uptake by Schiff base-chitosan was 112.34 mg/g for Pb(II) ion. The kinetics of Pb(II) on Schiff base-chitosan complied with the pseudo-second-order model. The equilibrium data were fitted to Langmuir and Freundlich isotherm models. The mechanism for Pb^{+2} adsorption onto adsorbent involved the interactions of N, O and also aromatic rings with heavy metal followed by their adsorption on the MCS-Sch.

Keywords: Schiff base, Modified chitosan, Heavy metal removal, Mechanism,

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The role of substituents on the complexation of thiols with copper ion

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Copper complex formation has been monitored along with thiols (RSH) in the non-enzymatic wine oxidation reactions [1]. The presence of different substituents can be effective in the stability of $Cu^{2+}\cdots RS2$ complexes. The effects of some substituents on the binding energy (ΔE) of $Cu^{2+}\cdots RS2$ complexes has been investigated in the present work. All calculations were carried out at the B3LYP/6-31G(d,p) level of theory and using the Gaussian09 program package [2]. The trend of $-\Delta E$ values is: $OCH_3 > CH_3 > H > Cl > NO_2$. The $Cu^{2+}\cdots$ RS2 complexes become more stable in the presence of electron-donating substituents (OCH_3 and CH_3), because of increase in the negative charge density on the S atom. A linear relationship is observed between $-\Delta E$ and the total Hammett constant, σ_t, ($\sigma_t = \sigma_{meta} + \sigma_{para}$ and R = 0.98).

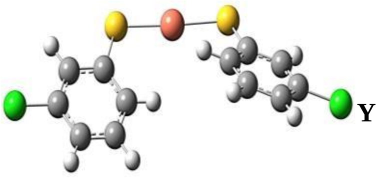

Fig. 1. The structure of $Cu^{2+}\cdots RS2$ complexes. The **Y** is OCH_3, CH_3, Cl and NO_2.

Table 1. The binding energy ($-\Delta E$ in kcal mol^{-1}) and σ_t values in $Cu^{2+}\cdots RS2$ complexes

Y	ΔE	σ_t
H	694.60	0.00
Cl	661.99	0.60
NO2	601.65	1.48
CH3	696.73	-0.24
OCH3	699.76	-0.16

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Incorporated palladium nanoparticles on mesoporous zinc ferrite as an effective catalyst for ethanol electrooxidation

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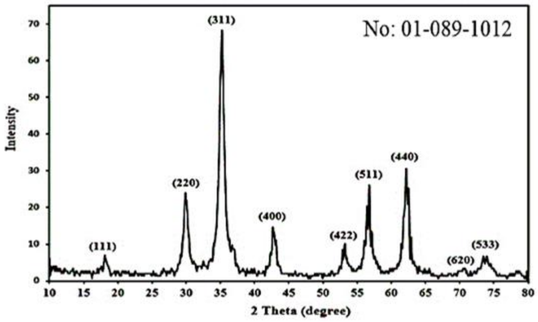
A main challenge in the commercialization of polymeric fuel cell is the improved performance of anode electrocatalyst. Recently, the porous structure materials have attracted much attention owing to low density, cheapness, great surface area [1], extra thermal conductivity [2], and easy charge- and mass-transport [3]. In order to disperse the catalytic noble metals and increasing their electrochemical surface area, employment of a porous support seems to be a sufficient solution. In the present work, solution combustion synthesis method (SCS) was utilized to synthesis mesopores zinc ferrite (mZF) powder. In the SCS, a self-sustained exothermic reaction is occurred among organic fuels (e.g., glycine) and oxidizers (e.g., metal nitrates). Gaseous products like H_2O, CO_2 H_2, CO, and N_2 that are produced from combustion of organic fuels leading to porous structure. As well as, the morphology and structure of mZF powder were characterized by using scanning electron microscope and X-ray diffractometer. Then, the palladium nanoparticles (PdNPs) were deposited onto the surface and into pores of mZF as support. The morphology and status of PdNPs-mZF were investigated by field emission scanning electron microscopy. The electrochemical studies were utilized to determine the characteristics and catalytic activity of PdNPs-mZF towards electrooxidation of ethanol.



The XRD pattern of as-prepared the synthesized mZF powder.

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Synthesis and characterization of meso-porous $NiFe_2O_4$ with a novel combustion method: Application as support for Pd nanocatalyst

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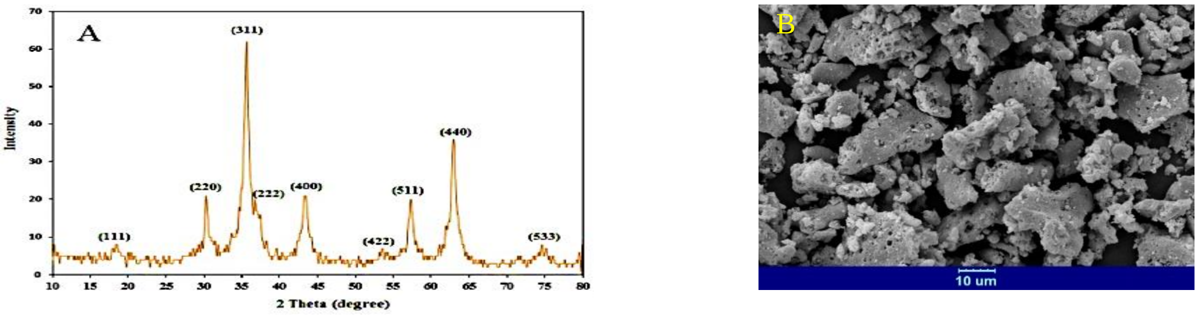
The cost and performance of electrodes are two major parameters in fabricating of polymeric fuel cells. Hence, the noble metals incorporated on supports are employed as electrocatalyst for liquid fuel oxidation [1]. Stable structure, high surface area, and good electronic and geometric properties of support in addition to appropriate interaction of the support and the metal are criteria to choose a support [2]. In the present study, nickel ferrite ($NiFe_2O_4$) powder was fabricated via a novel combustion method and applied as support for Pd nano catalyst. Scanning electron microscopy and X-ray diffraction techniques were employed to character morphology and structure of $NiFe_2O_4$ powder. Then, it was focused on the chemical reduction of Pd nanoparticle on $NiFe_2O_4$ powder. The catalytic activity of Pd-$NiFe_2O_4$ for the electrooxidation of diethylene glycol was investigated in sodium hydroxide solution by using the electrochemical techniques. The results proved that the association of Pd nanoparticles with $NiFe_2O_4$ support was effective to increase the current density and the transferred charge during the reaction of diethylene glycol electrooxidation.



The XRD pattern (A) and SEM image (B) of as-prepared the synthesized $NiFe_2O_4$ powder

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Preparation and characterization of Nickel oxide nanoparticle and its application in removal of food colors

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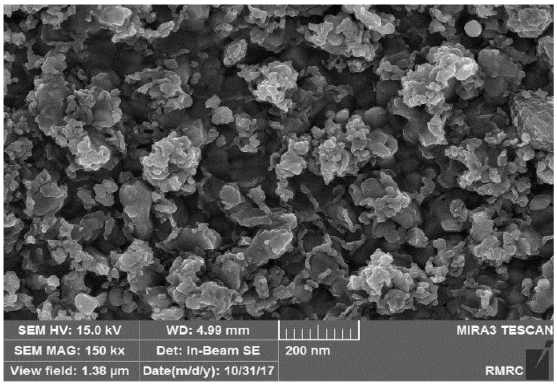
Preparation of nanoparticles is by chemical means different processes, such as: Chemical vapor deposition, Coexistence, Sonochemistry, Sol-gel, Hydrothermal.A important advantage of these methods is the possibility of achieving a high degree of chemical homogeneity [1]. In this study, nickel oxide nanoparticles was prepared by co-precipitation method and used as potential adsorbent for the removal of food color from aqueous solution in a laboratory scale. The sample characterized using Fourier transform infrared spectrophtometry (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectrometer (EDX).By Fourier transform infrared FTIR has proven bond forming of NiO in nickel oxide. X-ray diffraction pattern XRD,a sample is single phase and in the cubic crystalline network.The size of the formed nanoparticles is about 57nm. UV-VIS spectrophotometry showed that the nickel oxide nanoparticles can be prepared as an efficient Adsorbent for the removal of Food color Aqueous solution. The highest removal percentage of food color, was in pH=7and it's concentration was 15 ppm.

The obtained emperimental data in optimum condition was used to model the behavior of absorption in five isotherm equations such as: Langmuir, Freundlic–Langmuir, Toth. The adsorption data were fitted well to the Langmuier isotherm. The kinetics of adsorption interactions were examined with two adsorption mechanisms, pseudo-first-order and pseudo second-order . The obtained results showed that the adsorption data has the most conformity with, pseudo-second-order model.



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Preparation and identification of nanoparticles of nickel oxide and study of the adsorption isotherms of food color by them

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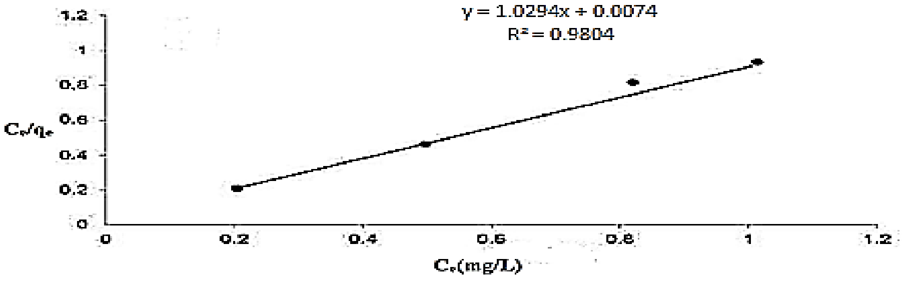
Co-precipitation is one of the methods for the preparation of nanoparticles. This method is very simple and cost effective.[1] In this study, first nickel oxide nanoparticles were prepared by co-precipitation then Its ability to absorb edible color in a laboratory scale has been studied. This compound characterized using FT-IR, X-ray diffraction (XRD), scanning electron microscopy (SEM) and energy dispersive X-ray spectrometer (EDX). Three types of adsorption isotherms including Langmuir isoterms, Langmuir-Freundlich, Thawts were investigated in different concentrations at pH=7. [2]Considering the amount of R obtained for the Langmuir isotherm, which is equal to 0.980, we conclude that the absorption of food color on the surface of the adsorbent is monolayer and uniform. The absorption of food color by nickel oxide nanoparticles is well suited to Langmuir isotherm.



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A Zigzag (8,0) Ni-doped $B_{32}N_{32}$ Nanotube as a New Catalyst for Generation of Hydrogen from Methylamine: a DFT Study

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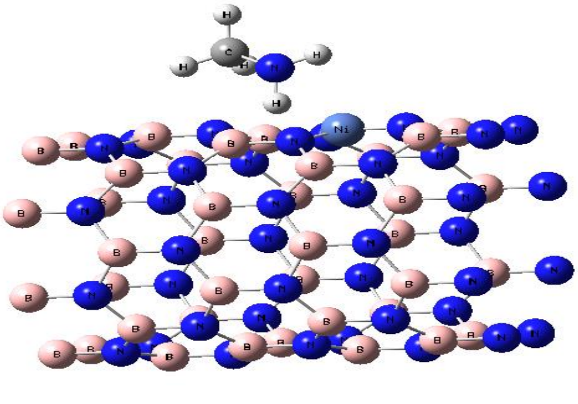
A zigzag (8,0) boron nitride nanotube (BNNT) with 64 atoms was chosen as the simulated model. The substitution ten 3d transition metal such as nickel in (8,0) BNNTs was investigated using density functional theory (DFT). The Ni-doped BNNTs with low dimension and high surface can be considered as a new catalyst for the generation of hydrogen from methylamine [1]. In this study, the decomposition of CH_3NH_2 (MA) on the surface of Ni-doped BNNTs was investigated. All the calculations were carried out with the Gaussian 09 program at the B3LYP/6-31G* level of theory. The adsorption energy (E_{ad}) of the MA on the surface of Ni-doped BNNTs is defined as:

$$E_{ad} = E\ (\text{MA-Ni-doped BNNT}) - E\ (\text{MA}) - E\ (\text{Ni-doped BNNT}) \qquad (1)$$

The decomposition of adsorbed MA on Ni-doped BNNTs may proceed along two pathways: $CH_3NH = CH_2NH + H$ and $CH_3NH = CH_3N + H$. However, the calculations shown that the first pathway is preferable. Intrinsic reaction coordinate (IRC) calculations were performed in the forward and reverse directions to determine minimum-energy pathways. Natural population analysis (NPA) and electron density difference maps were obtained at the B3LYP/6-31G* level of theory [2]. To investigate the changes of electronic structures in the Ni-doped BNNTs caused by adsorption of CH_3NH_2 molecule, total density of states (TDOS) and projected density of states (PDOS) of the pristine Ni-doped BNNT and CH_3NH_2–Ni-doped BNNT complexes are calculated. Our results demonstrated that CH_3NH_2 is adsorbed molecularly on the Ni-doped BNNT surface through its nitrogen lone pair electrons with the suitable adsorption energy. The adsorption process is an exothermic reaction with a negative ΔG_{298} value.



MA adsorbed on the surface of Ni-doped (8,0) BNNT

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The Role of intermolecular Interactions in the Supramolecular Architecture of a Series of Isostructural Group IIB Coordination Complexes

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The supramolecular chemistry of metal-containing compounds has attracted intense attention due to not only their fascinating structures,[1]. but also their potential applications in diverse fields such as ion and molecular recognition[2].The ultimate goal of supramolecular chemistry is to understand the inherent complexities of association mechanisms of molecular and ionic building blocks organized through non-covalent intermolecular interactions with prescribed properties and functions [3]. in continuation of our research program aiming at the understanding of the role of non-covalent interactions in the fabrication and self-assembly of metal-containing building blocks a series of coordination compounds, namely[ZnL_2I_2], [CdL_2Br_2] and [HgL_2I_2] where L is 2-(((2-methoxyphenyl)imino)methyl)phenol have been synthesized and characterized using X-ray crystallography and different spectroscopic techniques. The geometrical and Hirshfeld surface analyses and theoretical calculation reveal the importance of π-π stacking interactions as well as hydrogen bonding in governing the crystal packing of these series of isostructural metal-containing compounds. all compounds exhibit infinite 1D ladders in the solid state governed by the formation of H-bonding and π–π stacking interactions in the solid state

Keywords: Coordination compound, Crystal structure, Supramolecular chemistry, Noncolvalent interaction, Hydrogen bonding,

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Synthesis, characterization, antibactrial activities of Ag(I) complex containing the $SpymMe_2$= 4,6-dimethyle-2-mercaptopyrmidine and interaction Between Ag(I) complex with salmon fish DNA

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Human beings are often infected by microorganisms such as bacteria, yeasts, and viruses in the living environment. Resistance to antimicrobial agents by pathogenic bacteria has emerged in recent years and is a major health problem. Research in antibacterial material containing various natural and inorganic substances has been intensive. Since silver has antimicrobial properties [1] , we prepared the new complex of Ag with ligand 4,6-dimethyle-2-mercaptopyrmidine, which were characterized by spectroscopies and electrochemical techniques and elemental analysis [۲]. Additionally, in this research antibacterial activity of this Ag against the Bactria's of Staphylococcus aureus and Escherichia coli been investigated. Finally, the binding properties of Ag(I) with salmon fish DNA was investigated by UV-Vis spectroscopy and $K_b=1.2\times10^5$ was obtained.

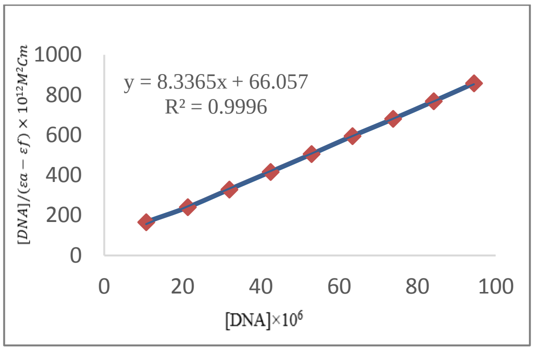

Figure1.Chart changes (εa-εf) / [DNA] according to [DNA] complex at room temperature

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Synthesis and characterization of new Schiff base complex and investigate the anticancer activity

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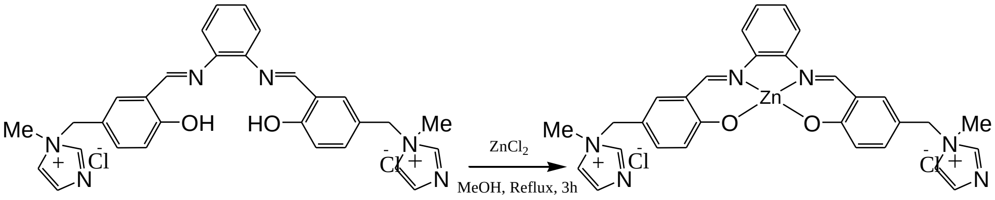
In 1864 a new condensation between an aldehyde and an amine was describe by Hugo Schiff [1]. Schiff bases are very strong ligands to coordinate metals through imine nitrogen or other groups. Nowadays, there are many reports for the different properties of Schiff base ligands from catalytic to biologic activity. Because of the ability of many Schiff base ligands to stabilize different metals in various oxidation state, active and well-designed Schiff bases ligands are considered privileged ligands [2]. In this study we synthesized a new complex of imidazolium salophen Zn(II) complex and characterized by spectroscopic methods (IR, UV-Vis, ^{1}H-NMR)and elemental analysis. Then, we investigated the anticancer effect of this complex. The IC50 result showed that imidazolium salophen Zn(II) complex has a moderate anticancer activity in compare with cisplatin in ovarian cancer.



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Two New Nickel(II) and Zirconium(IV) Schiff Base Complexes, Synthesis, Characterization and Luminescence Investigations

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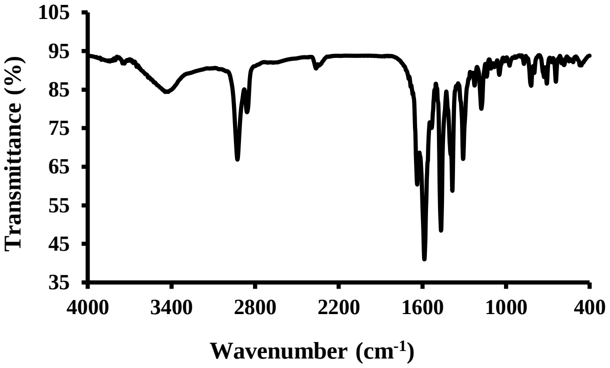
Schiff base ligands have been extensively studied in coordination chemistry mainly due to their facile syntheses, easily tunable steric, electronic properties, good solubility in common solvents and readily form stable complexes with most of the transition metals [1]. Multidentate Schiff bases have been widely used as ligands, because they can easily attached to metal ions due to the formation of high stability of coordination compounds. Also, the chemistry of transition metal complexes of Schiff bases has played an important role in the development of coordination chemistry as a whole. Metal complexes of S-, N-, and O-chelating ligands have attracted the considerable attention because of their interesting physico-chemical properties, pronounced biological activities and being models of metalloenzyme active sites [2]. In this research two new Schiff base complexes of nickel and zirconium have been synthesized by the reaction of $Ni(OAc)_2.4H_2O$ and $ZrCl_4$ with two moles of bidentate Schiff base ligand (containing a novel amine and 5-bromo-2-hydroxybenzaldehyd) at room temperature in methanol. In these complexes the ligands were coordinated to the metals via the imine N and enolic O atoms. The complexes have been found to possess 1:2 Metals:Ligands stoichiometry and the molar conductance data revealed that the metal complexes were non-electrolytes. The emission spectra of the complexes were studied in acetone. The metal Schiff base complexes have been characterized by FT-IR, ^{1}H NMR, UV/Vis, elemental analysis and conductometry.



FT-IR spectra of Nickel(II) Schiff base complex

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A nickel(II) complex including 2,6-pyridinedicarboxylate and metformin ions:Synthesis, characterization, crystal structure and electrochemical studies

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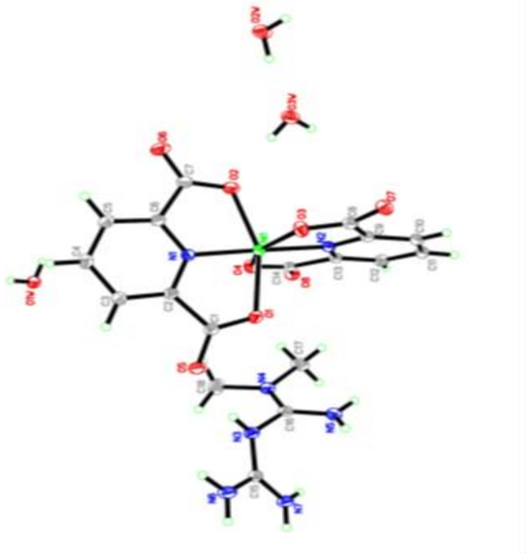
Metformin, N,N-dimethylbiguanide, a biguanide antihyperglycemic agent, has been extensively used throughout the world over the last four decades to treat type-2 diabetes mellitus and, more recently, to treat polycystic ovarian syndrome. It has a distinct advantage of lowering serum glucose levels without causing hyper-insulinemia and subsequent risk of hypoglycemia, or weight gain [1-3].The new complex $[H_2Met][Ni(dipic)_2].3H_2O$ ($dipicH_2$ = 2,6-pyridinedicarboxylic acid) and Met = metformin (N,N-dimethylebiguanidine), was synthesized and characterized by elemental analysis, FT-IR, and UV–Vis spectroscopy and single crystal X-ray method. The crystal system is triclinic with space group $P\bar{1}$. The unit cell dimensions for Ni(II) complex is a = 9.292 (8), b = 10.095 (8), c = 12.541 (11). In this complex, metformin is diprotonated and acts as counter ion. The intra and intermolecular hydrogen bonds stabilize the crystal structure of compound. The redox behavior of the complex was investigated by cyclic voltammetry.



The asymmetric unit of $[H_2Met][Ni(dipic)_2]$. $3H_2O$

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Sonochemical synthesis and characterization of some new four coordinated cadmium complexes: New precursors for nanostructure metal oxides, antimicrobial, and DNA cleavage potential

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Schiff bases represented a class of compounds having azomethine group (-CH = N^-) and considered as the potential sites for bio-chemically active compounds that are related to intermolecular hydrogen bonding and proton transfer equilibria [1]. Metal complexes of Schiff base ligands have gained considerable attention as the results of their spectroscopic properties and remarkable antifungal, antibacterial and antitumor activities applications [2].
In this work some new cadmium(II) Schiff base complexes $CdLX_2$ (where X = Cl^-, Br^-, I^-, SCN^-, N_3^-, NO_3^- and L is a new N_2-Schiff base ligand were synthesized and characterized by fourier transform infrared, proton and carbon nuclear magnetic resonance spectra, UV–visible, thermal analyses, and molar conductivity measurements. cadmium complexes have been also prepared in nanostructure sizes under ultrasonic irradiation confirmed by X-ray powder diffraction (XRD) and the morphology and size of ultrasound-assisted synthesized cadmium complex have been investigated using scanning electron microscopy (SEM). CdO nanoparticles were prepared by direct calcination process of cadmium iodide complex at 600°C under air atmosphere. antibacterial/antifungal activities of the compounds were screened by the disk diffusion method against the Gram-negative bacteria *Escherichia coli* and *Pseudomonas aeruginosa*, the Gram-positive bacteria *Staphylococcus aureus* and *Bacillus subtilis* and the fungi strain *Aspergillus oryzae*and *Candida albicans*. The antimicrobial activities were determined for all compounds and the complexation was found to enhance the inhibitory activity. Moreover, DNA cleavage potential of all compounds was investigated by agarose gel electrophoresis method. The results showed remarkable ability of some cadmium complexes for DNA cleavage.

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Synthesis, characterization, DNA binding studies of Pd (II) antitumor complexes

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Two new palladium complexes [Pd (8-QO)(AA)] (where 8-QO= 8-hydroxyquinoline and AA= amino acids with hydrocarbon (hydrophobic) side chains such as glycine and valine) have been synthesized by reaction between sodium salt of respective amino acid and Na_2 [$PdCl_4$] and subsequent addition of 8-hydroxy quinoline. The molar ratio of the three reactant was 1:1:1. This complexes have been characterized by FT-IR, UV-Vis and ^{1}H-NMR spectroscopic techniques and conductivity measurements. The novel antitumor Pd (II) complexes were evaluated for its binding to CT-DNA in physiological buffer (pH=7) by using absorption spectroscopy, fluorescence titration spectra studies. The result obtained from these analyses indicated that the complexes can bind to DNA cooperatively through astatic quenching procedure [1-3].

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Solid-State Synthesis and Characterization of Polyaniline/TiO_2 nanocomposite

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Organic–inorganic nanocomposites with an organized structure has been extensively studied because they combine the advantages of the inorganic materials (electrical, mechanical strength, thermal stability and magnetic properties) and the organic polymers (ductility, flexibility, dielectric and processibility), which are difficult to obtain from individual components [1]. Hybrid organic-inorganic nanomaterials are the focus of much attention due to their capacity to enhance electronic and conductance properties of both materials. One important feature is the nanostructuration of such nanocomposite [2,3]. In this work Polyaniline/TiO_2 nanocomposite was prepared by using solid-state synthesis method at room temperature. The structure and morphology of the naocomposites were characterized by the Fourier transform infrared (FTIR) spectra, ultraviolet-visible (UV–vis) absorption spectra and scanning electron microscopy (SEM). The electrochemical performances of the nanocomposites were investigated by cyclic voltammetry (CV). The results from FTIR and UV–vis spectra showed that the nanocomposites displayed higher oxidation and doping degree than pure PANI. The technology presented in this study has considerable potential for the low cost, large scale production of polyaniline.

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Optimizations and characterizations of Biosynthesis of Silver nanoparticles using leaf aqueous extract of *Cannabis Sativa* L.

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The plant extracts have been widely used as herbal reducing agents for green, easy, non-toxic and environmentally friendly nanoparticles synthesis. In this study, the extract of *Cannabis sativa* L. was used for synthesis of silver nanoparticles. The influences of various parameters including pH, volume of extract, extract concentration, concentration of silver nitrate and reaction times on the synthesis of silver nanoparticles were investigated [1]. The synthesized silver nanoparticles were characterized by some techniques such as; Transmission Electron Microscopy (TEM), X-Ray Diffraction (XRD), Fourier Transform Infra-Red (FT-IR) and UV-Vis spectroscopy. Afterwards, the antibacterial activity of these nanoparticles against human pathogenic bacteria was studied. The results showed that, the Ag NPs were spherical shape with particle sizes in the range of 5-22 nm. They also show maximum absorption at 420 nm due to Surface Plasmon Resonance (SPR). The optimum conditions for the synthesis of Ag NPs were determined as: pH = 8, 3 ml of extract, 0.5% concentration of extract, 1 mM of silver nitrate salt concentration and the reaction time of 20 minutes. Moreover, it was revealed that alkaloids and secondary metabolites act as both stabilizing and reducing agents. The Ag NPs showed a significant antibacterial activity.

Keywords: Biosynthesis, *Cannabis Sativa* L., Silver nanoparticles, Surface Plasmon Resonance

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Synthesis and characterization of $MgFe_2O_4$ by Solid- state method

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Magnesium ferrites are the potential materials for various applications due to their high electrical resistive. Many physical properties of $MgFe_2O_4$ depend on their microstructure, porosity, grain size, state of chemical order and the cation distribution [1-2]. The main objective of this study was to synthesize and characterization of $MgFe_2O_4$ using $MgCl_2$ and $FeCl_3$ at 900°C for 10 h by solid state reaction. The employed techniques are XRD, SEM and FT-IR. XRD pattern of powdered sample of $MgFe_2O_4$ is presentedin Fig.1. The XRD pattern provides information about single-phase formation of spinel structure with cubic symmetry. The crystallite size of $MgFe_2O_4$ sample was calculated from x-ray lines broadening of the reflections of (220), (311), (222), (400), (442), (511), (440), (533) and (444) using Scherrer's equation (D=31 nm). Also, the formation of spinel $MgFe_2O_4$ structure was further supported by FT-IR spectra (Fig.2). Fig.3 shows the FESEM image of sample. It shows that there are some multigonal structures including the triangle prism morphology. The optical properties of the obtained material showed that the material has strong absorption in UV light region. Direct optical band gap energy of the obtained material was 2.7eV.

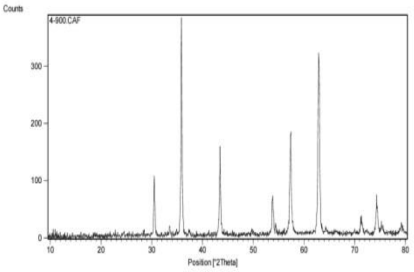

Fig 1: XRD pattern of $MgFe_2O_4$

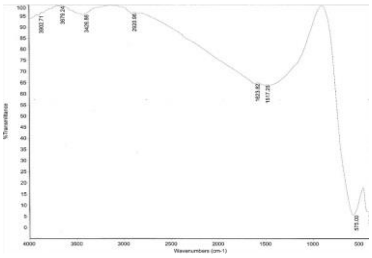

Fig 2: FT-IR spectra

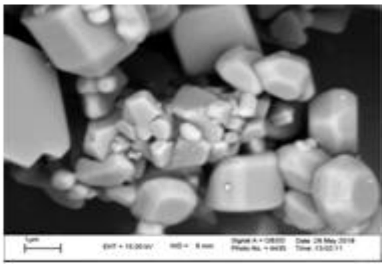

Fig 3 : FESEM image

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Synthesis and Characterization of New Nickel(II) and Zinc(II) Schiff Base Complexes Containing Disulfide Bond

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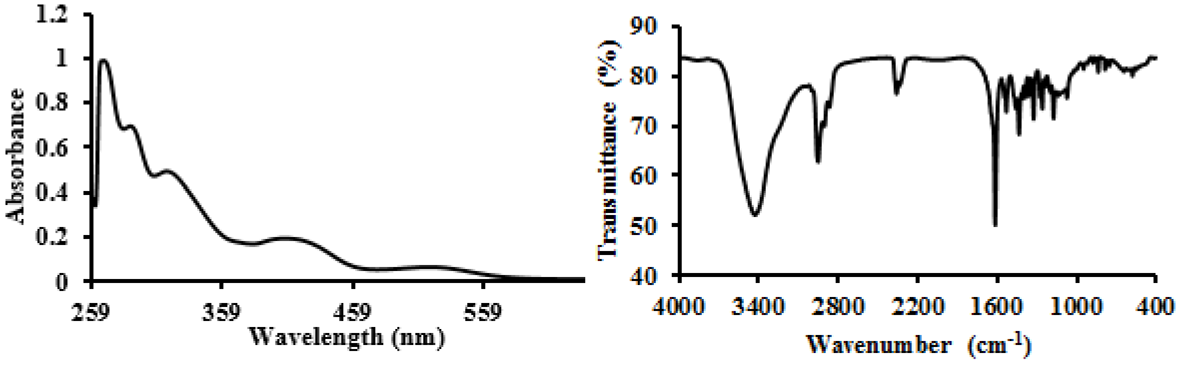
Schiff base complexes are compounds that contain the azomethine group (–CH=N–) in their structure which are generally synthesized by the condensation of primary amines and active carbonyl groups. The interest of studying Schiff base complexes containing different donor atoms such as ONS arise from their significant antifungal, antibacterial and anticancer activities [1]. In addition, the presence of both hard and soft donor groups in one compound increases the coordination ability towards hard as well as soft acidic metals. Also, the chelating properties of Schiff base ligands in their complexes display manifold applications in medicine, industry and agriculture [2]. Schiff base complexes recently have taken more attention in bioinorganic, biochemistry and medicine because of the fact that they have antimicrobial and chemotherapy features [3]. The biological activity potential of complexes containing sulfur and nitrogen may be the reason for this increased interest. In this work, two new complexes of nickel(II) and zinc(II) were synthesized by the reaction of $NiCl_2.6H_2O$ and $ZnCl_2.H_2O$ with two moles of bidentate Schiff base ligand in ethanol at 58℃. In these complexes NSO atoms were observed but Schiff base was coordinated as a bidentate ligand through NO donor atoms of phenolic and azomethine groups in metal complexes and the thiolic groups were oxidized and formed disulfide bond. The metal centers were coordinated to all the available functional groups on the double Schiff base ligand. These new complexes were characterized by the spectroscopic techniques such as UV–Vis spectroscopy, FT-IR, ^{1}H NMR and conductometry.



FT-IR and UV-Vis spectra of nickel(II) Schiff base complex

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Molybdenum(VI) complex with Schiff base ligand derived from nicotionhydrazide as catalyst for the oxidation of sulfides with H_2O_2

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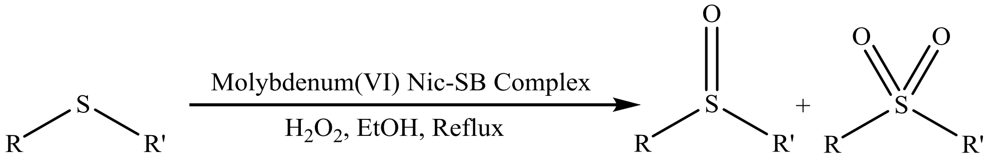
Schiff bases including N, O donor atom sets are renowned to match with different metal ions and this has fascinated lots of inventors. Not only the Schiff bases perform an important role in coordination chemistry, but also, their complexes have enough potential for property of catalyst. Molybdenum biochemical 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 and biochemistry of molybdenum [1-2]. In this study we prepared the new complex of molybdenum with nicotinohydrazide Schiff base ligand has been prepared and fully characterized. This complex was characterized by spectroscopic methods (FT-IR, UV-Vis, ^{1}H-NMR and ^{13}C-NMR). The prepared complex was used for oxidation of sulfides with aqueous hydrogen peroxide under reflux conditions. The reaction parameters such as catalyst amount, kind of solvent; oxidant amount and temperature were optimized in the oxidation of diphenyl sulfide (Scheme 1). The use of the complex as a catalyst for oxidation of sulfides was explored, using H_2O_2 as primary oxidant. First, the amount of catalyst was optimized. Next, the choice of solvent was optimized in the model reaction. Different solvents were investigated, and the highest yield of products was obtained with ethanol. In comparison with the data reported in the oxidation of organic sulfides by various Schiff base complexes, our system shows the following advantages: the cheapness, easy availability and non-toxicity of oxidant.



(Scheme 1)

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Synthesis, spectral characterization and investigation of biological properties of Cu(II) Schiff base complex derived from 4-aminoantipyrine

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As early as 1884, Knorr discovered the antipyretic (temperature reducing) action of a pyrazole derivative in humans, and due to its antipyretic property he named the compound Antipyrine. Transition metal complexes of pyrazolone derivatives are of great interest due to their biological activities, especially pyrazolone Schiff-base derivatives. Schiff base of 4-aminoantipyrine and its complexes have a variety of applications in biological, clinical and pharmacological areas [1–3]. In this research, we report the synthesis of Cu(II) complex containing Schiff base derived from 4-aminoantipyrine and 5-hydroxysalicylaldehyde. The Schiff base ligand was prepared using reaction of 5-hydroxysalicylaldehyde with 4-aminoantipyrine in ethanol at room temperature. This ligand was characterized by ^{1}H-NMR, ^{13}C-NMR, FT-IR and single crystal X-ray diffraction. Complex was prepared by direct reaction between the Schiff base ligand and the corresponding metal salt. The metal center possesses a distorted square planar geometry with N_2O_2 donor atoms coordinating from Schiff base ligand. Even though the ligand is tridentate in nature, it binds the Cu(II) ion, in a bidentate fashion through the deprotonated phenolic oxygen of the phenyl ring and nitrogen of the azomethine group, leaving the antipyrine exocyclic ketonic oxygens free. The steric strain imposed by the methyl substitution on the antipyrine moiety restricts the ligand towards bidentate coordination from its tridentate nature. The *in vitro* biological screening effects of the synthesized compounds were tested against different microbial kinds via MIC test. Our results revealed the more antimicrobial activity of the ligand than their Cu(II) complexe.

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Kinetics and Mechanism of Tetrahydrobenzo [b] pyran Derivatives Catalyzed by Glycine as Inorganic compound

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In the present investigation, the reaction between malonitrile and dimedon with derivatives of benzaldehyde have been studied spectrophotometrically for the one-pot Tetrahydrobenzo [b] pyran derivatives in the presence of glycine as a catalyst at different temperatures. The special advantages of is neutral and mild environmental conditions, lack of toxicity, giving high to excellent yields of products [1-2]. Experimentally, the reactions were found to be of second-order and observed rate constants were determined using UV-vis spectrophotometry. The proposed mechanism was adapted in accord with the experimental results and the steady-state assumption. Kinetic values (k and Ea) and associated activation parameters ($\Delta G^{\neq}.\Delta S^{\neq}$ and $\Delta H^{\neq}$) of the reactions were determined [3]. Furthermore, from studying the effect of solvent, concentration and catalyst on the reaction mechanism, useful information was obtained.

Keywords: kinetics, Glycine, Tetrahydrobenzo [b] pyran, Catalyst, UV-vis Spectrophotometry

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Quantum Mechanical Evaluation of Intramolecular Proton Transfer IPT in a New Hydrogen-Bonded [(DPAH)+(dipicH)−.H2O] Complex formed: NBO analysis and AIM Calculation, HOMO-LUMO

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In this work, we showed theoretically the aromatic system of the hydrogen-bonded complex, [(DPAH)+(dipicH)−.H2O] formed by the reaction between 2,2'-dipyridylamineand (DPA) and 2,6-pyridine dicarboxylic acid (dipicH2) established the π–π stacking interactions, which have an important role in the stabilization of crystals with distance centroid-centroid (d: Cg-Cg). The proton transfer investigated theoretically and thermodynamic parameters such as $\Delta H^{\ddagger}$, $\Delta G^{\ddagger}$, $\Delta S^{\ddagger}$ were calculated for this process [1-2]. Moreover, intramolecular hydrogen-bonding interaction has been recognized by calculating the electron density $\rho(r)$ and Laplacian $\nabla^2 \rho (r)$ at the bond critical point (BCP) using Atoms-In-Molecule (AIM) method. Also, the interaction between electron acceptor (σ^*) of OH with the lone pair of the nitrogen atom as an electron donor was evaluated using Natural Bond Orbital (NBO) analysis [3].

Keywords: Hydrogen-Bonded Complex, Stacking Interactions, Proton Transfer, AIM, NBO

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Three-dimensional architecture of Pd-Ag aerogel as a unique class of inorganic modern polymers toward formic acid oxidation

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Three-dimensional architectures of noble metal aerogels are considered as a unique class of inorganic modern polymers. Until now, various approaches have been published for the creation of noble metal aerogels, while their development and synthesis suffer from time-consuming multistep procedures. Herein, we propose a simple and useful strategy for the fabrication of Pd-Ag aerogel. This method offers several advantages over other methods such as being one-pot synthesis, simplicity and fast. This three-dimensional polymer was prepared by the reduction of H_2PdCl_4 and AgCl in the presence of sodium carbonate by using glyoxylic acid monohydrate as a reducing agent followed by supercritical CO_2 drying. The Pd–Ag aerogel was applied as a support-less catalyst for electrooxidation process of formic acid, and depicts much higher electrocatalytic activity and durability compared to the Pd/C. The higher electrocatalytic activity of the Pd-Ag aerogel compared to the Pd/C catalyst is attributed to the unique characters of this three-dimensional polymer. Mesoporous character creates a high surface area, which allows faster mass transport through the profuse pores, and macroporous character guarantees easy access of molecules to the active sites. Moreover, the self-supporting property of the Pd-Ag aerogel may prevent the loss of stability observed in Pd catalyst supported on carbon due to corrosion. We believe that the exceptional three-dimensional inorganic modern polymer fabricated by this route is powerful and promising catalysts for application in direct formic acid fuel cells (DFAFCs), which may open great opportunities for widespread applications such as catalysis, sensors, optoelectronics, electrochemical energy systems, etc.

Keywords: Inorganic modern polymers, Three-dimensional architecture, Aerogel, One-pot synthesis method, Formic acid oxidation

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Synthesis and characterization of a supramolecular structure bearing manganese(II) and pyridine-2,5-dicarboxylic acid *N*-oxide

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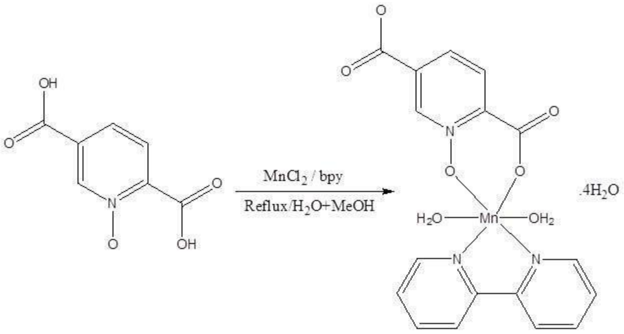
Purposeful design and organization of molecular building blocks into extended architectures with specific dimensionalities and properties is an important goal for scientists. In fact, the idea of preparing designed crystals with desired properties is known as "crystal engineering" and since the 1990s, this field has been flourishing. Also, it would be wonderful if we could predict what the resulting reactivity patterns would be for a given set of donor atoms on a particular metal center. An important way to achieve this goal is to study the geometry of ligands as well as to examine their effects on the spatial arrangement of the crystal lattice. H_2pydco (isocinchomeronic acid or pyridine- 2,5- dicarboxylic acid *N*-oxide) is an appropriate candidate for construction of new metal-organic compounds through coordination to metal ions as well as simultaneous participation in non-covalent interactions (typically π-stacking interactions) that promote the dimensional architectures of the complex. It is well known that Mn complexes containing *N*- oxide family of ligands have been utilized as anti- HIV agents, gas adsorbents, luminescent agents, *etc* [1-3]. In this work, we report preparation of a new coordination complex based on pydco, 2,2'-bipyridine (bpy) and manganese metal. It is characterized by physico-chemical approaches such as elemental analysis (CHN), IR spectroscopy and melting point. Based on the obtained data it can be formulated as $[Mn(pydco)(bpy)(H_2O)_2]\cdot 4H_2O$. Also, many aspects of this category of complexes such as single crystal X-ray diffraction, supramolecular interactions and biological tests are remain to be investigated; we plan to carry out this investigation in the future.

Keywords: crystalline engineering, pyridine- 2,5- dicarboxylic acid *N*-oxide, isocinchomeronic acid, 2,2'-bipyridine.



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Synthesis and characterization of molecular-crystal structure of a coordination complex based on zinc and pyridine-2,5-dicarboxylic acid *N*-oxide

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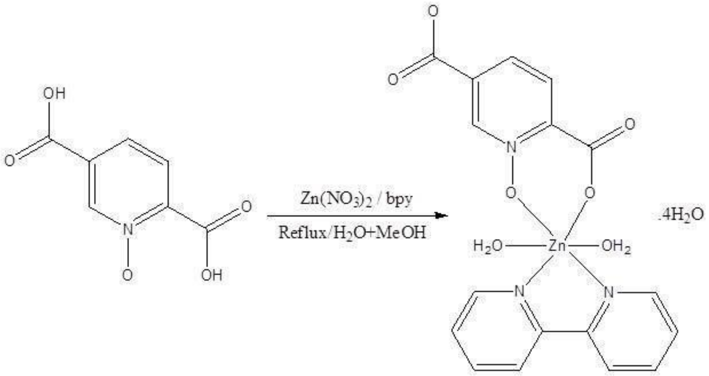
Chemistry of coordination compounds is an interesting and growing field of research; design and construction of novel compounds with favorable properties have fascinating applications ranging from nanotechnology, catalysis, macromolecular crystallography and medicine. *O*-donor ligands are of particular interest because their complexes with biologically important metals have potential medical applications. Furthermore, planar and rigid heterocyclic *N*-donor π-electron-deficient ligands, are widely used in supramolecular chemistry and/or in the molecular biology as DNA cleaving reagents and *etc*. The aim of the present study is to produce an organized structure possessing a combination of both properties using the mixed ligands.

In this work, we select pyridine-2,5-dicarboxyxlic acid *N*-oxide (pydco) as a versatile *O*-donor ligand with -COOH groups in a *p*-arrangement. It can be used to construct coordination polymers or link monomeric or dimeric compounds by hydrogen bonding through its uncoordinated carboxylate group at the position 5 [1-3]. Herein, we report successful preparation of a new coordination complex based on pydco, 2,2'-bipyridine (bpy) and zinc metal, which is characterized by physico-chemical approaches such as elemental analysis (CHN), IR spectroscopy and melting point. Based on our data it may be formulated as $[Zn(pydco)(bpy)(H_2O)_2]\cdot 4H_2O$. This category of complexes remains little-investigated in aspects such as single crystal X-ray diffraction, supramolecular interactions and biological tests; therefore we intend to extend our studies.

Keywords: Mixed ligands, pyridine-2,5-dicarboxylic acid *N*-oxide, 2,2'-bipyridine.



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Gas transport membranes based on novel optically active polyester/ cellulose/ZnO bionanocomposite membranes

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In this work, at first commercially available ZnO nanoparticles were modified with biodegradable nanocellulose through ultrasonic irradiation technique [1]. Then, optically active bionanocomposite (BNCs) membranes composed of polyester (PE) and cellulose/ZnO BNCs are synthesized, as a novel process to enhance gas separation performance. The obtained PE/BNCs were characterized by Fourier transform-infrared spectroscopy, thermogravimetry analysis (TGA), X-ray powder diffraction, field emission-scanning electron microscopy, and transmission electron microscopy (TEM). TGA data indicated an increase thermal stability of the PE/BNCs in compared to the pure polymer. From TEM image of PE/BNCs, it can be found that the surface-modified ZnO with diametric size of less than 40 nm, uniformly dispersed in the obtained PE matrix. The results obtained from gas permeation experiments with a constant pressure setup showed that adding cellulose/ZnO to the polyester membrane structure increased the permeability of the membranes. From biodegradation test observed that the degradation occurred in a faster rate in the presence of cellulose/ZnO in the PE matrix [2].

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Investigation of the possibility of silver recovery in the ethylene oxide catalyst for reuse in catalyst preparation

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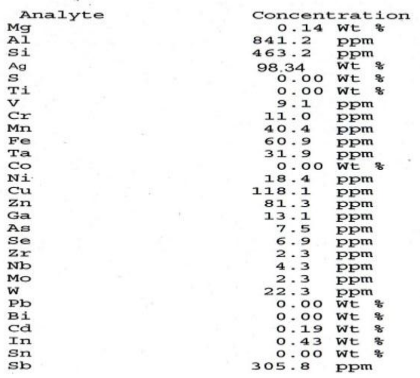
Due to The environmental problem of burying spent catalysts , considerations of sustainable development , Economic value and high usage of the noble metals , Recovery of these precious metals from spent catalysts , have attracted a great deal of attention and importance in recent years[1] . In this Research , recovery of the precious metal of silver from Ethylene oxide spent catalyst(Ag /Al_2o_3) , has been investigated .in the recovery process, silver , in the from of Nitrate solution has been recoverd by Nitric Acid as the extractant solvent , and after separating it from the solution and purifying it with recrystalyzation process , it has been converted to silver oxid (I) by Hydroxide Sodium[2] .Experimental results as well as the measurement of the extracted silver , determined using Atomic Absorption and XRF method , show the recovered silver with a purity of 99.99% .



Analyte	Concentration
Mg	0.14 Wt %
Al	841.2 ppm
Si	463.2 ppm
Ag	98.34 Wt %
S	0.00 Wt %
Ti	0.00 Wt %
V	9.1 ppm
Cr	11.0 ppm
Mn	40.4 ppm
Fe	60.9 ppm
Ta	31.9 ppm
Co	0.00 Wt %
Ni	18.4 ppm
Cu	118.1 ppm
Zn	81.3 ppm
Ga	13.1 ppm
As	7.5 ppm
Se	6.9 ppm
Zr	2.3 ppm
Nb	4.3 ppm
Mo	2.3 ppm
W	22.3 ppm
Pb	0.00 Wt %
Bi	0.00 Wt %
Cd	0.19 Wt %
In	0.43 Wt %
Sn	0.00 Wt %
Sb	305.8 ppm

Silver XRF in Silver Nitrate

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Binding mode investigation between a platinum (II) complex and BSA by fluorescence spectroscopy

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Serum albumins, the most abundant proteins in blood plasma, have long been the center of attention of pharmaceutical industry due to their ability to bind a verity of metabolites and drugs. This outstanding binding capacity often seriously impacts pharmacokinetic properties of drugs [1]. In this study, the interaction between a platinum (II) complex of formula $[Pt(en)(2\text{-}pyc)]NO_3$ (where en = 1,2-diaminoethane and 2-pyc = 2-pyridinecarboxylate anion), as a potential anti-tumor agent, and bovine serum albumin (BSA), as a protein model, was studied by fluorescence spectroscopy. To this purpose, a solution of BSA with a fixed concentration in Tris-HCl buffer of pH = 7.00 was titrated with a stock solution of the Pt(II) complex. After each addition, the sample was excited at excitation wavelength of BSA and the emission spectrum was recorded. The obtained results indicated that the Pt(II) complex strongly quench the intrinsic fluorescence of BSA. The binding constant (K_b), the number of binding sites (n) and the Stern–Volmer constant (K_{sv}) were calculated based on the obtained results. Furthermore, the fluorescence quenching mechanism was also investigated *via* examining the fluorescence quenching process at three different temperatures. The results demonstrated that the probable quenching mechanism of BSA by the Pt(II) complex is a static quenching, because the equilibrium constants have been decreased by rising temperature. The negative values of ΔH^o and ΔS^o show that hydrogen bonds and van der Waals force play a major role in the binding of the Pt(II) complex to BSA [2].

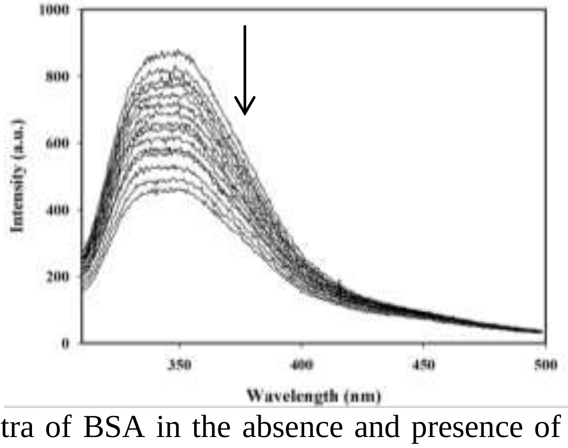

Fig. 1. The emission spectra of BSA in the absence and presence of increasing amounts of the Pt(II) complex at 300 K.

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Synthesis and photocatalytic properties of $BaZrO_3$

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Perovskite-based photocatalysts are of significant interest in the field of photocatalysis. Barium zirconate ($BaZrO_3$) has been extensively studied and widely used in various applications, such as thermal barrier coating material for aerospace industries. It has distinctive physical and chemical properties such as high thermal stability, excellent chemical durability, low coefficient of thermal expansion, and good structural compatibility [1]. Barium zirconate ($BaZrO_3$) with ideal perovskite structure is a value-added material for the refractory industry as well as a good substrate for the manufacturing of high temperature superconductors due to its structural compatibility and chemical inertia [2].

Ceramic was characterized by Energy dispersive X-ray analysis (EDX), FT-IR, SEM, UV-vis spectroscopy and X-ray diffraction (XRD). XRD analysis and SEM reveal pure perovskite phase structure and uniform grain size.

Parameters such as concentration of substrate, amount of photocatalyst, pH of the solution, temperature of reaction medium and time of irradiation of light for photocatalysis degradation of Eosin Y (EY) were investigated. Ceramic show the maximum adsorption at high pH hence the photodegradation also found maximum at high pH.

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Photocatalytic Activity of Ag-$BaZrO_3$ Nanoceramics

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Ceramic materials with perovskite type structure are value-added materials used for several functional applications such as transducers and wireless communications [1]. Perovskite oxides have been deemed as promising materials for photocatalysis due to their tunable electronic structures. Different from the mechanism of $BaZrO_3$ doping, previous investigations showed that Ag additions can improve the photocatalyst activity [2].

The Ag-BZO nanoceramic was prepared by sol-gel method . In a typical procedure, 0.40 g of barium chloride was dissolved in deionized water. In another beaker, zirconium oxychloride was added to silver chloride in deionized water. Then, a solution of NaOH added to them. Finally, precipitation was calcinated at 700 ˚C.

Ceramic was characterized by EDX, SEM and XRD. XRD analysis and SEM reveal pure perovskite phase structure. Parameters such as concentration of substrate, amount of photocatalyst, pH of the solution, and time of irradiation of light for photocatalysis degradation of Eosin Y were investigated. Ceramic show the maximum adsorption at neutral pH hence the photodegradation also found maximum at neutral pH.

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Aerobic Oxidation of Alcohol Using Molybdenum(VI) Oxide Immobilized on Mesoporous Silica

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First KIT-6 silica support, which possess ordered pores in nanoscale with high surface area, was synthesized through hydrothermal method and then Molybdenum oxide nanoparticles was located in the pores via wetness impregnation method.

The prepared catalyst was characterized with different techniques such as XRD, TEM, N_2 adsorption- desorption, UV-Vis, Raman and FT-IR. It is notably, existence of Molybdenum(VI) oxide was proved using Raman spectrum of MoO_3-KIT-6. This catalyst was tested for alcohols oxidation reaction with air as oxidant at 80°C in solvent free conditions which can oxidize alcohols to aldehydes in relatively short times.

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Comparison between Cu(II) schiff base complex immobilized on SBA-15, Fe_3O_4 and Fe_3O_4/mesoporous silica catalysts for alcohols oxidation

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In this study, Cu(II) Schiff base complex was synthesized and immobilized on a silica layer and magnetic core that was prepared through inverse microemulsion and precipitation method respectively. Structural and magnetic properties of the catalyst were characterized using XRD, TEM, FT-IR and VSM methods. XRD pattern of Fe_3O_4 nanoparticles showed a pure cubic phase. TEM image of nanoparticles confirmed spherical morphology containing magnetic core about 20 nm and silica layer around 50 nm thicknesses. VSM curve of Fe_3O_4 nanoparticles showed superparamagnetic property. Fe_3O_4@nSiO_2@mSiO_2@Cu(II) Schiff base catalyst was synthesized and their structural properties were characterized with TEM and IR methods. TEM image of the nanoparticles confirmed the presence of a magnetic core with diameter of 300 nm, amorphous silica layer ~ 15 nm and mesoporous silica layer ~ 70 nm.

These catalysts were compared with SBA-15-Cu(II) Schiff base for alcohols oxidation. Interestingly, Fe_3O_4@ SiO_2@Cu(II) Schiff base had the highest catalytic performance for oxidation of benzyl alcohol in the presence of hydrogen peroxide in water at 80°C and in contrast, SBA-15@Cu(II) Schiff base had the highest catalytic activity for benzyl alcohol oxidation in the presence of tert-Butyl hydroperoxide and acetonitrile as solvent at 60 °C.

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Synthesis and characterization of metal complexes by tridentate NOS Schiff Base ligand

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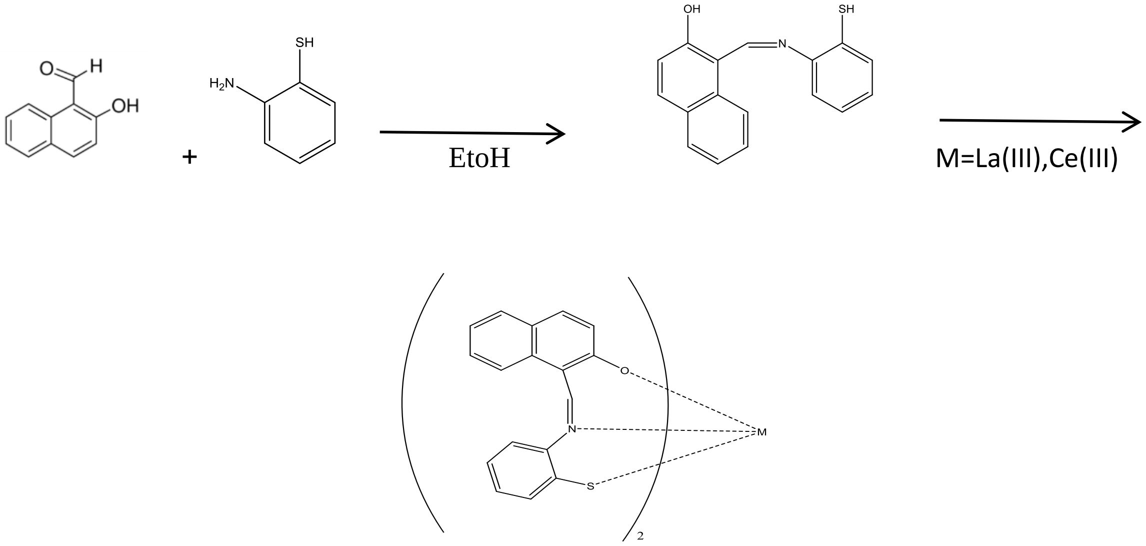
Transition metal complexes with nitrogen, oxygen and sulfur donors ligands have been prepared since the beginning of the development of coordination chemistry and there is continuing interest in these complexes [1]. The presence of both hard and soft donor atoms in the backbones of unsymmetrical Schiff bases ligands, they readily coordinate with a wide range of transition metal ions[2]. The synthesis of transition metal complexes of unsymmetrical Schiff bases ligands with nitrogen, oxygen and sulfur atoms is an important area of study with implications in bioinorganic chemistry catalysis and medical chemistry [3]. In this study, tridentate NOS Schiff base ligand prepared by reaction of 2-aminothiophenol with 2-hydroxy-1-naphtaldehyde. La (III), Ce (III) Schiff base complexes of this ligand were synthesized. The Schiff base ligand and related complexes were characterized by FT-IR, UV-vis, NMR, Mass spectrometry, conductivity and elemental analyses. The results show that the ligand is coordinated to metal ions through imine N and hydroxyl O and thiol S atoms.



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Interaction Between La(III), Ce(III) Schiff base complexes with salmon sperm DNA

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Metal Schiff base complexes, which are known as drugs in cancer chemotherapy, could inhibit in vitro tumor cell growth and can affect the function of proteins, target nucleic acids, catalyze the formation of ROSs and are able to bind and cleave DNAwhich leads to cell cycle arrest and apoptosis[1]. The synthesis of transition metal complexes of unsymmetrical Schiff bases ligands with nitrogen, oxygen and sulfur atoms is an important area of study with implications in bioinorganic chemistry catalysis and medical chemistry [2]. This type of complexes, show strong intercalation with DNA and good biological activity and have received special attention. [3].

In this research work, we prepared the new complexes of La,Ce with NOS schiff base ligand has been prepared and fully characterized . The crystalline form of this complexeswere characterized by spectroscopic methods (FT-IR, UV-Vis, ^{1}H-NMR, and luminescence), elemental analysis, and the cyclic voltammetric methods. The fluorescence properties of the compounds have also been investigated. Their binding properties of La(III) and Ce(III) with salmon sperm DNA were investigated using several methods, and the results showed that the intercalated ligand had an important effect on the binding affinity of the Lanthanum and Cerium complexes with DNA. The interactions of that compound with salmon sperm DNA have been investigated by UV–Vis, fluorescence spectroscopies and gel electrophoresis.

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Synthesis, characterization and DNA-binding studies of a Palladium(II) containing mixed-ligands of 1,10-phenanthroline and salicylic acid complex

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The novel antitumor Pd(II) complex of formula [Pd(phen)(SA)] (where, phen=1,10-phenanthroline, SA=Salicylato) from the interaction of molecules $[Pd(phen)(H_2O)_2](NO_3)_2$ and sodium salt of salicylic acid (SA.Na) have been synthesized. The complex has been characterized by conductivity, elemental analysis, UV-Vis, FT-IR and ^{1}H-NMR techniques. The studies indicated that this complex is nonelectrolyte and the salicylato ligand is bidentately bound to Pd(II) ion through two oxygen atoms. The interaction of Pd(II) complex with calf thymus DNA (CT-DNA) was investigated by UV–Vis spectroscopy. This experiment imply the Pd(II) complex interact with DNA. The intrinsic binding constant (K_{app}) of interaction between CT-DNA and mentioned complex was obtained 11.25×10^4 (M^{-1}) 310K, respectively. The concentration of this complex in the midpoint of transition, $[L]_{1/2}$, at 300K and 310K are 0.011 μM M and 0.015 μM, respectively. This means that the complex can unfold CT-DNA at low concentrations and if this is used as antitumor agent, very low doses will be needed, which may have fewer side effects[1-3].

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Synthesis and characterization of nano-oxide (Co_3O_4)And(CeO_2) using precursor [(phen)$_2$(OH_2)Co(μ-SCN)Ce(μ-SCN)$(SCN)_4$Co(OH_2)$(Phen)_2$]NO_3

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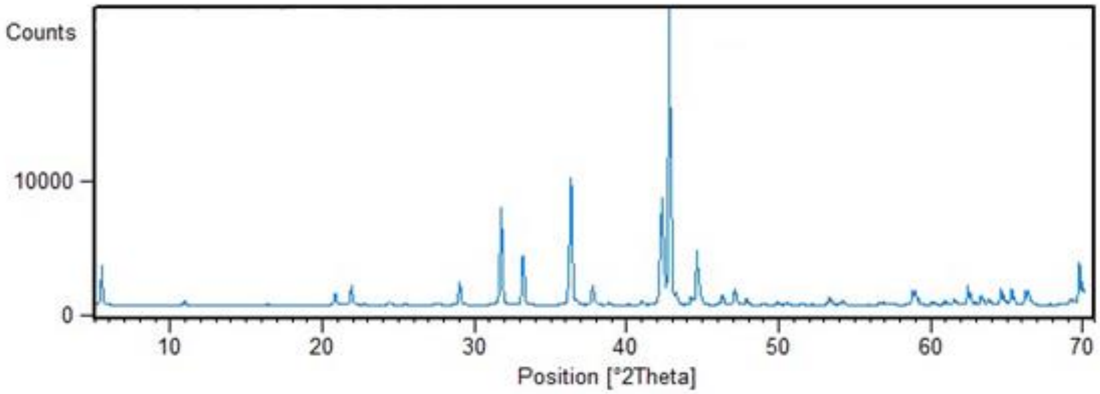
The hetero nuclear complex, [(phen)$_2$(OH_2)CO(μ-SCN)Ce(μ-SCN)$(SCN)_4$CO(OH_2)$(Phen)_2$]NO_3 (1) (phen = 1,10-phenanthroline and SCN= thiocyanato) has been prepared in aqueous solution at room temperature. This complex was purified and characterized by FT-IR , UV-Vis and atomic absorption spectroscopes.

The purpose of this research, synthesis of triple-core complex Co(II) and Ce(III) with SCN and Phen as ligand. The linear thiocyanate group can as a ligand a monodentate ligand coordinated to sulfur or nitrogen, or a bridging ligand. This complex characterized using FT-IR, UV-Vis spectroscopy and cyclic voltammetry (CV) method for electrochemical studies. To prepare nano-oxide , amount of compound **(1)** was placed in a furnace with a temperature of 1000. After calcination of this compound, sample studied using XRD and SEM techniques. Particle size was measured from the XRD data based on Debye- Scherrer¼equation. The X-ray diffraction patterns revealed that, highly pure and crystallized Co-Ce nano-oxide as (Co_3O_4)And(CeO_2) formula with Rhombohedral phases in 1000°C, with an average particle size of about less than 100nm for both nano-oxide. SEM figure show that the particles have same morphology with a uniform porous surface[1].



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Synthesis, characterization and DNA-binding studies of a metal complexes of anthranilic acid

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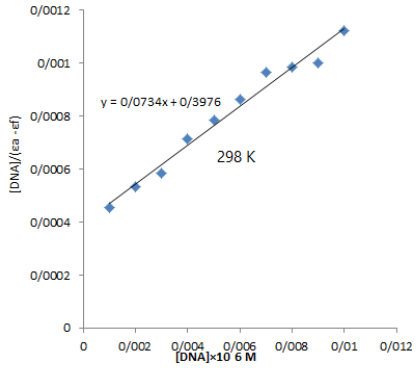
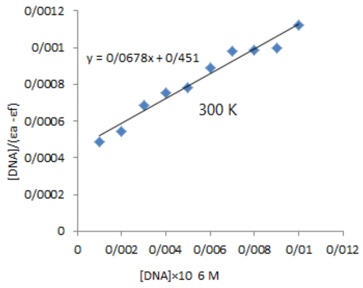
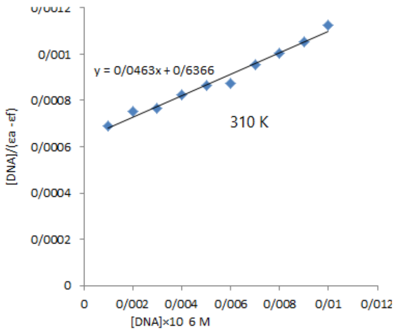
The project first synthesizes, detects and investigates the spectroscopy of complexes of Ni, Cu and Zn binomial intermediates with anthranilic acid ligands. Synthesized complexes characterized using FT-IR, UV-vis and ^{1}H-NMR. The electron spectra of these complexes have absorption bands in the region of 200-400 nm and intra-ligand transitions (n → π *, π → π *) of anthranic acid. Bands in the range of 400-800 nm attributed to d-d transitions. The results obtained from the ^{1}H NMR study are also consistent with the theoretical results [1]. Investigation of the interaction of synthetic complexes with DNA at 298, 300 and 310 Kelvin temperatures was carried out using electron-absorption spectrophotometry technique, and K_b was obtained for the bonding of the complex with DNA. The thermodynamic parameters, such as ΔG °, ΔH ° and ΔS °, were calculated [2].







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Utilization of Olive Kernel and its modified form for adsorptive dye removal

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Abstract

The wastewater of textile industries possesses toxic materials that it is needed to be removed before discharge into the environment. Several methods for dye removal from of textile plants are used. Adsorption is the most effective between these methods. In the study, Olive Kernel has been applied for dye removal. Methylene blue was selected as test probe. The experiments were carried out in a bench scale using batch system. The effect of various parameters such as initial dye concentrations (25-150 mg/L), adsorbent dosage (0.10-0.50 g), contact time (10-70 min) and the solution pH (2.0-12.0) on the removal of dye were investigated. The results indicated that the increase in adsorbent dose led to increasing of the removal efficiency. According to the results, adsorption efficiency was increased with increasing of pH and exposure time. Higher removal was observed with increasing of pH toward alkaline conditions. In order to evaluate the suitability of the introduced bioadsorbent for dye removal, isotherm and kinetic investigations were also performed. The results obtained showed that olive kernel is a cost effective and efficient adsorbent that can be applied for dye removal successfully.

Keywords: Olive Kernel , adsorbtion , methylene blue.

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Green synthesis of NiO nanoparticles using Green Tea extract

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In recent years, nanoparticles are synthesized using plant extract. Plant extract has been used an reducing and capping agent for the synthesis of nanoparticles with could be advantageous over photochemical reduction, electrochemical reduction methods[1-2]. Present research work focoused on to synthesis of NiO nanoparticles from leave extract of Green Tea plant using Green synthesis method. To synthesis the NiO nanoparticles dissolve 7g of $Ni(NO_3)_2.6H_2O$ in 50 ml of distilled water. Added leaves extract under constant stirring and achieve PH of solution became 7. The mixture was subjected to stirring for 48h on heater continuously. Afterwards in ultrasonic radiation for 30 min. Then the solution was sealed in a Teflon-lined autoclave and maintained at 80℃ for 24h, after cooling to room temperature and washed with distilled water and absolute ethanol. Next dried at 60℃ for overnight and calcined at 700℃ for 3h. The obtained NiO nanoparticles have been characterized by XRD, FTIR , SEM. The appearance of sharp band at 1457.62 cm^{-1} in the FTIR spectrum confirms the synthesis of NiO (Fig.1). The XRD pattern showed that the product consist of NiO with no characteristic peak of other impurities (Fig.2). SEM image reveals the uniformity of the average particles size and shape of the obtained NiO nanoparticles (Fig.3). The results indicate that NiO nanoparticles are in spherical shape. We can observe that the particles are highly agglometered and they are essentially a cluster of nanoparticles.

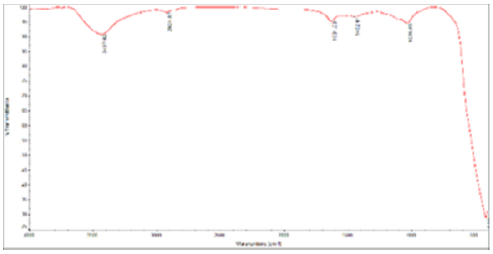

Fig 1: : FT-IR spectra

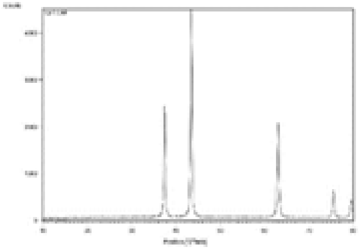

Fig 2: XRD pattern of NiO

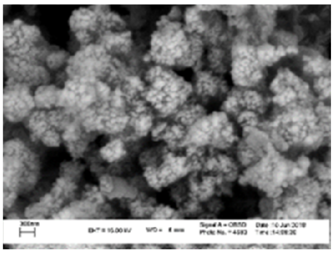

Fig 3 : FESEM image

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Synthesis, Characterization and Photoluminescence Studies of New Zinc(II) and Zirconium(IV) Complexes Containing Pyridyl Rings

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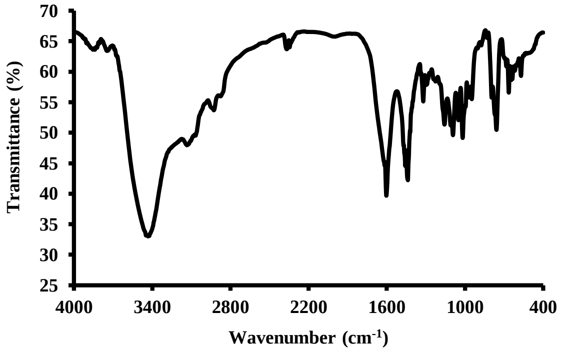
Schiff base ligands are one of the most important electron donors in coordination chemistry. Schiff bases are usually formed by condensation of primary amine and an aldehyde or a ketone [1]. The transition metal complexes of Schiff bases derived from heterocyclic compounds containing nitrogen, sulfur and/or oxygen as ligand atoms are of current interest as simple structural models of biological. Schiff base ligands and their metal complexes have a variety of applications including clinical, analytical, industrial, and organic synthesis. Schiff base metal complexes are also interesting for their contributions in material science such as photochromism, thermochromism, and catalysis such as reduction, oxidation and epoxidation process [2]. In this study new Schiff base complexs of zinc(II) and zirconium(IV), were synthesized using the Schiff base ligand containing 2-aminoethanethiol and a macrocyclic ketone with pyridyl rings and zinc(II) chloride and zirconium(IV) chloride in 1:1 molar ratio. The molar conductivity values of complexes in dichloromethane solvent implied the presence of nonelectrolyte complexes. The fluorescence properties of these complexes were studied. The Schiff base complexes were characterized by FT-IR, ^{1}H NMR, UV/Vis spectroscopies, elemental analysis, and conductometry.



FT-IR spectra of zinc(II) complex

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Essey access of various dihydropyranopyrazole derivatives promoted via Sno$_2$ nano-thin films as efficient and reusable catalyst

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With increasing interest in green chemistry, the development of new eco-friendly methods such as one-pot multicomponent reactions (MCRs) with using recyclable heterogeneous catalysts has been raised. In this study, the catalytic activity of SnO_2 based nano thin-films which prepared by spray pyrolysis technique on the inside of beakers has been reported for one-pot synthesis of dihydropyrano[2,3-*c*]pyrazoles. This catalyst is found to be efficient heterogeneous catalysts for the multicomponent reaction of 3-methyl-1-phenyl-2-pyrazolin-5-one/hydrazine monohydrate, ethyl acetoacetate with malononitrile and aryl aldehydes. The results confirm that SnO_2 nano-thin films are a potential catalytic compound for synthesis relevant to pyrazole scaffolds in high yields. Catalyst being heterogeneous lead to reused several times without a significant decrease of catalytic activity, which is in agreement with the principles of green chemistry. SnO_2 nano-thin films were developed as an efficient catalyst for the greener synthesis of dihydropyrano[2,3-*c*]pyrazoles in high yields without any troublous by-products, besides the ease of work-up and purification[1-3].

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The first report on the green catalytic activity of water extract of *Elaeagnus angustifolia L.* leaves for the synthesis of diverse 4*H*-Pyrans

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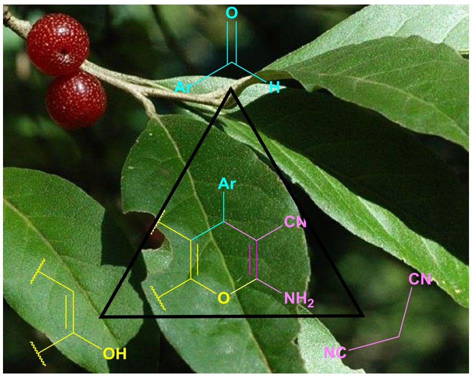
4*H*-pyran ring is a fascinating component in a broad variety of naturally occurring compounds, to the extent that the presence of 4*H*-pyran scaffold in organic compounds possessing a wide spectrum of biological properties such as anticancer, antimalarial, antimicrobial, antidyslipidemic as well as anti-inflammatory has been proven. It is remarkable to say that in order to treat some chronic diseases such as urinary incontinence, hypertension as well as ischemia, a number of drugs containing 4*H*-pyran moiety are prescribed. In the present study, a green and versatile approach for the synthesis of a variety of 2-amino-3-cyano-4*H*-pyrans is achieved via multicomponent reaction of an aldehyde, malononitrile and a CH-acid including 4-hydroxycoumarin, 3-methyl-1-phenyl-2-pyrazolin-5-one or ethyl acetoacetate/hydrazine hydrate. The reaction is properly progressed with taking advantage of extract of *E. angustifolia L.* leaves as a safe and natural catalyst. Moreover, the introduced approach is featured by mild reaction condition, short reaction time, simple work-up, easy to purification of products as well as avoiding the use of toxic solvents [1,2].



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Synthesis core shell SAPO-18/SAPO-34 as Methanol to olefin catalysts

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A series of SAPO-18/ASPO-34 nano catalysts with hierarchical porosity were synthesized by new two stage hydrothermal method using inorganic aluminum and Si sources and different type of template (Tetraethyl ammonium hydroxide and di-isopropyl ethyl amine). The properties of core-shell SAPO-18/SAPO-34 catalyst and SAPO-34 catalyst are analyzed by XRD, N_2-adsoption, FTIR and NH_3-TPD. With adding SAPO-18 to SAPO-34 zeolite gel, external surface area, total pore volume, particle size of SAPO-34 decrease but crystalinity is almost constant and SAPO-5 is not appeared in XRD diffraction. Finally, their catalytic activity in methanol-to-olefin (MTO) reaction was evaluated at 425-445 °C, These core shells catalysts showed the higher performance to propylene and C4-C5 than SAPO-34 catalysts. The working lifetime in the SAPO-18/34 catalysts was remarkably more than SAPO-34. The SAPO-18/34 catalysts were regenerated perfectly.

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Modified seeding method of hierarchical Fe-ZSM-5 SCR catalysts

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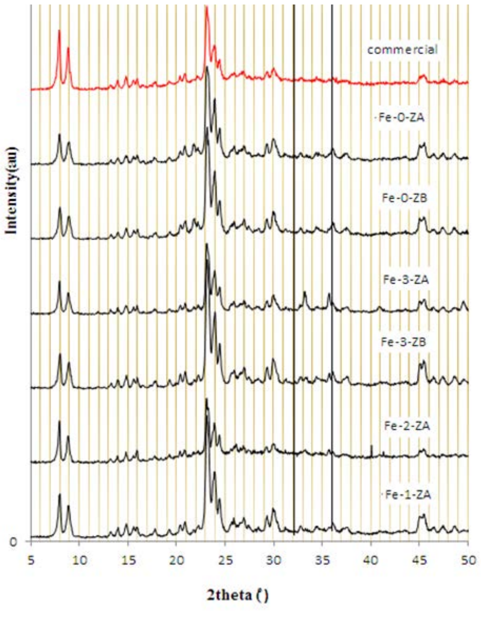
A series of FeZSM-5 nano catalysts with hierarchical porosity were prepared by the modified seed-induced method, using silicate-1 and different amounts of functionalized iron oxide in the final composition as seeds. The effect of the Fe/TMAOH ratio in iron seed and Fe/Al ratio in initial synthetic gel on the properties of Fe-ZSM-5 catalyst were analyzed by XRD, SEM, N_2-adsoption, FTIR, TPR and NH_3-TPD. By adding iron to ZSM-5 initial gel, external surface area, total pore volume, particle size,amount of aluminum in the zeolite framework and micro-porosity percent decreased but the crystallinity was almost constant and Fe_2O_3 was not appeared in XRD diffraction patterns. ZSM-5 with hexagonal structure without agglomeration were formed by increasing amount of iron in the initial gel. The catalytic performance of these samples was between 95 to 98% in nitrogen oxide catalytic reduction with ammonia.



XRD patterns of synthesized samples as well as the commercial ZSM-5 zeolite

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Green synthesis and characterization of silver nanoparticles

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The green synthesis of nanoparticles is considered as a nontoxic, clean and eco-friendly method compared to other chemical and physical methods [1]. Various types of metal nanoparticles such as silver, copper, gold, zinc, titanium, magnetite and nickel are synthesized using parts of the plants. Ag NPs have many applications in biomedicine, catalysis, energy, materials, etc [2]. In this study, silver nanoparticles were prepared with green synthetic methods using aqueous extract of galls of Quercus infectoria (Q. infectoria) as a reducing, capping and stabilizing agent. The biosynthesized Ag NPs were characterized using various techniques. UV–visible spectrum of silver nanoparticle solution showed two absorption peak at 220 and 310 nm. Scanning electron microscopy (SEM) analysis revealed that Ag NPs have spherical in shape with an average particle size of 33 nm. Transmission Electron Microscope (TEM) confirm that the synthesized AgNPs are in spherical structures and the particles have sizes of 16-38 nm. X-ray diffraction (XRD) revealed the Ag nanoparticles size that calculated using Scherrer equation is 18 nm. The spectra data show the five diffraction lines (111), (200), (220), (311), and (222), which are according with the standard pattern. This is a simple, reliable and clean procedure which could promote green industrial production of Ag NPs. Green synthesis provides an eco-friendly route for the synthesis of safe nanoparticles.

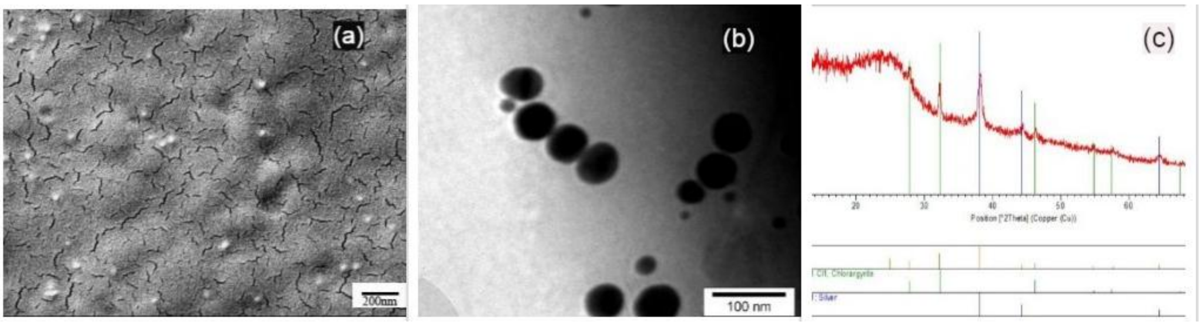

Fig. 1. a) SEM, b) TEM and c) XRD analysis of Ag nanoparticles

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Green synthesis, characterization and antibacterial activity of copper nanoparticles

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Nanoparticles are synthesized by chemical and physical processes. These methods are suffering from problems like dangerous reaction condition, expensive reagent, longer time, difficultly process to isolate nanoparticles. Green synthetic methods using plant extracts have been produced metal nanoparticles without the use of physical/chemical processes [1,2]. In this work, copper nanoparticles (Cu NPs) were prepared with green synthetic methods using aqueous extract of galls of Quercus infectoria (Q. infectoria) as reducing and capping agent. Fourier transform infrared (FT-IR), ultraviolet-visible (UV–Vis) spectrophotometry, scanning electron microscopy (SEM), energy dispersive X-ray (EDX), Transmission Electron Microscope (TEM) and spectrum X-ray diffraction (XRD) were used to characterize the samples. The results from the characterization techniques proved the formation copper nanoparticles by this novel reduction method. Highly stable Cu NPs have spherical morphology with average size about 20 nm in diameter. Antibacterial activity of the Q. infectoria galls extract and copper nanoparticles was evaluated against two Gram-positive bacteria (Bacillus cereus, Staphylococcus aureus) and four Gram-negative bacteria (Escherichia coli, Klebsiella pneumonia, Acinetobacter baumannii and Pseudomonas aeruginosa). The galls of Quercus infectoria extract and Cu NPs showed excellent antibacterial activity toward six types of bacteria. The result proved that galls extract as compared to the conventional physical and chemical processes is a very good eco-friendly and nontoxic source for the synthesis of Cu NPs.

Bacteria	B. cerus	S.aureus	P. aeruginosa	E.coli	K. pneumonia	A.baumannii	Negative control (DMSO
extract	22 mm	25 mm	22 mm	25 mm	30 mm	30 mm	0 mm
CuNPs	24 mm	31 mm	20 mm	25 mm	35 mm	28 mm	0 mm

The antimicrobial effect of the Q. infectoria galls extract and copper nanoparticles against six pathogenic bacteria

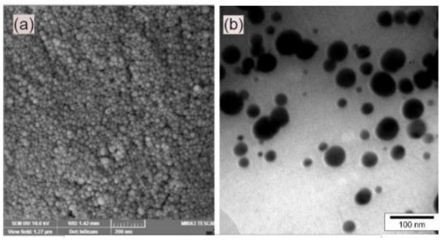

Fig. 1. a) SEM and b) TEM, analysis of Cu nanoparticles

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Fe_3O_4@CuO core–shell nanoparticles: magnetically recyclable visible-light photocatalyst

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Fe_3O_4@CuO core-shell nanoparticles synthesis by a fast, simple and low-cost method. The photocatalytic activity of this nanoparticle has investigated the removal of methylene blue (MB) in the presence of visible light. The core-shell nanoparticle was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), EDS analysis, transmission electron microscopy (TEM) and vibrating sample magnetometer (VSM). The effects of some operational parameters were studied such as H_2O_2 concentration, nano photocatalyst dosage, pH and temperature on the removal efficiency. Maximum photocatalytic activity was obtained at pH=6 and the best catalysis dosage was 0.01g. In addition, the most efficient of H_2O_2 concentration was 2 ml at 71°C. Eventually, this photocatalyst can be recovered by the external magnet from the solution.

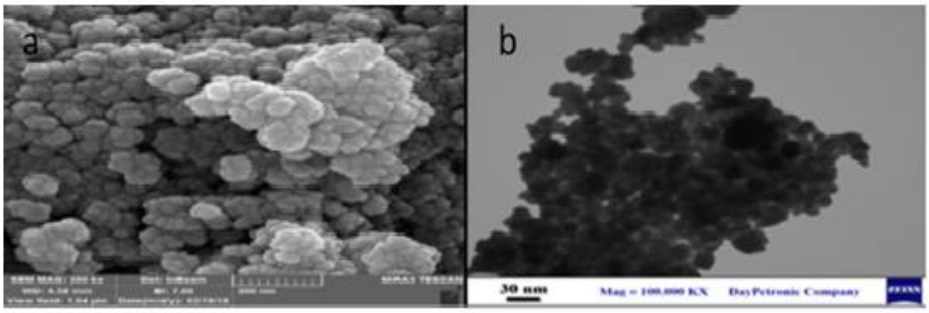

Figure 1. (a) SEM image of Fe_3O_4@CuO, (b)TEM image of Fe_3O_4@CuO

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Synthesis and characterization of nanoparticle $BaFe_2O_4$ using precursor $[Fe(bpy)_3]_2[Ba(acac)_2(SCN)_2(H_2O)_2]$

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In this investigation, we report a new nanostructured was prepared from cationic-anionic complex of formula $[Fe(bpy)_3]_2[Ba(acac)_2(SCN)_2(H_2O)_2]$ (bpy= 2 2'-bipyridine, acac=Acetylacetone).

The complex has been characterized by FT-IR, UV-Vis, conductivity measurements, elemental analysis and cyclic voltammetry (CV) method for electrochemical studies. The infrared spectroscopy results showed that bpy ligand connected to metal center by two nitrogen atomes of bpy[1]. Vibration frequencies in the region of 2052 cm^{-1} (NCS-stretching) and 843cm^{-1} (CS-stretching) confirmed that, the NCS ligand connect to metal center through nitrogen atom. Also, in this study, barium- iron nano-oxid $BaFe_2O_4$ are prepared from the complex $[Fe(bpy)_3]_2[Ba(acac)_2(SCN)_2(H_2O)_2]$ at 750°C. The nanoparticles was investigated using FT-IR, XRD (X-Ray Diffraction), SEM (Scanning Electron Microscopy), and EDX (Energy Dispersive X ray). XRD results all peaks in the XRD pattern were identified as belonging to $BaFe_2O_4$. The average size of the particles is 14.1 nm. In SEM image, it was observed that the nanoparticles with the same morphology had a uniform porous surface. The percentages of the components were obtained through EDX.

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Barium hexaferrite magnetic fluid: preparation, characterization and the *in vitro* identification of cytotoxicity and antibacterial activity

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As an alternative way to encounter antibiotic-resistant strains of bacteria, we report here a harmless magnetic fluid, which can be targeted to infections using external magnetic field and destroy the target. In this research the ultrafine $BaFe_{12}O_{19}$ nanoparticles were synthesized through hydrothermal method and for the first time, they were coated by citric acid to form the stable aqueous suspension. Characterization of the prepared (coated) oxide was performed on Furrier transform infrared spectroscopy (FT-IR), powder X-ray diffraction (XRD), field-emission scanning electron microscopy (FE-SEM), dynamic light scattering (DLS) and energy-dispersive X-ray spectroscopy (EDS) analysis. The *in vitro* cytotoxicity as well as the antibacterial activity of the surface modified nano-oxide were measured against eukaryotic cells and samples from both Grams of bacterial strains, respectively. Results showed that the superparamagnetic crystals of barium hexaferrite were successfully surface modified to form a water-based stable magnetic fluid. The magnetic fluid measured to be extremely bio compatible by 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2H-tetrazolium bromide (MTT) test. Disc diffusion and minimum inhibitory concentration (MIC) methods revealed that the surface modified nano-oxide is fetal for both the Gram-negative Escherichia coli (E. coli) and the Gram-positive Staphylococcus aureus (S. aureus). However, the fatality of the nanoparticles is lower for the Staphylococci strain.

Keywords: Barium hexaferrite. Hydrothermal. Magnetic fluid. Antibacterial activity. Cytotoxicity.

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Synthesis and characterization of nanoparticle ($NiCo_2O_4$) using precursor $\{[Co(phen)_2]_2Ni(SCN)_6\}.2H_2O$

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Abstract

In this investigation , we report a new nanostructured was prepared from heteronuclear complex of formula $\{[Co(phen)_2]_2Ni(SCN)_6\}.2H_2O$ (1) (phen = 1,10-phenanthroline and SCN= thyocyanide) has been prepared in aqueous solution at room temperature. This complex was purified and characterized by FT-IR , UV-vis and atomic absorption spectroscopes.

The purpose of this research, synthesis of triple-core complex Co(II) and Ni(II) with SCN and Phen as ligand. The linear thiocyanate group can be present in compounds as an anion or as a ligand a monodentate ligand coordinated to sulfur or nitrogen, or a bridging ligand. This complex characterized using FT-IR, UV-vis spectroscopy and cyclic voltammetry (CV) method for electrochemical studies. To prepare nanoparticles, amount of compound **(1)** was placed in a furnace with a temperature of 900. After calcination of this compound, sample studied using XRD and SEM techniques. Particle size was measured from the XRD data based on Debye-Scherrer¼equation. The X-ray diffraction patterns revealed that, highly pure and crystallized Co-Ni nanoparticles as $NiCo_2O_4$ formula with Cubic phases in 900°C, with an average particle size of about less than 100nm for both nano-oxide[1]. SEM figure show that the particles have same morphology with a uniform porous surface.

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New Synthesis and Characterization of Zeolite Y-Platinum Nanoparticles by Ultrasonic Irradiation

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Zeolites are inorganic crystalline aluminosilicates with a network of pores classified as micro porous materials. Their micro pore topology, well-proportioned surface functionality, and high stability have led to the application of zeolites in catalysis, molecular separation, and water treatment [1]. Recently, the use of ultrasonic irradiation has been extensively studied, as a new source of energy and environmentally compatible [2]. There are reports about the use of ultrasound in many areas such as sonocatalysis, preparation of materials, polymer chemistry, organic chemistry, extraction, enzymatic catalysis, electrochemistry, biomass conversion, environmental remediation [3]. Also, platinum is a noble and expensive metal with high catalytic activity and stability that has many technological applications. In this work, first zeolite Y was prepared by ultrasonic method and then platinum nanoparticles were deposited on the surface of zeolite Y using ultrasonic irradiation. The structure and morphology characteristics of the product were investigated by Fourier transform infrared (FT-IR), X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Figure 1 shows SEM and TEM images of the synthesized zeolite Y-platinum nanoparticles.

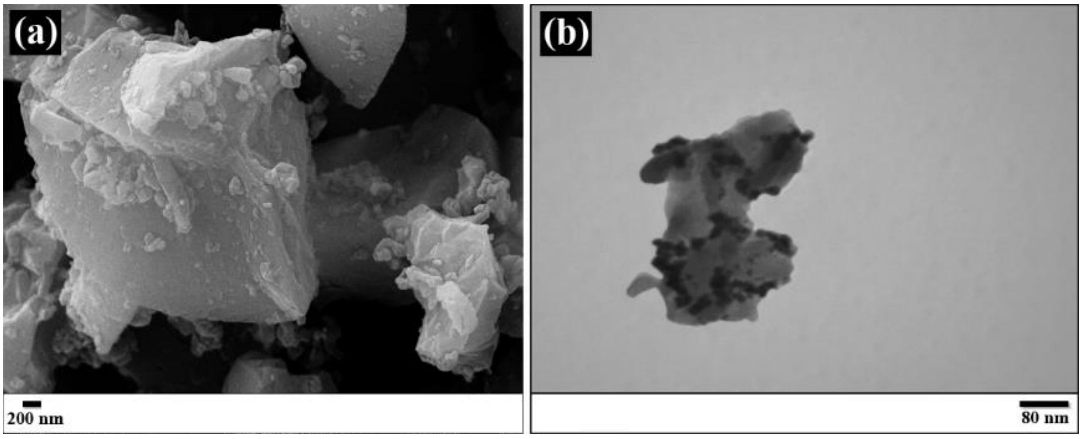

Figure 1: a) SEM image and b) TEM image of the synthesized zeolite Y-platinum nanoparticles

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Green Synthesis and Characterization of Zeolite X-Palladium Nanoparticles as a Suitable Catalyst for Suzuki Coupling Reaction

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Zeolites are nanoporous crystalline materials with a uniform pore size distribution on a molecular scale and with high thermal, mechanical and chemical stability [1]. Zeolites have shown their potential for several emerging applications, with exciting examples appeared in the field of heterogeneous catalysis, ion-exchange, adsorptive separation, storage and biomedical-related applications. Ultrasonic wave is a type of mechanical energy, distinguished by vibrations with a frequency greater than 20 kHz. When the ultrasonic wave interacts with a liquid, local high pressures and high temperatures are generated. There are many reports about the use of ultrasound as source energy in the synthesis of micrometer sized molecular sieves [2]. The palladium-catalyzed Suzuki coupling reaction between an aryl halide and a phenylboronic acid has been among the most powerful tools for constructing C-S, C-N and C-C bonds in organic synthesis [3]. Because biaryl moieties are used as the building block of a wide range of pharmaceuticals, herbicides, natural products, polymers, and etc [4]. In this study, a simple and green energy method, sonochemical, was applied to synthesis of zeolite X-palladium nanoparticles. The advantages of this method are applying green energy, short time synthesis, and creating regular zeolite. The structure and properties of zeolite X-palladium nanoparticles were characterized by various techniques. To investigate the performance of zeolite X-palladium nanoparticles, it was used in Suzuki coupling reaction as catalyst. The zeolite X-palladium nanoparticles showed high activity in carbon-carbon coupling reaction, and, interestingly, fluorobenzene could react with phenylboronic acid in presence of this catalyst.

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Synthesis and Characterization of Copper (II) Coordination Polymer with 1,3,5-Benzenetricarboxylic Acid Ligand.

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Abstract

In recent years, metal-organic frameworks (MOFs) or coordination polymers (CPs) have attracted attention due to their potential applications for gas storage, catalysis, molecular magnetism and sensors. The combinations of metal ions and organic ligands are designed in the form of one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) frameworks. The coordination geometry of the metal ions and the organic ligand geometry affect the structure and topology of the MOFs. In this research, a novel metal-organic framework (MOF) formulated as, $[Cu_2(Hbtc)_2(H_2O)_6]$ (1), has been synthesized with reaction between copper (II) and 1,3,5-benzenetricarboxylic acid. The product has been characterized by IR spectroscopy and X-ray diffraction. The complex (1) is crystallized in the monoclinic crystal system with P21/n space group. Crystal data for complex (1): a= 6.7575(3), b= 18.8415(6), c= 8.5187(5)[Å], $\beta = 92.366(4)$[°], Z= 2.

Keywords: Coordination polymer, Metal-Organic framework, Copper complex, 1,3,5-benzenetricarboxylic acid

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Chemical and Biological Sensing using Nano-Structured Single-Mode Fiber Bragg Grating

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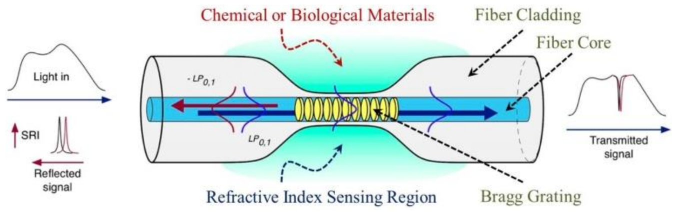
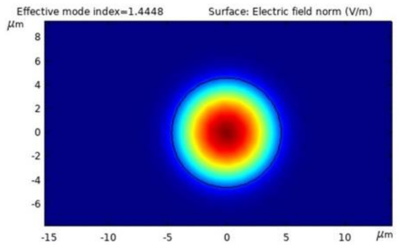
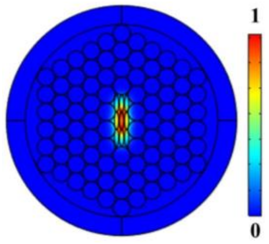
In this paper, we report a specified refractive index based sensor which is used to identify different types of chemical and biological materials using a fiber Bragg grating (FBG) structure. In nano- and micro-grating optical fibers, the wavelength of the transmitted and reflected wave would be changed by altering the chemical and biological materials around or inside the fiber Bragg grating, thus the optical property helps to detect the mentioned materials [1,2]. The functionality of this type of label-free optical sensor can be improved by optimizing structures containing a cavity in the middle of Bragg mirrors. Moreover, at the desired position the evanescent wave can be introduced and controlled to interact with these materials and consequently affect the wavelength of the photonic modes. In this paper, design and simulations for the fiber Bragg grating sensor are done by finite element method based Comsol Multiphysics commercial software. Some design strategies have been proposed to measure the reflection wavelength to improve the performance of the sensing system (Fig. 1).







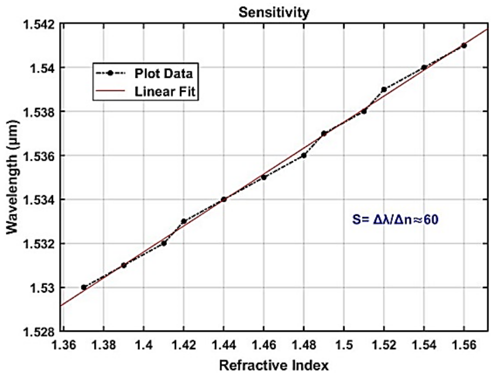


Fig. 1: Results for different micro-fiber Bragg grating based refractive index sensing of the material

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The electronic and molecular structures of some new Cu(II) complexes with tripodal amine ligands: DFT studies

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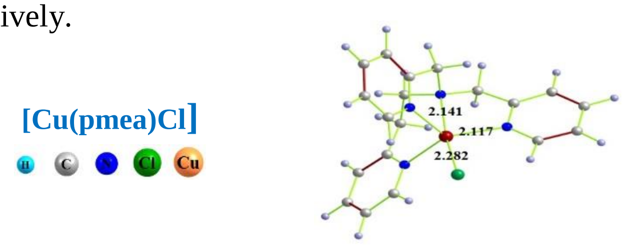
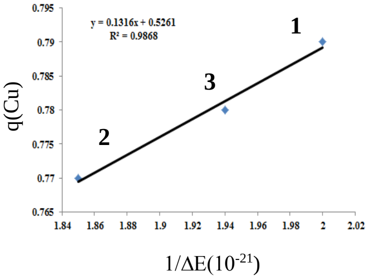
Abstract

The new anticancer complexes with tripodal ligands formulated [Cu(pmea)Cl] **(1)** **(**pmea = Bis[(2-pyridyl)methyl]-2-(2-pyridyl)]ethylamine), [Cu(pmap)Cl] **(2)** **(**pmap = Bis[2-(2-pyridyl)ethyl]-(2-pyridyl)]methylamine), and [Cu(bpdmpz)Cl] **(3)** (bpdmpz = bis[((2-pyridylmethyl)-di(3,5-dimethyl-1H-pyrazolyl)methyl)]amine) have been used for calculations at B3LYP/LANL2DZ/6-311+G (*d*, *p*) level of density functional theory (DFT)[1]. Their CIFs with CCDC (**1**) 1491458 (**2**) 1491471, and (**3**) 1558493 show that they crystallizes in triclinic, monoclinic, and monoclinic systems with *P1*, $P2_1/c$, and *C2/c* space groups, respectively[2]. The structural comparison of the mentioned complexes could followed through their physicochemical properties such as, electronic transmission in UV-Visible spectroscopy, chemical shift of metal center NMR, total energy, and frontier molecular orbitals (FMOs) energy. The relation of structure especially ligand electron donating ability with these properties has been discussed. The calculated electronic absorption spectra confirm the experimental data with electron-transition bands of intra-ligand charge transfer (ILCT) with $\pi \rightarrow \pi^*$, metal to ligand charge transfer (MLCT) with $\pi^* \rightarrow n\,(d)$, and ligand to metal charge transfer (LMCT) with $\pi \rightarrow n(d)$ character for **1**, **2**, and **3**, respectively.





Relationship between q (Cu) and 1/ΔE

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Ultrasound-assisted gadolinium-doped manganese oxide nanocatalyst and the investigation of Catalytic properties

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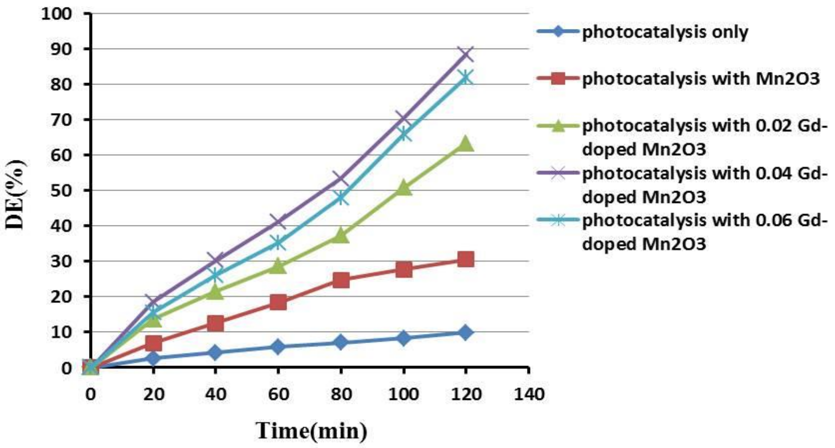
Degradation of hazardous organic pollutants existing in industrial wastewater via advanced oxidation processes (AOPs) has been an active area of research [1, 2]. Gadolinium (Gd^{3+})-substituted nanocrystalline Mn_2O_3 ($Mn_{2-x}Gd_xO_3$) was obtained by oxidation of $Mn(NO_3)_2$ at ambient conditions under ultrasound sonication in basic solution. Gd^{3+} substitution into the structure of Mn_2O_3 resulted in a material with new physical properties, composition, and morphology. The SEM, XRD, EDX, TEM, HRTEM, XPS techniques were used for characterization of as-prepared material. Increasing the amount of Gd^{3+} ions during synthesis did not increase significantly the percent substitution in the final product beyond 6%. The influence of substitution of Gd^{3+} ions into Mn_2O_3 caused a red shift in the absorbance and a decrease in the band gap. The as-synthesized compounds were used for photocatalytic degradation of Methylene Blue (MB). 6% Gd-doped Mn_2O_3 displayed the elevated photocatalytic activity considering various amounts of gadolinium. The order of inhibitory effect of radical scavengers was 1, 4 Benzoquinone > SO_3^{2-} > t-BuOH > I^- > $C_2O_4^{2-}$**.** The influence of various specifications like catalyst amount, initial dye concentration, and ultrasonic power was explored.



Photocatalytic degradation of methylene blue by Gd-doped Mn_2O_3

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Manganese Vanadate/Graphene Oxide Nanocomposites as High Energy Density Supercapacitor Materials

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The electrochemical supercapacitors have been studied extensively in recent years as an alternative type of energy storage device, owing to their fast charge and discharge rates, long cycle lifetime, and reliability. They have much larger energy density than conventional capacitors, and much larger power density and charging/discharging rate capability than batteries [1]. Transition metal oxides are good electrodic materials candidates for pseudocapacitors, which use faradaic reactions for storing energy [2]. Recently, manganese oxides have been attracted a lot of attention for this issue because of their earth-abundant and non-toxic nature [3]. In this study, nanostructured manganese vanadate as a ternary manganese oxide has been synthesized using hydrothermal method. Its crystal structure and morphology were determined by XRD and TEM, respectively. Then the surface of a piece of stainless steel has been covered by nanostructured manganese vanadate using electrophoretic method, which was used as working electrode in electrochemical tests. The specific capacity of manganese vanadate was determined using cyclic voltammetry, charge-discharge curves and electrochemical impedance spectroscopy. To modify its electrical conductivity, some nanocomposites containing manganese vanadate and different amounts of graphene oxide were prepared and their capacitive behavior were investigated.

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Ultra-Sensitive Chemical Gas Sensor based on Slot and Cavity Strip Silicon Waveguide

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Identification and analysis of chemical compounds and products are of great importance for researchers in Chemistry, especially in the Organic and Analytical Chemistry. Accordingly, chemical sensors due to their sensitivity to change and certain chemical compounds, can identify these compositions, and provide information which needed by researchers to analyze. In this paper, an ultra-sensitive optical sensor ($S \approx 2.5$) is introduced for chemical gases such as CH_4, CO, CO_2, NO, N_2O and H_2O as well. Due to the high optical power, and consequently, the increased risk of the reaction of combustible chemical gases in the earlier sensors, the ineffectiveness and the high risk of using those sensors have become more and more recognized. Since the maximum optical absorption of CH_4 is in the wavelength of $\lambda = 3.39$ μm, therefore He-Ne laser can be used in the studies. Another reason to choose such exciting optical sources are their lower power and thereby they can eliminate the risk of explosion of the combustible gases such as CH_4[1,2]. The proposed optical sensor structure in this paper is a slotted strip waveguide in the Silicon core that comprises two cavities (with radius R) which is grown on Silica substrate. The optical interaction of the evanescent field with CH_4 gas changes optical parameters such as the effective refractive index [1]. These changes are the basis of sensing in such optical sensors [2]. Hence, in this research, we try to increase the confinement of the electric field in the slotted region and therefore increasing the possibility of optical interaction with CH_4 in this region (Fig. 1). This combined configuration causes the proposed sensor to perform extraordinary sensitivity to the gaseous fluids passing through the gap region.

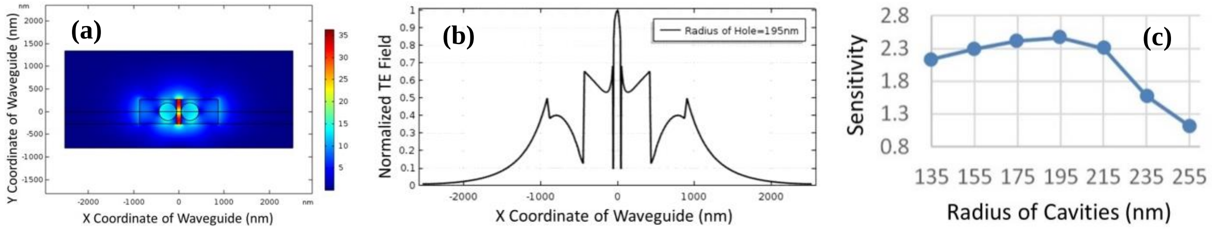

Fig. 1: a) Quasi TE mode distribution, and b) Normalized transverse electric (TE) field, in the sensor. c) The sensitivity of the sensor for different radius of the cavity.

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Green synthesis of Ni/NiO nanocomposite using Calotropis procera plant

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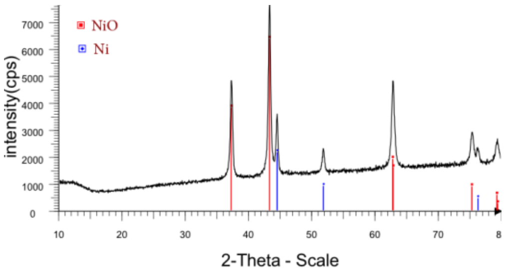
Nanocomposite (NC) materials have gained much attention and interest of scientists in recent years because of their improved properties than the single metal nanoparticles. Nanocomposite is a combination or matrix, in which different materials combine to develop new properties of the materials ensuring that one of the materials have size in range of 1-100nm. There are hence two parts on NC i.e. continuous phase and discontinuous reinforcing phase. Nanocomposite can be prepared from any combination of materials that can be categorized into three basic building blocks i.e. metals, ceramics and polymers [1].The nanocomposite can have a combination or have markedly different mechanical, electrochemical, electrical, catalytic, thermal and optical properties from the component materials [1, 2]. Further, these NC have emerged as materials of 21st century that offer number of technological and business breakthroughs in all the sectors of life.

In this work, Ni/ NiO nanocomposite was synthesized using Calotropis procera plant. For this aim, at first, 5 ml distilled water was added to 0.085 g of this plant. This bio nanocomposite was characterized by SEM,TEM,XRD and AFM. The average size of Ni nano particle and nickel oxide nano particle were 5 and 75 respectively.

Calotropis procera



Ni/NiO nanocomposite

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Synthesis and characterization of CdO nanoparticles starting from Calotropis procera

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Nanoparticles have attracted great interest recently due to their unique physical and chemical properties, which are different from those of either the bulk materials or single atoms. In recent years, many researchers have focused on cadmium oxide (CdO) due to their applications in several areas of research, specifically in optoelectronic and other applications, including solar cells, phototransistors, photodiodes, transparent electrodes and gas sensors [1]. Cadmium oxide (CdO) is n-type semiconductor used as a transparent conductive material prepared as a transparent conducting film back. Various methods have been used for the synthesis of CdO nanoparticles such as thermal process, precipitation method, sonochemical method and microemulsion, but these methods have limited control to achieve technological grade particles for their industrial applications and these procedure are not cost-effective and complex approach is involved which are not environmental friendly [2]. Hence, green synthesis of CdO is so important approach for industrial application.

In this work, CdO nanoparticles were prepared by simple and cheap strategy using *Calotropis procera* plant. These green CdO bio-nanoparticles were characterized by TEM, SEM, XRD and DLS.

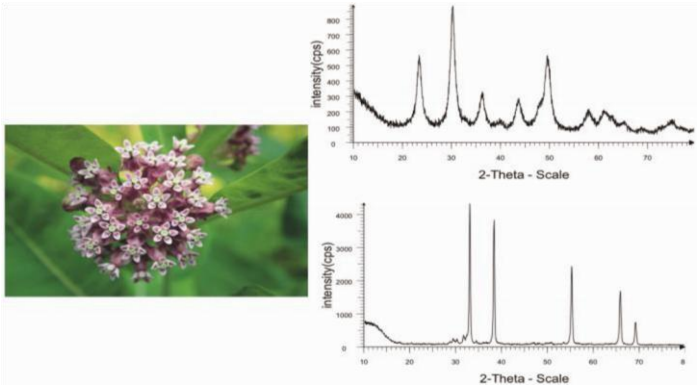

Fig.1. The synthesis of CdO nanoparticles using *Calotropis procera*

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Synthesis and characterization of metal complexes with Schiff Base ligand derived from 2-aminobenzoic acid with 2-nitrobenzaldehyde

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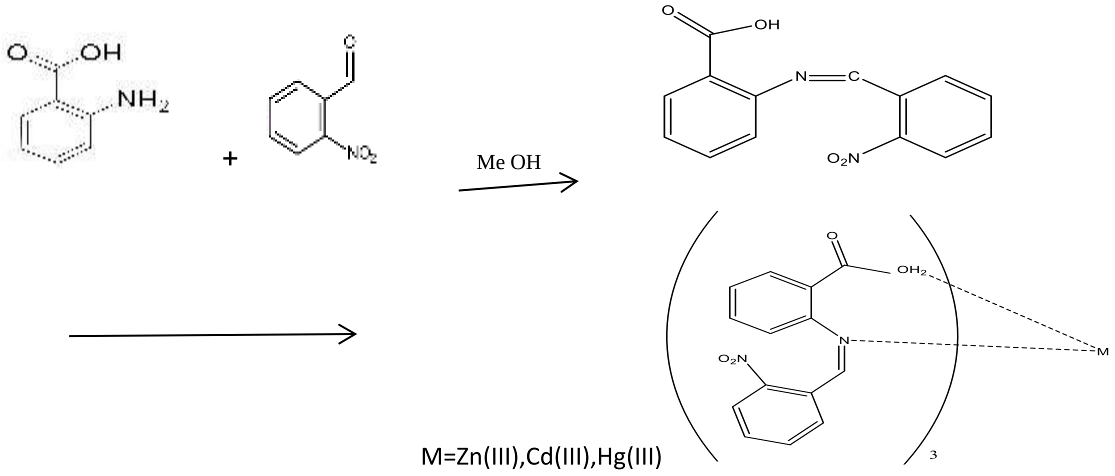
The Schiff bases are based on the first type of amine condensation with carbonyl compounds, the functional group of which is Azometine or Amine, which has a double bond of nitrogen The magnitude of these ligands can be attributed to the magnetic properties, drug properties, catalytic properties, fluorescence properties, and nonlinear and biological optical properties [1]. Schiff Bases are a group of organic compounds with a C = N-R functional group and because of the easy availability of nitrogen, they are used as intermediates for the metal as a ligand[2]. Also to evaluate the thermal stability of the synthesized complexes and to examine their antimicrobial activity against different species of bacteria and fungi [3]. In this research work, NO Schiff base ligand prepared by reaction of 2-amino-benzoic acid with 2-nitrobenzaldehyde. Zn(III), Cd(III) and Hg(III) Schiff base complexes of this ligand were synthesized. The Schiff base ligand and related complexes were characterized by IR, UV-Vis, NMR, Mass spectrometry, conductivity and elemental analyses.



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Use of palladium nanosheets on graphene substrate for oxidation of formic acid in fuel cells

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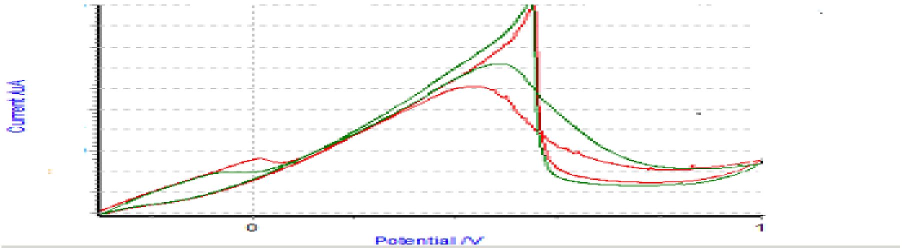
Palladium nanosheets have many uses in industry, medicine, biotechnology and etc. Also it useful for interaction in chemical reaction and Formic acid oxidation that use as fuel in fuel cells. One of its most important applications in the medicine for cancer treatment.Its clinical application are hindered by many particle problems such as low accumulation in tumors, high laser power density and high bioxicity in the body. Herein, it can serve as pH – responsive drug carriers to efficiently delivered DOX into cancer cell and tumors. In this paper, we study the nanosheets of palladium to oxidize the Formic acid in an acidic environment in the presence of ethanol.This process is contained in four steps: The first step preparation of nanosheets was made by Pd(acac)$_2$ and reduced by Co. Two step is the construction of the electrode. And tree step use it for Formic acid oxidation in the fuel sell on the acid environment. Then cyclic voltammetry (CV) and (CAM) method for electrochemical studied. Data CV shows that Alcohol oxidation generates flow in the forward reaction and climbing the curve to the oxidation of primary oxidation products (Figure1).Data CV show that when the electrode is placed in a constant potential, rapid oxidation of alcohol occurs at the Electrode level and over time, the flow decreases exponentially. Finally, we reach a stable state and the flow is fixed.



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Selective adsorption of cationic dyes from aqueous solution by polyoxometalate based metal– mineral framework composite

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The pigment obtained is suitable for the textile industry and the dyeing process of fibers, yarns and fabrics, and is in line with environmental and anti-allergenicity.A novel environmental friendly adsorbent H6P2W18O62/MOF-5 was synthesized by a simple one-step reaction under solvothermal conditions and characterized by XRD, FTIR, thermogravimetric analyses (TGA) and N2 adsorption–desorption isotherms. The removal rate of H6P2W18O62/MOF-5 was quite greater (85%) than that of MOF-5 (almost zero), showing that the adsorption performance of porous MOF-5 can be improved through the modification of H6P2W18O62. Further study revealed that H6P2W18O62/MOF-5 exhibited a fast adsorption rate and selective adsorption ability towards the cationic dyes in aqueous solution. The removal rate was up to 97% for cationic dyes methylene blue (MB) and 68% for rhodamine B(Rhb) within 10 min. However, anionicdye methyl orange(MO) can only reach to 10%. The influences including initial concentration, contacttime, initial solution pH and temperature of MB adsorption onto H6P2W18O62/MOF-5 were investigated in detail. The kinetic study indicated that the adsorption of MB onto H6P2W18O62/MOF-5 followed the pseudo second-order model well. The isotherm obtained from experimental data fitted the Langmuir model, yielding maximum adsorption capacity of 51.81 mg/g. The thermodynamic parameters analysis illustrated that the MB adsorption onto H6P2W18O62 immobilized MOF-5 was spontaneous and endothermic process. Besides, these results implied that designing a novel material polyoxometalate-based metal–organic frameworks is great potential for removing cationic organic pollutants and even extended to improve other specific application.

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Synthesis and Characterization of a new magnetic Fe(III)Salophen complex as a heterogeneous bio-relevant catalyst

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Schiff-bases derived from an amino and carbonyl compound are an important class of ligands that coordinate to metal ions via azomethine nitrogen and have been studied extensively. They have wide applications in food industry, dye industry, analytical chemistry, catalysis, fungicidal, agrochemical and biological activities [1]. With the increasing incidence of deep mycosis, there has been increasing emphasis on the screening of new and more effective antimicrobial drugs with low toxicity. Schiff-base complexes are considered to be among the most important stereochemical models in main group and transition metal coordination chemistry due to their preparative accessibility and structural variety [2]. Not only have they played a seminal role in the development of modern coordination chemistry, but also they can be found at key points in the development of inorganic biochemistry, catalysis and optical materials. To improve the stability and activity of Schiff base complexes in catalysis, many functional materials, and in particularly magnetic nanoparticles (MNPs) have been intensively investigated [3]. In this work, we designed a new magnetic nanocatalyst via anchoring of Fe(III)salophen complex on γ-Fe_2O_3 providing a heterogeneous catalyst. The structural integrity of as-prepared nanomaterial was confirmed by several analytical techniques such as FT-IR, EDS, VSM and TGA. Then, its catalytic oxidation activity was compared with free Fe(III) salophen complex.

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Catalytic Decolorization of Rhodamine B by magnetic nanoparticles modified with Fe(III)Salophen complex

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Dyes are extensively used in printing, textile and food industries. It is estimated that about 10 – 15% of unused dyes are discharged into the water environment during production and utilization [1]. Several methods such as adsorption, coagulation and biodegradation have been investigated and developed for dye wastewater treatment [1]. But due to their limitations, these methods were not efficient to destructively degrade dyes. Advanced oxidation processes (AOPs) have been proven to be effective technologies for the degradation of dyes in recent years [2]. Persulfate ($S_2O_8^{2-}$) was investigated as a suitable oxidant for the degradation of organic pollutants such as azo dye, diphenylamine and trichloroethylene [3]. In this study, Fe(III)salophen complexe supported on γ-Fe_2O_3 was synthesized as heterogeneous catalyst to activate persulfate to effectively degrade Rhodamine B (RhB).The effects of some operational parameters such as initial solution pH, amount of catalyst, initial concentration of RhB and persulfate, and reaction temperature were studied. Finally, the free radicals participating in the process were classified by radical quenching studies, and a rational mechanism was proposed based on obtained results to understand the catalytic process.

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A novel eco-friendly procedures, for the Synthesis of Spiro-Oxindole derivatives via alcoholic extractive of Angustifolia leaves as the catalyst and solvent

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Heterocyclic compounds such as spiro-oxindoles occupy a particular place in chemistry, because of their 'privileged structure' in a wide spectrum of pharmacological and organic chemistry. Spiro-oxindole framework represents the biological and pharmacological activities such as anti-fungal, anti-microbial, anti-oxidant, anti-malarial and anti-tumor. Because of their unique chemopreventive, the expansion of synthetic methods providing easily obtained to this heterocycle are still desirable [1]. Herein, we investigated Angustifolia leaf extract as a new catalyst to a known synthesis of spiro-oxindole derivatives via condensation of isatin derivative, malononitrile, and 1, 3-dicarbonyl compounds under mild reaction conditions (Fig. 1). This efficient route and green methodology for novel synthesis of spiro-oxindoles derivatives has a number of advantages such as short reaction time, high yields (87–95%), use an alcoholic extract of Angustifolia leaves [2] as the solvent and catalyst [3], simple workup procedures and avoidance of hazardous or toxic organic solvents and catalysts. The structure of desired compounds have been described by their physical and spectral data (such as melting points, ^{1}H NMR and ^{13}C NMR spectra and elemental analyses).

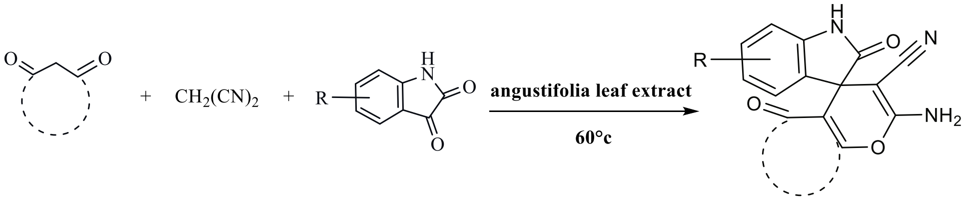

Fig. 1. Synthesis of spiro-oxindole-pirane derivatives in Angustifolia leaf extract

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Synthesis and Characterization of Lead(II) Complex with a Terpyridine Derivative Ligand

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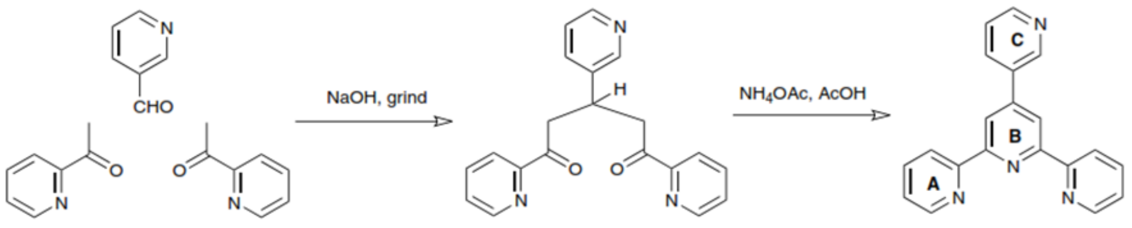
The complexes containing terpyridine derivatives have been widely studied. Terpyridine complexes may be used in photochemistry to design fluorescent devices or as sensors for converting light to electricity. In clinical chemotherapy and biochemistry, functional therapeutic agents have received a wide range of potential uses from colorimetric determination to DNA bonding materials and anti-tumor research [1]. In this project (4′-(3-pyridile)-2,2′:6′,2″-terpyridine) was synthesized. On the other hand lead has attracted much attention among the metals in the main group. Not only because of biological activity, but also because of its great radius, variable stereo chemical activity and flexible coordination, which provides unique opportunities for obtaining new coordination mode [2]. In this study the aim is preparation and identification of lead(II) complex with a ligand of the derivatives of the terpyridine. The ligand and the complex were evaluated by different spectroscopy methods.



Synthesis of 4′-(3-pyridile)-2,2′:6′,2″-terpyridine

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Investigation of interaction between [Pd(en)(2-pyc)]NO_3 and bovine serum albumin (BSA) using fluorescence spectroscopy

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Many drugs are transported in the blood while bound to albumin. Therefore, investigation of the Drug-protein interaction is important to know mechanism of the transport of a drug in the body. In the present study, bovine serum albumin (BSA) has been used as the protein model because of the abundance, cheapness and similarity with the human serum albumin[1]. Herein, the interaction between a recently made palladium(II) complex of formula [Pd(en)(2-pyc)]NO_3 (where en = 1,2-diaminoethane and 2-pyc = 2-pyridinecarboxylate anion), as a potential anti-tumor agent, and BSA was studied by fluorescence spectroscopy. The fluorescence titration experiments in Tris-HCl buffer of pH = 7.00 were performed at a fixed BSA concentration while varying the concentration of metal complex. The obtained data indicated that the Pd(II) complex strongly quench the intrinsic fluorescence of BSA. Analyzing of the data using Stern–Volmer equation, the quenching constant (K_{sv}), binding constant (K_b), number of binding sites (n) and the bimolecular quenching rate constant (k_q) have been calculated. Using these date, thermodynamic parameters were calculated too. Decreasing the equilibrium rate constants with increasing the temperature indicates that the quenching mechanism of BSA by the Pd(II) complex is static quenching. The negative values of ΔH^o and ΔS^o show that hydrogen bonds and van der Waals force play a major role in the binding of the Pd(II) complex to BSA [2].

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Synthesis and characterization of new Schiff Base N-donor ligands with metal complexes and investigation of biological effect of them

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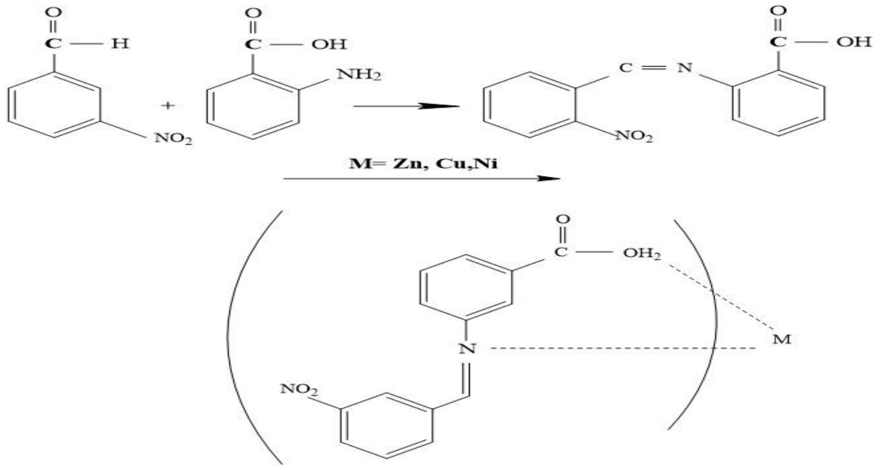
Schiff bases, named after Hugo Schiff [1], are formed when any primary amine reacts with an aldehyde or a ketone under specific conditions. Structurally, a Schiff base (also known as imine or azomethine) (Fig. 1) is a nitrogen analogue of an aldehyde ketone in which the carbonyl group (C = O) has been replaced by an imine or azomethine group.Schiff bases are some of the most widely used organic compounds. They are used as pigments and dyes, catalysis, intermediates in organic synthesis, and as polymer stabilisers [2].Schiff bases have also been shown to exhibit a broad range of biological activities, including antifungal, antibacterial. antimalarial, antiproliferative, anti-inflammatory, antiviral, and antipyretic properties [2,3]. Imine or azomethine groups are present in varios natural, naturalderived, and non-natural compounds (see Fig. 2 for some examples). The imine group present in such compounds has been shown to be critical to their biological activities.In this research work,No, Schiff base ligand prepared of 2-amino benzoic acid with 3-nitro benz aldehyde. Zn(II), Cu(II) and Ni(II) Schiff base complexes of this ligand were synthesized. the Schiff base ligand and related complexes were characterized by IR, UV-Vis, NMR, Mass spectrometry.



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Modifying of Nanostructured $MnWO_4$ by Ca-, Cu- and Co-Doping towards Artificial Photosynthesis Applications

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Nowadays, the human societies encountered some serious environmental problems because of population growth and industrialization. One of them is increasing the amount of CO_2 in the atmosphere [1]. It has been shown that during natural photosynthesis water oxidation happens on the surface of a Mn-Ca oxide complex and produced proton travels to another site which CO_2 reduction occurs on it [2, 3].

In this study, we prepared nanostructured manganese tungstate by reflux method and modified it by doping with Ca^{+2}, Co^{+2} and Cu^{+2} ions. The morphology and crystal structure of prepared materials were investigated by TEM and XRD techniques, respectively. The specific surface area of prepared samples were determined using BET and their bandgaps were determined with a combination of DRS and electrochemical impedance spectroscopy. Finally, their abilities towards electrochemical water splitting and CO_2 reduction were investigated by linear sweep voltammetry.

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Kinetic studies of complex formation between Co(II) ion and 2, 2'-bipyridine with UV-Vis and Stopped Flow techniques

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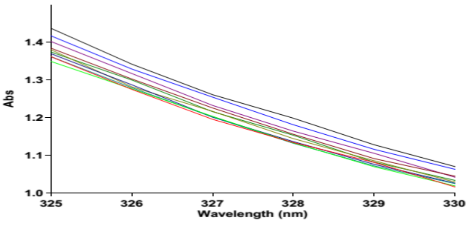
Macrocycle molecules are an interesting class of compounds that have attracted much attention in recent years. Specifically, the coordination chemistry community has been interested in the study of such compounds due to the increased kinetic inertness and thermodynamic stability of their metal complexes compared to their acyclic analogues [1,2]. In this project kinetics and mechanism of the reaction between cobalt(II) choloride and 2,2'-bipyridine as a bidentate ligand were investigated using UV-Vis spectrophotometry technique. The results indicated that reaction follows a second order reaction. Overall rate constants (k_{obs}), activation energy (E_a) and other parameters ($\Delta S^{\ddagger}$،$\Delta H^{\ddagger}, \Delta G^{\ddagger}$)were reported. In addition, useful information were obtained on the rate of reaction from study of effects of temperature and solvent. Experimental data exhibited that second step of each reaction is a rate determining step (RDS). In addition, fast step of reaction was studied by Stopped – Flow method. Also determination of reaction stoichiometries was recognized by the Yoe and Jones method. The results indicated that the cobalt (II) and 2,2'-bipyridine stoichiometric ratio is 1: 3.



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DFT Study of Thermodynamic Parameters of One New Schiff Base Ligand and Their Complexes

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To investigate the stability of [H_2L] Schiff base ligand (where: L = derived methyl-2-(1-methyl-2'-aminoethane)amino-1-cyclopentenedithiocarboxylate) and their Ni(II) and Cu(II) complexes in gas phase, some properties such as HOMO-LUMO energies, chemical hardness and binding energy were obtained by using the gradient corrected density functional theory (DFT) method with the B3LYP functional [1] and LANL2DZ and 6-311G* basis sets. The optimized geometries of [H_2L] shows the mentioned ligand can act as an NNOS tetradentate chelating agent using the thion sulfur atom (S), the nitrogen atom (N) from (N=CCH_3) group, the primary nitrogen atom (N) and the hydroxyl oxygen atom (O). The title ligand contains two planar fragments, *vis.* the cyclopentene and salicylate derivatives moieties. The ligand uses its four atoms to link the metal ion. Therefore, the metal centre is in a tetracoordinated environment and the geometry about the metal ions could be described as square planar for [NiL] and square planar distorted for [CuL]. A large HOMO-LUMO energy gap increase stability and decrease chemical reactivity [2]. The calculation results confirm that the [CuL] complex is the most stable than [NiL] complex. This finding is further supported by the fact that the experimental formation constants of these complexes.

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pH-stable porous mechanically interlocked 2D metal-organic polyrotaxane for in situ organochlorine insecticide encapsulation, sensing and removing

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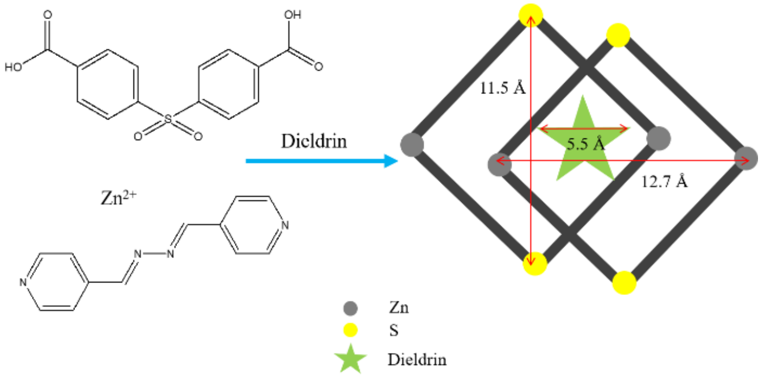
Mechanically interlocked structures such as rotaxanes, catenanes, and borromean rings are new materials [1], which are known for their interesting structures and have made an impact with their potential applications in different fields such as molecular machines so that the 2016 Nobel Prize for Chemistry was awarded for work on such systems [2]. 4,4′-Sulfonyldibenzoic acid (H_2sdba) is a V-shaped organic ligand (Scheme 1), which is used in many mechanically interlocked molecular architectures such as interlocked supramolecular metal-organic frameworks (MOFs) and coordination polymers (CPs) [3]. In this work we introduce a new porous 2D metal-organic polyrotaxane, $[Zn_2(sdb)_2(4\text{-bpdb})]\cdot 2DMF$ (**1**) 4,4′-sulfonyldibenzoate (sdb),4-bis(4- pyridyl)-3,4-diaza-1,3-butadiene (4-bpdb), possesses channels that could in situ encapsulate and remove dieldrin as a harmful organochlorine insecticide to form a host-guest system. pH stability, strong luminescence nature, very sensitive and complete quenching in presence of dieldrin introduce **1** as a precious sensor for dieldrin.



Synthesis route of **1** and dieldrin@**1** with dieldrin and void space dimensions from side and cross views

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Synthesis and characterization coordination of polymers of a new Cd(II) with bidentate flexible ligands

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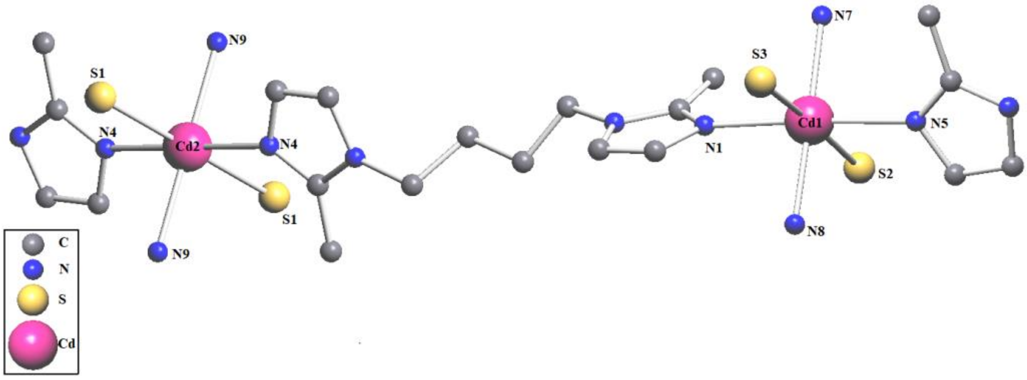
A new coordination polymer, $[Cd(\mu_2\text{-}SCN)_2(bib^{Me})]_n$ (**1**), was prepared at room temperature by the reaction of appropriate salt of cadmium(II) with the flexible linker ligands 1,4-bis(imidazolyl) butane (**bib**) and methylimidazolyl)butane (**bib^{Me}**). The compound was characterized by elemental analyses, IR spectroscopy and single crystal X-ray diffraction. In the polymeric structure of **1**, the Cd(II) ion adopt the CdN_4S_2 pseudo-octahedral geometry and two bib^{Me} ligands are coordinated to one central Cd(II) to form 2D framework with new topology (Point symbol: $3^9.4^{10}.5^2$).



View of the coordination environment of Cd(II)

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Active and Recyclable Graphene Encapsulated Fe_3O_4 Magnetic Organometallic Photocatalyst for Degradation of Congo Red

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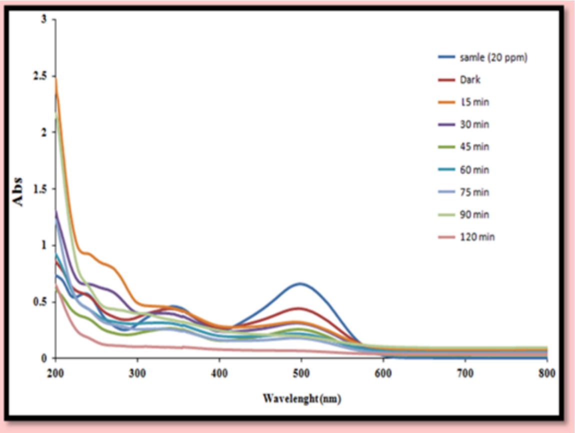
In this work, a novel photocatalyst, reduced graphene oxide encapsulated Fe_3O_4–Pd magnetic nanohybrid was synthesized and characterized. Then, this magnetic catalyst showed high catalytic activity for the degradation of Congo red under visible light irradiation. Magnetic separation is an environmentally-friendly alternative method for the separation and recovery of catalysts, since it minimizes the use of solvents and auxiliary materials, reduces operation time, minimizes catalyst loss by preventing mass loss and oxidation. Also High yield, low reaction time and non-toxicity of the catalyst are the main merits of this protocol.



Dependence of degradation of Congo red to the presence of light and catalyst.

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Synthesis, characterization DNA / BSA interaction and antibacterial studies of Zn(II) N_2O-Schiff base complex

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Schiff base of ortho-phenylenediamine and acetylacetone alone and their Zn(II) complexes have a variety of biological applications including antibacteriale, antifungal, anticancer and other properties[1-3].The present investigation includes in situ synthesis of 4-(2-amino-phenylimino)-pentene-2-ol (acac-o-PhdaH) ligand and its Zn(II) complex. This complex of formula [Zn(acac-o-phdn)Cl] have been characterized by FT-IR , UV-Vis and ^{1}H-NMR spectroscopic techniques and conductivity measurements. These studies showed coupling of 1:1 stoichiometric ratio of ortho-phenylenediamine and acetylacetone. DNA / BSA and antibacterial studies of the above mentioned Zn(II) complexes are in progress.

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Synthesis of $ZnFe_2O_4$ nanostructure for supercapacitor application

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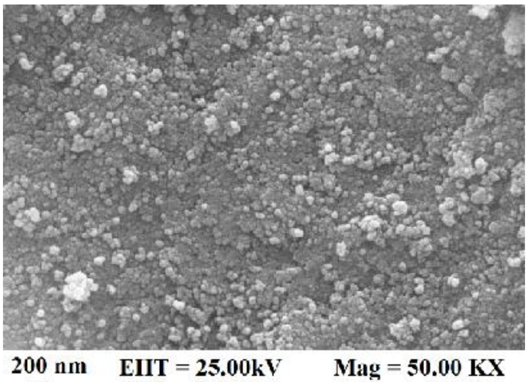
Worldwide growing demand for portable electronic devices and electric vehicles has motivated the research and development of energy storage devices like supercapacitors [1-2]. Among the various energy storage systems, supercapacitors are important source of energy storage devices and power outputs. Typically, supercapacitor shows reasonable energy with high power density and long cycle life [3]. In this work, $ZnFe_2O_4$ nanoparticles have been prepared by sonochemical method. $Fe(NO_3)_3.9H_2O$ and $Zn(NO_3)_2.6H_2O$ were used as reagents and the resulted precursor was calcined in the air. The precursor and resultant product were characterized using thermogravimetric analysis (TGA), fourier transform infrared (FT-IR), X-ray powder diffraction (XRD), scanning electron microscopy (SEM) as well as Transmission Electron Microscope (TEM). Cyclic voltammetric (CV) measurements gave a maximum specific capacitance of 490 F/g at a scan rate of 1 mV/s. For this sample 95% of this specific capacitance was retained after 5000 cycles.



SEM image of $ZnFe_2O_4$ nanoparticles.

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A facile and green sonochemical route for the synthesis of $ZnFe_2O_4$ nanoparticles

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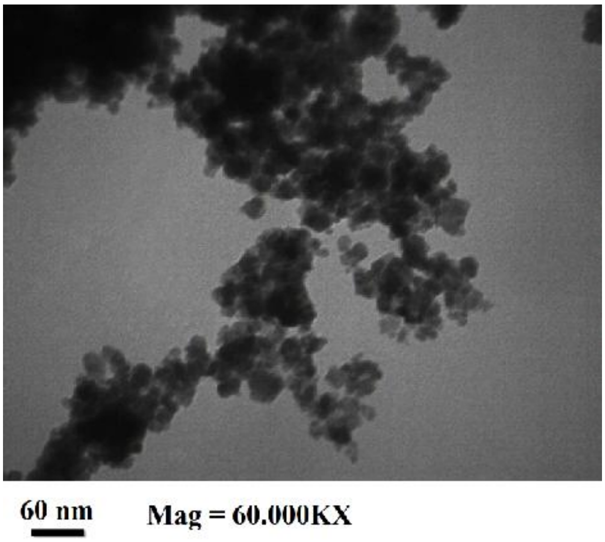
Recently spinel transition metal oxides (AB_2O_4) containing two metal elements have gained great attention as promising electrode materials. Particularly, among the spinel metal ferrites (MFe_2O_4), $ZnFe_2O_4$ is the most promising due to its low toxicity, high specific surface area, good chemical performance and ultralow-cost, environmental benignity and rich abundance [1-2]. In this research, $ZnFe_2O_4$ nanoparticles have been prepared by sonochemical method via weak ultrasonic irradiation at DI water. $Fe(NO_3)_3.9H_2O$ and $Zn(NO_3)_2.6H_2O$ were used as reagents and the resulted precursor was calcined in the air at 400°C for 3hours. The precursor and resultant product were characterized using thermogravimetric analysis (TGA), fourier transform infrared (FT-IR), X-ray powder diffraction (XRD), scanning electron microscopy (SEM) as well as Transmission Electron Microscope (TEM).



TEM image of $ZnFe_2O_4$ nanoparticles.

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Kinetic and Mechanism of H_2O_2 Decomposition on Keplerate $\{Mo_{72}Fe_{30}\}$ Nanoball

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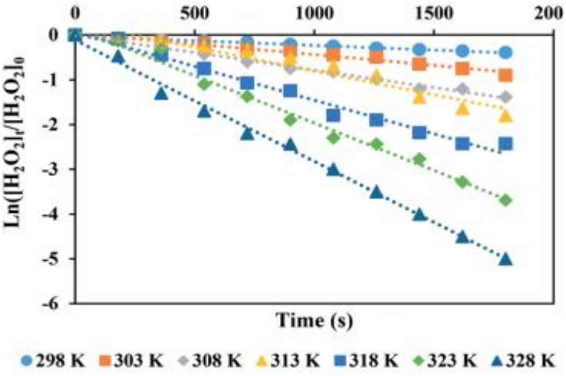
Hydrogen peroxide (H_2O_2) is an important regulator of cellular events leading to glucose transport activation in mammalian skeletal muscle. However, the hydroxyl radical produced by hydrogen peroxide causes DNA and membrane damage, lipid peroxidation, and cell death [1]. It is widely used as bleaching and oxidizing agent in medicine and chemistry. It has been previously reported that the catalytic decomposition of hydrogen peroxide follows the first-order kinetics with respect to H_2O_2 [2]. In this study, the kinetics and mechanism of hydrogen peroxide decomposition on the surface of Keplerate nanoclusters containing $Fe^{(III)}$ and $Mo^{(VI)}$ is investigated. The first-order kinetics with a rate constant of 3×10^{-4} s^{-1} at T=298 K was obtained for the decomposition of H_2O_2. To determine the activation energy, the rate constants as a function of temperature in the temperature interval T = [298–328] K was obtained. The activation energy of the reaction was found to be 58.74 kJ mol^{-1}. The second-order rate constant for the reaction at 298 K was 3×10^{-8} ms^{-1}. The negative results of scavenging experiments using terephthalic acid and methanol as OH radical trapping agents led us to propose a non-radical mechanism for hydrogen peroxide decomposition on the surface of cluster molecules.



ln $[H_2O_2]_t / [H_2O_2]_0$ as a function of reaction time for T = 298, 303, 308, 313, 318, 323 and 328 K

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Photochemical Properties of Iron (III) containing Polyoxomolybdate Nanoclusters

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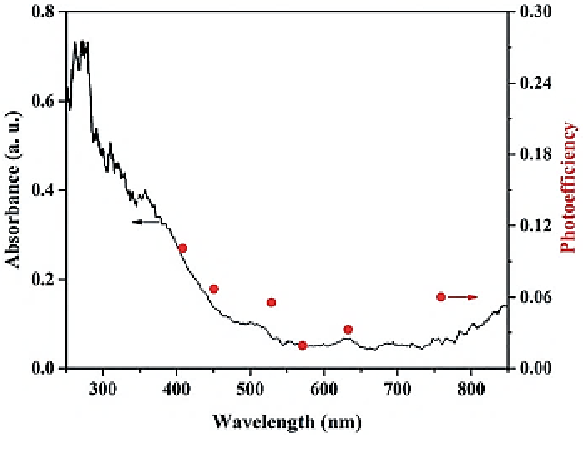
The photocatalytic reaction demonstrates the possibilities of converting light energy into chemical energy. Recently, much attention has been paid to the use of visible light to drive chemical reactions because of the abundance of visible light, its benign environmental impact, and sustainability. Polyoxometalates (POMs), a large group of metal oxide clusters, having electronic and structural diversity possess broad applications in many fields of science, such as catalysis, materials science, and biology [1]. In this work, we investigated photocatalytic decomposition of H_2O_2 on iron (III) containing polyoxomolybdates as the catalyst. When the reaction was subjected to visible light irradiation, H_2O_2 decomposed completely in less than 1h. The optical properties of the nanoclusters were evaluated by diffuse reflectance UV-vis spectroscopy. According to the band gap value (2.12 eV), the clusters could be visible light sensitive photocatalysts. The effect of different light wavelengths on the H_2O_2 decomposition in the presence of this nanoclusters was examined under visible light irradiation using different cut-off filters. The initial rate of the H_2O_2 decomposition was found to be wavelength dependent [2]. The photoefficiency is in good accordance with the diffuse reflectance absorption spectrum which further suggests that the catalyst is efficient in the visible region.



Photocatalytic action spectrum for H_2O_2 decomposition on iron (III) containing nanoclusters

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Synthesis and characterization of Mn(III), Ni(II), Cu(II), Zn(II), and Cd(II) complexes containing a new tridentate Schiff base ligand

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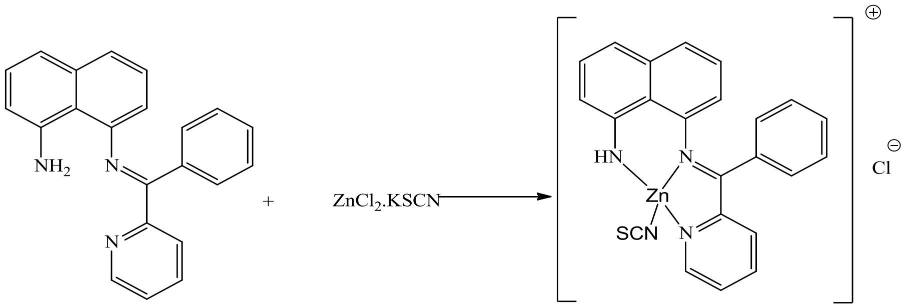
Schiff bases are an important class of organic compounds, which are known as donor-acceptor systems in coordination chemistry [1]. These compounds are synthesized by the condensation of primary amines with carbonyl groups [2]. The Schiff base complexes are used as catalysts, antimicrobial and antitumor components, etc. [3].

In this research project, at the first step, a new tridentate Schiff base, ((E)-N1-(phenyl(pyridin-3-yl)methylene)naphthalene-1,8-diimine) was synthesized by the reaction of 2-benzoylpyridine and 1,8-diaminonaphthalene in 1:1 mole ratio. At the next step, some of the transition metal ions such as: Ni(II), Cu(II), Zn(II), and Cd(II), were reacted with the Schiff base ligand. At last, it was followed by the reaction with potassium thiocyanate to produce the desired Mn(III), and Zn(II) complexes containing an isothiocyanato monodentate ligand. The ligand and its complexes were Characterized by FT-IR, UV-Vis, and ^{1}HNMR spectroscopic data, thermal and elemental analysis, magnetic and conductivity properties.



Synthesis of Zn(II) complex containing the Schiff base and isithiocyanato ligands

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Synthesis and identification of Fe(II), Ni(II), and Zn(II) complexes containing a tetradentate Schiff base ligand

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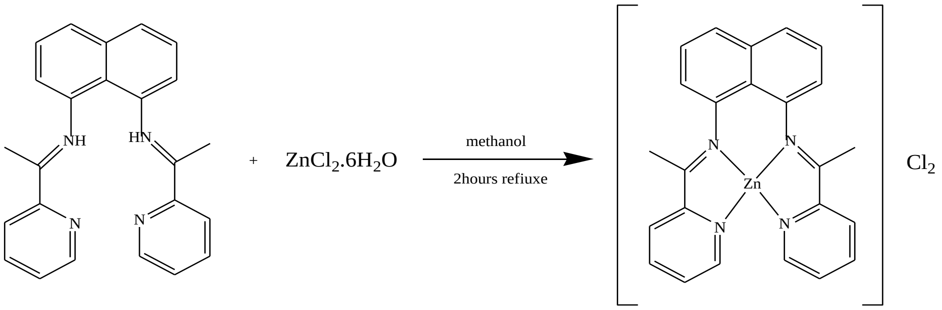
Schiff base compounds are synthesized by the condensation of amines with carbonyl/aldehyde groups. These compounds and their metal complexes have been synthesized because those are able to stabilize metal ions in various oxidation states [1]. Schiff base complexes are often utilized as catalysts with high performance for producing organic compounds. A well known series of the complexes containing a tetradentate Schiff base moiety can be used as oxygen carriers which are useful models for biochemical processes [2].
In this reseach project at the first step, a new tetradentate Schiff base ligand of N,N-bis-(2-acetylpyridine)-1,8-diamino naphthalene, (L) was synthesized. The ligand was confirmed by various analytical technics. At the second step, its Fe(II), Ni(II), Cu(II), and Zn(II) complexes were synthesized in a 1:1 molar ratio. The mentioned complexes investigated and characterized by using Gouy balance, elemental and thermal analysis, conductometry, and FT-IR, UV-Vis, spectroscopic techniques. FT-IR spectra of all the complexes exhibit the imine (C=N) bond which is shifted with respect to the imine peak of the Schiff base ligand. Besides, all the complexes, except for Zn(II), are paramagnetic with the appropriate unpaired electrons.



Synthesis of M(II)L complex

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Inorganic salts effect as further study on the reaction mechanism and kinetics of 2-dimethyl 2 (2,4dioxothiazolidin-3-yl) fumrarate: Experimental approach

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In the present work, the kinetics and mechanism of the reaction among dimethyl acetylendicarboxcylate (**DMAD**), Thiazolidine-2, 4-dione (**TZD**) and triphenylarsine (**TPA**) as a catalyst was conducted in the methanol solvent using UV/vis spectrophotometry technique, for the generation of 2-Pyrrolidin-1-yl-but-2-enedioic acid dimethyl ester [1]. Increasing the reaction rate with the lowest cost can be an extra large challenge. Accordingly, the effect of different salts on the reaction rate [2] were considered. Enhancing the polarity of the solvent from ethanol (ε = 24.5) to methanol (ε = 32.7) increased the reaction rate about five times but the addition of salts to the solution has a much stronger effect on the reaction rate. The reaction rate among DMAD, TZD and TPA in the methanol solvent with salt content is about 68.5 times higher than the reaction rate [2] in the absence of salt. Activation energy (E_a= 25.74kJ.mol^{-1}) and its related parameters were determined ($\Delta H^{\ddagger}$ = 23.39 J.mol^{-1}, $\Delta S^{\ddagger}$ = -175.59 J.mol^{-1}K^{-1}, $\Delta G^{\ddagger}$ = 75.83 kJ.mol^{-1}). And associative mechanism, chemically and enthalpy-controlled being of the reaction documented. Pursuant to the effect of changing the reaction medium by temperature, solvent and salt step$_4$ recognized as RDS [3]. The overall order of the reaction was two, and partial orders of reactants **DMAD** and **TZD** were one and one, respectively. Also, the order of catalyst (**TPA**) was experimentally determined to be one.

Keywords: Inorganic salts effect, triphenylarsine, kinetics and DMAD

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A Novel Combustion Method to Fabricate of Porous NiO: Application as Catalyst Support to Immobilize Palladium Nanoparticles for Methanol Electrooxidation

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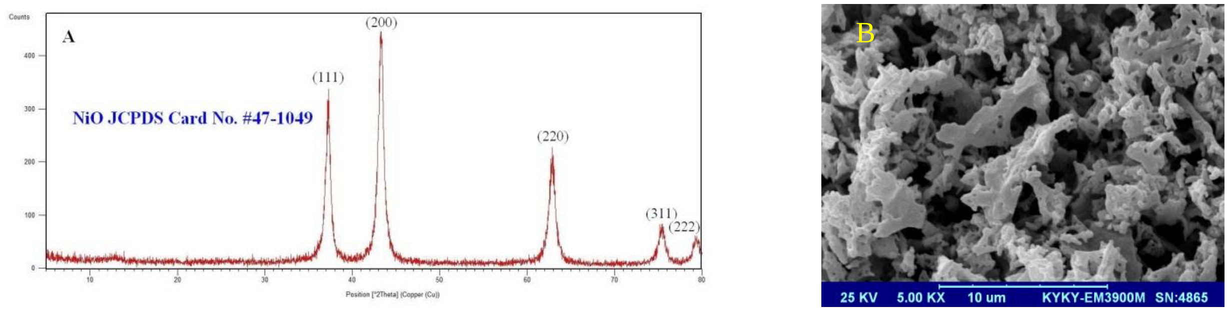
A significant percentage of researches on fuel cells are focused on the presentation of electrocatalysts for the oxidation of alcohols [1]. Due to different properties of metal oxides such as: low thermal conductivity, great thermal stability and high resistance to chemical degradation [2]; they can be a convenient support for catalytic particles. In the present study, the solution combustion synthesis method (SCS) was utilized to fabricate NiO with high surface area and large porosity using glycine as a fuel. A self-sustained exothermic reaction among organic fuels (e.g., glycine) and oxidizers (e.g., metal nitrates) is occurred in SCS; so that, the combustion of organic fuels produced a much amount of gaseous products like H_2O, CO_2 H_2, CO, and N_2, leading to porous structures. In the following, the crystalline phases of as-prepared NiO were identified by X-ray diffractometer. Also, the morphology and particles size of the powder were detected through the scanning electron microscope. Then, the palladium nanoparticles were reduced onto the surface and into pores of NiO powder. The electro-catalytic activity of resultant nanocomposite was investigated towards the oxidation of methanol in alkaline solution by using electrochemical techniques.



XRD pattern (A) and SEM image (B) of as-prepared the synthesized NiO powder

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Synthesis and identification of 2-(((E)-(2-hydroxy naphthalen-1-yl)methylene)amino)-3-(((E)-thiophen-2-ylmethylene)amino)maleonitrile schiff base ligand and its Ni(II), Cu(II), Mn(II), Cd(II), Zn(II) complexes

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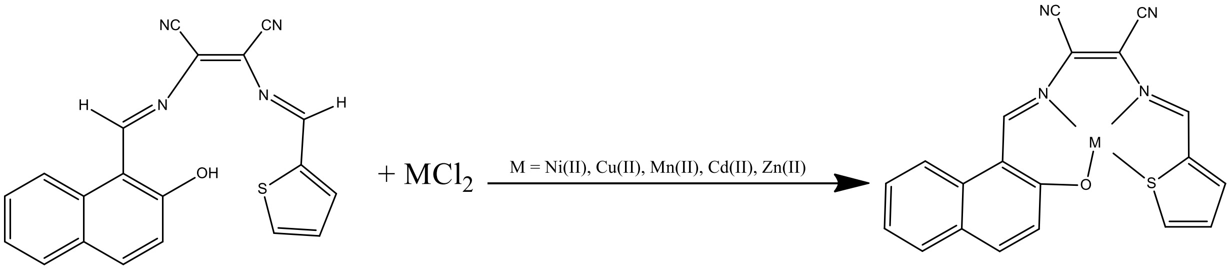
Schiff base compounds, play a key role in the coordination chemistry. These ligands can form stable complexes as chelating ligands [1]. Metal complexes derived from Schiff base ligands that have both hard atoms, such as oxygen and nitrogen, and soft atom as sulfur in their structure, show interesting chemical properties. These complexes have been used as models for biological systems. The synthesis and use of asymmetric Schiff base as catalysts for various types of reactions have been considered more than before [2]. The main purpose of this study is synthesis and identification of Ni(II), Cu(II), Mn(II), Cd(II), Zn(II) complexes containing a new derivative of the diaminomaleonitrile which reacts as a tetradentate ligand. In this project an asymmetric Schiff base ligand, 2-(((E)-(2-hydroxy naphthalen-1-yl) methylene) amino)-3-(((E)-thiophen-2-ylmethylene) amino) maleonitrile was synthesized. The ligand and its complexes were charactrized by different analytical methods, such as FT-IR and UV-VIS spectroscopy, CHN, TG-DTA and ICP analytical techniques and magnetic susceptibility measurement.



synthesis of MCl_2, [M = Ni(II), Cu(II), Mn(II), Cd(II), Zn(II)] with 2-(((E)-(2-hydroxy naphthalen-1-yl)methylene)amino)-3-(((E)-thiophen-2-ylmethylene)amino)maleonitrile

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Chalcogen bonding in copper(I) complexes of sulfur-containing ligands: structural and charge density analyses

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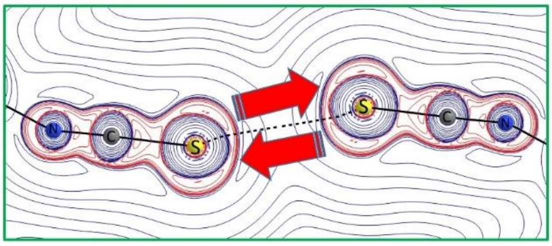
Chalcogen bonding involving synthesized sulfur-containing compounds have crucial importance in supramolecular chemistry and crystal engineering [1], which involves finding the subtle role of non-covalent interactions in controlling the supramolecular architecture of coordination compounds. Even though the reports on electronic anisotropy in non-covalent interactions involving sulfur was negligible in the past, it has been highlighted in dozens of recent studies [2,3]. Herein, we report on the synthesis of new copper(I) complexes with sulfur-containing ligands. The influence of sulfur interactions on the supramolecular assemblies has been investigated by geometrical analysis and theoretical calculations. Topological analysis has also been employed, with respect to the Laplacian of electron density, in order to inspect the physical characteristic of the CB interactions. The non-covalent sulfur interactions in crystalline structures have been evaluated by wave function and DFT methods to acquire intuition into the CBs. So, the S···X (X= S, O, N, Cl) interactions, can be categorized as a lump-hole interaction; a region of charge depletion (hole) of sulfur, interacts with a region of charge concentration (lump) of another involved atom in the valence shell charge concentration (VSCC) which forms a chalcogen bond.



Lump-hole interaction

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A novel highly selective colorimetric sensor for Cu(II) ion using azo-azomethine derivatives

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The development of highly sensitive and selective probes for the sensing and recognition of environmentally and biologically important ionic species, especially metal ions, has been of great interest in recent years [1]. Among the metal ions, the design and synthesis of sensitive and selective probes for the detection of Cu2+ has attracted much attention, as it is the third most abundant essential trace element after iron and zinc in biological systms and plays a vital role in a variety of fundamental physiological processes in organisms ranging from bacteria to mammals[2].Copper is an essential nutrient for life and its homeostasis is connected to severe diseases such as Menkes, Wilson and Alzheimer's disease [3]. In the present work, we have developed a novel azo–azomethine receptor, for colorimetriction of Cu^{2+} ions. To reach receptor **L**, 5-(4-CH_3-phenyl)-azo-salicylaldehyde was introduced into the naphthol skeleton to afford effective metal binding sites via nitrogen and oxygen heteroatoms. The new receptor was characterized by IR, ^1H NMR and mass spectrometry. To investigate the selectivity of receptor **L,** the UV–Vis absorption spectral behavior upon addition of metal ions was monitored. The proposed sensor shows a reasonable discrimination ability towards Cu^{2+} ion in comparison to some alkali, alkaline earth transition and heavy metal ions (Fig.1). The resulting Cu(II)-complex was characterized by IR and mass spectrometry.

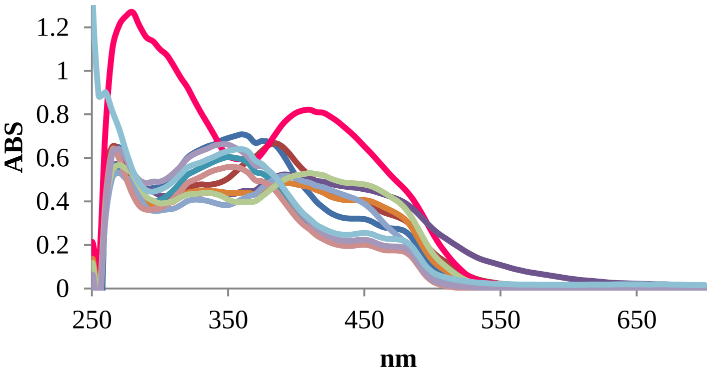

Fig.1. UV–Vis absorption spectra of receptor **L** in the presence of 10 equiv. of various metal ions

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Triple-decker lanthanide Schiff base complex

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Salen type Schiff-base ligands as one of the best known organic ligands with an N_2O_2 cavity has been modified to various derivatives in respect to the expected functions. These type ligands have played an important role in coordination chemistry for over half a century. It is known that salen type ligands are able to stabilize various different metals in various coordination environments [1, 2]. Polynuclear lanthanide complexes and double- and triple-decker complexes has attracted considerable attention in the field luminescent and magnetic properties because of their potential applications in the preparation of new optical, quantum computing, high-density information storage, and molecular spintronics [3]. Our recent studies have focused on the use of a salen-type Schiff base ligand to stabilize Tb(III) centers and to provide the antenna for lanthanide luminescence. An interesting emerging feature exhibited by these complexes is the self-assembly of stacked “multi-decker” structures in which Tb(III) ions are sandwiched between alternating layers of the Schiff base ligand. the reaction of equimolar amount (N,N_0-bis(1-naphthaldiamine)-*O*-phenylenediamine) and $Tb(NO_3)_3$ $.xH_2O$ in absolute MeCN, afforded the “triple-decker” ($[Tb_2L_3]$) architecture (fig.1). The resultant product was identified via IR and Mass spectroscopic methods.

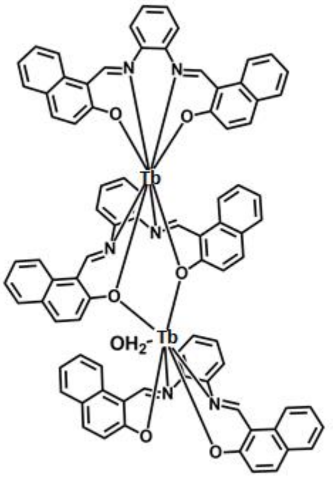

Fig.1.

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Novel inorganic precursor for Fischer-Tropsch synthesis

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The Fischer–Tropsch synthesis (FTS) is highly noteworthy for production of clean fuel from syngas [1,2]. Conversion of the hydrogen and carbon monoxide to hydrocarbons at the presence of a catalyst is a fundamental step in the FTS process. Hence, selecting a suitable catalyst plays a key role in crop distribution [3]. A novel coordination polymer formulated as $[Co_{1.68}Ni_{1.32}(btc)_2(H_2O)_{14}].4H_2O$ (**1**) was synthesized with reaction between cobalt nitrate, nickel nitrate and 1,3,5-benzenetricarboxylic acid. The complex (**1**) was characterized by elemental analysis, FT-IR spectroscopy and its structure was determined by single crystal X-ray diffraction. Silica and alumina-supported Co-Ni catalysts were prepared through thermal decomposition of respective inorganic precursors and also by the impregnation method as reference catalysts. The catalytic activity of these catalysts was evaluated for Fischer–Tropsch synthesis (FTS) at a fixed bed reactor. The catalytic performance of the synthesized catalysts was superior to the catalysts produced by the impregnation procedure. The catalysts were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), and BET specific surface area.

Keywords: *Fischer–Tropsch synthesis, inorganic precursor, impregnation.*

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Reduction of nitrofurazone in aqueous solution by a novel catalyst based on Ag nanoparticles on mesoporous silica

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Among the different noble metal nanoparticles, silver nanoparticles (Ag NPs) have attracted immense attention due to their wide applications in various fields such as biology [1], and catalysis [2]. Several investigations have been reported on preparation and catalytic activity of Ag NPs. Nitrofurazone is a type of antibiotic and has been widely used in food-producing livestock. Cytotoxicity and DNA damage by nitrofurazone has been reported [3]. Hereby we report the synthesis of a novel catalyst based on Ag nanoparticles on mesoporous silica and its application as an effective catalyst in reduction of nitrofurazone in aqueous solution. The synthesized Fe_3O_4@SiO_2@KIT-Ag nanomaterial was characterized by powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM), and scanning electron microscopy (FE-SEM). For example, FT-IR spectrum of Fe_3O_4@SiO_2@KIT-6-NH_2 nanocomposite is shown bands at 462 and 561 cm^{-1} are attributed to the Fe-O vibrations of Fe_3O_4 in tetrahedral and octahedral sites. In addition, the broad and intense peak at 1072 cm^{-1} is attributed to asymmetric stretching vibrations of Si-O-Si. Also, stretching vibration of the N-H functionalities was observed at 3421 cm^{-1}.

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Effect of pH for Lead removal from Aqueous Solution applying Montmorillonite

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Wastewaters containing heavy metals as contaminants originate from a large number of metal-related industries and mines. Heavy metals are toxic and nonbiodegradable, and their presence in streams and lakes leads to bioaccumulation in living organisms, causing health problems in animals, plants, and human beings [1]. To avoid water pollution, treatment, that is, the removal of heavy-metal ions from industrial wastewaters is needed before disposal. Several conventional techniques are used for removing heavy metals from aqueous solutions [2]. Compared with other conventional techniques, adsorption appears to be an attractive process in view of its efficiency and simplicity of operation in the treatment of wastewaters containing heavy metals, as well as the availability of a wide range of adsorbents [3]. Large-scale sorption processes for the treatment of wastewaters containing heavy metals demand inexpensive, nontoxic, and available sorbents with known kinetic parameters and sorption characteristics. Clay minerals are good adsorbents for metal ions from aqueous solutions owing to their high cation exchange capacities, high abundance and local availability, nontoxicity, chemical and mechanical stability, Brønsted and Lewis acidity, low costs, and ability to be recycled.

In this study, the effect of pH on Lead elimination from Aqueous Solution using montmorillonite has been investigated (Fig.1). The montmorillonite clay before and after of Pb adsorption was characterized by X-Ray Diffraction (XRD) and Field emission scanning electron microscopy (FE-SEM).

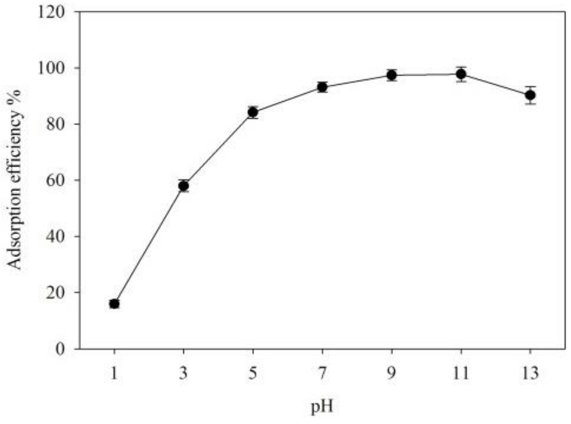

Fig.1 Effect of pH on the removal rate of Pb(II) (50 ppm) using montmorillonite (20 mg), contact time (15 min) .

Refs.

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Effective Removal of Lead (II) Ions from Aqueous Solution Using Montmorillonite/TiO_2 Clay

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Lead (Pb) is the third-most common toxic element in the heavy metal toxicity list. It is also one of the 10 chemicals that the WHO has set out as a cause for significant public health concerns [1]. The removal of Pb (II) has become a great concern globally due to these toxic effects of Pb (II) on living beings. In the past few years, various techniques have been used for lead removal [2]. Among these methods, adsorption has the advantages of being easy to perform and having a low cost and high efficiency. Thus, it has been used commonly in the heavy metal pollution treatment of water [3]. Clay as an adsorbent is widely used for the removal of heavy metals and has great applicability due to its being economical and having an environment-friendly nature, a high adsorption capacity, and a wide pH range.

In this study, montmorillonite/TiO_2 (Mont/TiO_2) mineral was made nano-size and characterized by FT-IR, XRD and FE-SEM. Then nano Mont/TiO_2 was used to adsorb Pb(II) in the aqueous solution. Figs.1a, b shows the effect of dosage of adsorbent and contact time on the removal of Pb(II) ion in the presence of Mont and Mont/TiO_2, respectively. The obtained results show that the efficiency of these adsorbents is such that a small amount of adsorbent, even 20 mg can eliminate a significant amount of lead ion (II) (50 ppm) over a short period of time (5 minutes).

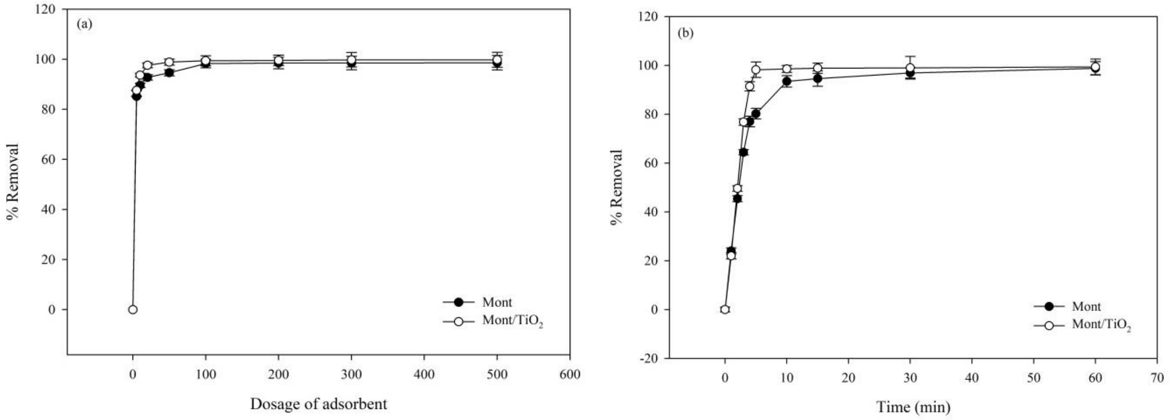

Fig.1 Effect of (a) adsorbent dosage and (b) contact time on the removal rate of Pb (II) (50 ppm), pH 7.

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Synthesis and characterization coordination of polymers of a new Zn (II) with bidentate flexible ligands

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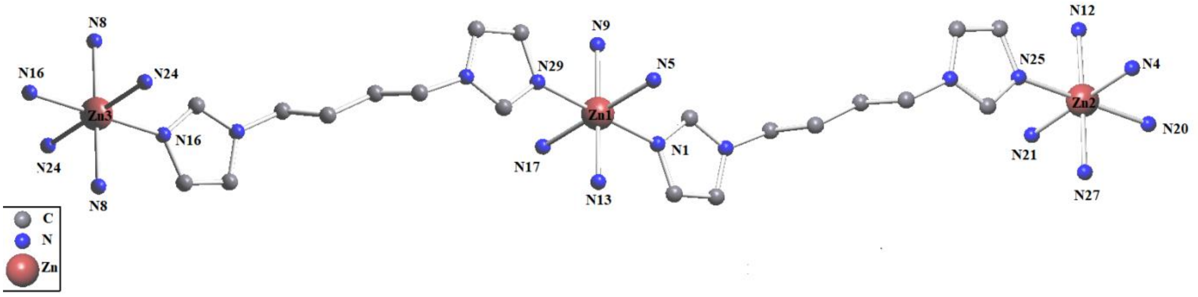
A new coordination polymer, $\{[Zn(bib)_3](ClO_4)_2\}_n$ (**1**), was prepared at room temperature by the reaction of appropriate salts of zinc(II) with the flexible linker ligands 1,4-bis(imidazolyl) butane (**bib**) and methylimidazolyl)butane (**bib**^{Me}). The compound was characterized by elemental analyses, IR spectroscopy and single crystal X-ray diffraction. In the polymeric structure of **1**, the Zn(II) ions lies on an inversion center and adopts the ZnN_6 octahedral geometry. In compound **1**, six bib ligands are coordinated to one central zinc(II) to form an open 3D 2-fold interpenetrating framework of the a-polonium (pcu) type topology.



View of the coordination environment of Zinc(II)

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Synthesis and characterization of $Nd_xSr_2As_2O_{7+\delta}$ by solvothermal method

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Mixed metal oxides have drawn considerable attention in many applications such as immobilization of fission products, catalysis [3], and solid electrolytes [10]. They have also been used in various environmental and bio-industrial applications such as in degradation of organic pollutants. The main objective of this study was to synthesize and characterization of $Nd_xSr_2As_2O_{7+\delta}$ using As_2O_3, $Sr(NO_3)_2$ and Nd_2O_3 by solvothermal method (ratio H_2O:Ethanol was 1:1) at 200 °C for 24 h(pH=12) . The employed techniques are XRD, SEM and DRS. XRD pattern of powdered sample is presented in Fig.1. Rietveld analysis showed that the obtained material was crystallized well in the monoclinic and tetragonal crystal structures . The crystallite size of the sample was calculated from x-ray lines broadening of the reflections of using Scherrer's equation(D=24 nm). Fig.2 shows the FESEM image of sample. It shows that the product is consisted of high-length rods and sheets.The optical properties of the obtained material showed that the material has strong absorption in UV light region. The direct optical band gap energies of the two samples show that there are two distinct band structures. So, two band gap energies are present in the spectra at about 3.00 and 3.40 eV.

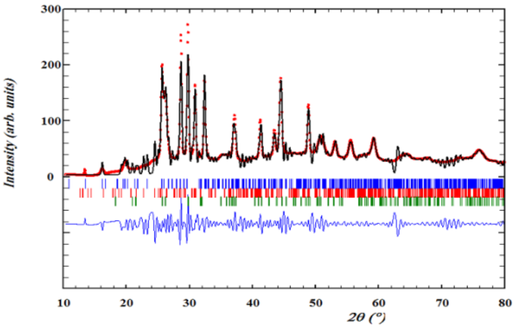

Fig 1: XRD pattern of sample

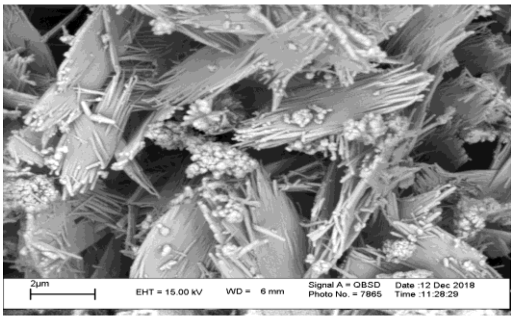

Fig 2: SEM spectra

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Scanometry Method Study, Structural and Spectroscopic Aspects of Schiff Base Ligands Containing N and S Donor Atoms

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The tetradentate Schiff base ligand methyl-2-{[1-methyl-2-(aceton) ethylidynenitrilo]ethyl}amino-1-cyclopentenedithiocarboxylate, (H_2cdacacMeen), was synthesized and characterized by elemental analysis, IR, ^{1}H NMR, UV-Vis and mass spectrometry. The characterization of the scanometry method [1,2] based sensor membrane is described for the determination of Schiff base ligand on the immobilization of some metals such as Fe, Mn, Cu, and Ni on a triacetylcellulose membrane. The application of silica gel polymer as a reagent for determination of metal ion based on single drop scanometry was described. After mixing sample solution containing Schiff base ligand with silica gel polymer, reaction was done and one droplet of final solution injected on the glass plate, before drying the droplet, glass plate was scanned with flatbed scanner. Image of solution single droplet was analyzed to color values in the various color spaces such as RGB, CMYK, HSL, HSV, XYZ, and correlation between any color values and concentration was studied. The characterization of single droplet, the sampling box location in the single drop and the effect of times on the reaction was studied by scanometry method.

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Synthesis and characterization of nano oxid (CeO_2) And (NiO) using precursor [$(phen)_2(OH_2)Ni(\mu\ SCN)Ce(\mu SCN)(SCN)_4Ni(OH_2)(phen)_2$] NO_3

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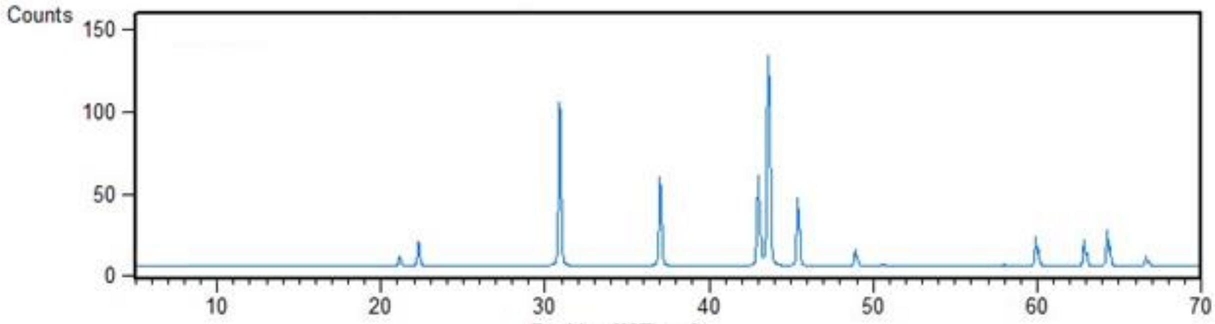
In this investigation, we report facile synthesis of transition metal oxide (CeO_2) And (NiO) as nano oxid. The process contained two steps: first preparation of complex [$(phen)_2(OH_2)Ni(\mu\ SCN)Ce(\mu SCN)(SCN)_4Ni(OH_2)(phen)_2$] NO_3**(1)** where phen=1,10-phenanthroline and SCN= thiocyanate. Then the precursors were complex **(1)** synthesized using a mix of ethanolic solution of Ni(NO3)2(2mmol), and phenanthroline(4mmol) and Ce(NO3)3(1mmol) , SCN(6 mmol). Then desired product was collected by suction filtration and characterized using Fourier transform infrared (FT-IR), Ulcalcination. In first step, tra Violet-Visible (UV-vis) spectroscopy and cyclic voltammetry (CV) method for electrochemical studies. The next step to prepare nano oxid, amount of compound **(1)** was placed in a furnace with a temperature of 700. After calcination of title compound, this sample studied using XRD (X-ray Diffraction)and SEM (Scanning Electron Microscopy) techniques. Particle size for several diffraction and average crystallite size were measured from the XRD data based on Debye- Scherrer¼equation. The X-ray diffraction patterns at room temperature revealed that, highly pure and crystallized Ni-Ce nano oxid as form(CeO_2) And (NiO) ula with Hexagonal phases in 700°C, with an average particle size of about less than 100nm for both nano-oxide. SEM figure show that the particles have same morphology with a uniform porous surface[1].



1- . N. Raman^{a,*}, S. Sobha ^{a}, L. MituDesign ^{b}, synthesis, DNA binding ability, chemical nuclease activity and antimicrobial evaluation of Cu(II), Co(II), Ni(II) and Zn(II) metal complexes containing tridentate Schiff base. Journal of Saudi Chemical Society.

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Synthesis and Characterization of Magnetically Recyclable Natural Thomsonite Zeolite Supported on $Fe_3O_4@SiO_2$ Nanoparticle Catalyst and its use for the Preparation of Biginelli Reaction under Solvent-free Conditions

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Thomsonite Zeolite ($NaCa_2[Al_5Si_5O_{20}].6H_2o$) is a natural and heterogeneous catalyst that used broadly in the synthesis of specialty and fine chemicals [1]. In this study we used from heterogeneous catalyst (natural thomsonite zeolite) to linked superparamagnetic nanoparticle (NP), which providing quasi-homogeneous reaction conditions. After doing and complete reaction, the magnetically heterogeneous catalyst is easily separated by an external magnet and provide an easy work-up.Biginelli reactions for the synthesis of 3, 4-dihydropyrimidin-2-(1*H*)-ones derivatives have been shown many important biological properties such as antibacterial and anti-inflammatory, antifungal, antihypertensive effects, anticancer, anti HIV agent [2]. Magnetically recyclable natural thomsonite zeolite supported on $Fe_3O_4@SiO_2$ core-shell nanoparticles was prepared for the first time. The natural nanocatalyst was characterized by various techniques such as FT-IR, TGA/DTA, SEM, SEM-EDS, XRD, VSM, and UV analysis. This magnetically recyclable catalyst was used for the rapid synthesis of 3,4-dihydropyrimidin-2(1*H*)-one derivatives from ethylacetoacetate, urea, and aromatic aldehydes under thermal solvent-free conditions.

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Synthesis, Characterization and Photocatalytic Application of $LaFeO_3$,$NdFeO_3$ Magnetic Nanocomposites in Removal of Organic Wastes Water

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The development in the field of nano scale science and engineering provides us with unprecedented understanding and control of matter at atomic and molecular levels. The later advances in nanotechnology allow us to make more and more advanced materials with unusual magnetic, electric, optical, and biological properties [1] Organic dyes are widely used in different fields and seriously decrease water pollution. Most of the industrial dyes are toxic, carcinogenic, and teratogen [2]. Photocatalysis can play an important role in new technologies of water and wastewater purification [3]. The present work shows preparation of $LaFeO_3$,$NdFeO_3$ nanocomposites as effective photocatalysts. The prepared products were characterized by x-ray diffraction pattern (XRD).Transmission electron microscopy (TEM) and Fourier transfer infrared (FT-IR) spectroscopy. Alternating gradient force magnetometer (AGFM) illustrates magnetic behavior of $LaFeO_3$, NdFeO3 nanocomposites. The photocatalytic behavior $LaFeO_3$,$NdFeO_3$ nanocomposites were evaluated using the degradation metile violet, malachite under ultraviolet light irradiation .the results show that $LaFeO_3$,$NdFeO_3$ nanocomposite have application magnetic and photocatalytic performance.

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Preparation, Characterization And Study Of Biological Potency In Binuclear Zinc(II) Complex Of Dithiocarbamate Derivatives

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It is, essential to investigate the interactions between drugs and carrier proteins in order to specify the pharmacology and pharmacodynamics of drugs (1). A binuclear dithiocarbamate Zn(II) complex $[(phen)Zn(\mu\text{-pr-dtc})Zn(phen)](NO_3)_2$ (where phen = 1,10-phenanthroline, pr-dtc = propylenebisdithiocarbamate, Fig. 1) was synthesized and characterized in the present study. The formulated complex was evaluated for *in vitro* antioxidant activity as radical scavengers against 1,1-diphenyl-2-picrylhydrazyl radicals (DPPH.). According to the results, antioxidant activity of Zn complex (IC_{50} = 21 mg L^{-1}) was effective. Biophysical techniques along with computational modeling were employed to examine the binding of this complex with bovine β-lactoglobulin (βLG) as the model protein. The trial findings revealed an interaction between binuclear complex and βLG with a modest binding affinity ($K_b = 6.01 \times 10^4$ M^{-1}. An intense fluorescence quenching of protein through a static quenching mechanism was occurred due to the binding of complex to βLG. Hydrogen bonds and Van der Waals forces was the main stabilizing forces in the development of drug-protein complex. Analysis of protein-ligand docking demonstrated binding of complex to residues placed in the site B of βLG .

Keywords: Carrier protein; Antioxidant agent; Molecular docking

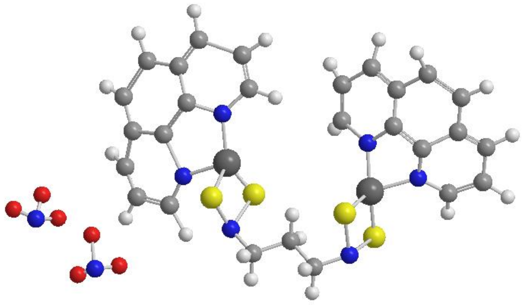

Fig. 1 Molecular structure of Zn(II) complex.

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Synthesis, characterization, and antibacterial activities of a cobalt (II) complex of bipyridine derivative

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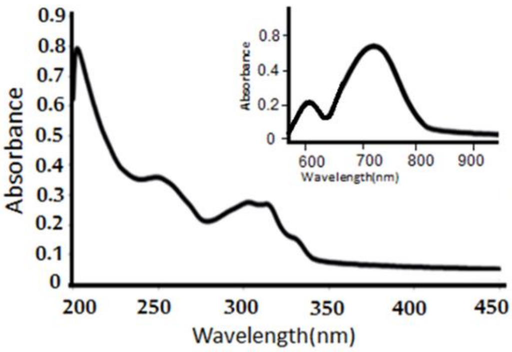
The cobalt(II) complex of the formula [Co(5,5´-dmbipy)$_2$ (NCS)$_2$], was obtained by the reaction of $Co(NO_3)_2{\cdot}6H_2O$ with 5,5´-dimethyl-2,2´-bipyridine and NaSCN. The metal complex was characterized through FT-IR, UV–Vis, ^{1}H-NMR and elemental analysis. In vitro biological screening of the free ligand, complex and its metal salt against diverse microorganisms was done using Macro-dilution (tube) broth method. The antibacterial effects of complex have also been examined in vitro against standard bacterial strains. The minimum inhibitory concentration (MIC), minimum bactericidal concentration (MBC) and inhibition zones (IZ) of the complex, its ligand (5,5´-dmbipy) and its metal salt $Co(NO_3)_2{\cdot}6H_2O$ against the growth of microorganisms (one Gram- positive standard strain of Staphylococcus aureus; S. aureus ATCC 25923, and one Gram-negative standard strain of Escherichia coli; E. coli ATCC 25922) are obtained. Comparison of the antimicrobial activities of the synthesized cobalt compounds with similar complexes in the literature shows that our new compounds are more strong [1,2].



The electronic absorption spectrum of the [Co(5,5´-dmbipy)$_2$ (NCS)$_2$] complex in methanol

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Synthesis, characterization, thermal study, and luminescent a complex of Iron (III)

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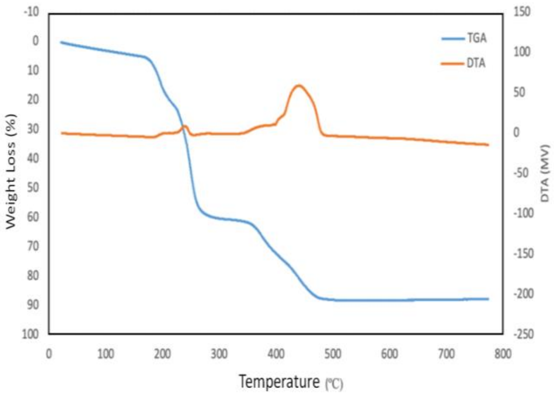
The binuclear iron(III) complex of the formula $\{[Fe(5,5'\text{-dmbpy})_2(OH_2)]_2(\mu\text{-}O)\}(NO_3)_4$ **(a)** was prepared from the reaction of $Fe(NO_3)_3{\cdot}9H_2O$ with 5,5´-dimethyl-2,2´-bipyridine. The complex **(a)** was characterized by FT-IR, UV–Vis, TGA, ^{1}HNMR spectroscopy, elemental analysis and luminescence measurements. Its structure was investigated by the single-crystal diffraction method. Crystal structure analysis showed that both Fe(III) cations are coordinated by two bidentate ligands, one water molecule and one bridging oxygen atom, resulting in coordination by four nitrogen atoms of 5,5´-dmbipy ligands and two oxygen atoms. The coordination polyhedrons are distorted octahedral. The thermal stability and fluorescence property of (a) have also been investigated [1,2].



Thermogravimetric analysis (TGA) and (DTA), analysiscomplex (a)

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Green Synthesis and Kinetics of Functionalized Piperidines promoted by Tartaric Acid as a Naturally Catalyst under Green Solvent

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Synthesize of the substituted piperidine from the one-pot reaction between aromatic aldehydes, anilines and β-ketoesters in the presence of tartaric acid as a catalyst has been investigated at ambient temperature in both methanol and ethanol media [1]. Using of tartaric acid had many advantages such as mild reaction conditions, simple and readily available precursors and inexpensive catalyst [2]. Different conditions of temperature and solvent were employed for calculating the thermodynamic parameters and obtaining an experimental approach to the mechanism. Based on the spectral data, the overall order of the reaction followed the second order kinetics. Methanol was optimized as a desirable solvent in the synthesis of piperidine, nevertheless, ethanol in a kinetic investigation had none effects on enhancement of the reaction rate than methanol. The results showed that the first step of the reaction mechanism is a rate determining step [3]. The proposed mechanism was confirmed according to the obtained results and the steady state approximation.

Keywords: Kinetics; Catalyst; Tartaric acid; Piperidine

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20th Iranian Inorganic Chemistry Conference

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The catalytic role of triphenylarsine in the formation of (Z)-N-vinyl Inorganic compound: an experimental mechanistic study

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Abstract:

In the current work, the kinetics and mechanism of the reaction between dimethyl acetylendicarboxcylate **2** (DMAD) and phthalimide **3** (N-H heterocyclic compound) in methanol environment in the presence of triphenylarsine **1** (TPA) as a catalyst was undertaken using UV/vis spectrophotometry technique, for the generation of N- vinyl heterocyclic compound [1]. The reaction followed second-order kinetics and the partial orders of DMAD and phthalimide are one and one, respectively. Also, the fourth step (step 4, k_4) of the reaction mechanism was recognized as a rate determining step (RDS). In the previous works, when triphenylphosphine (TPP) was employed instead of (TPA) as an another reactant (not catalyst) for the similar reaction with DMAD and N-H heterocyclic compounds to yield different ylides, the partial orders in related to DMAD, TPP and different N-H heterocyclic compounds were one, one and zero, respectively. Herein, on the contrary with the current work, the first step ($step_1$, k_1) of the reaction mechanism was determined as a rate determining step. In both the previous and current works, TPP or TPA, participates in the first step ($step_1$, k_1) of the reaction mechanism in order to react with DMAD, but TPA acts as a more stronger nucleophile than the TPP, hence the rate of the first step ($step_1$, k_1) speeds up remarkably in the current work. As a result, this step could not be a rate-determining step as well as the first step of the previous works, so the different reactivity and nucleophicity of TPA in comparison with TPP can influence kinetics and mechanism of the mentioned reaction, herein, this behavior has been described on competitive mechanism. From the temperature, concentration and solvent studies, the activation energy and the relevant activation parameters (E_a, $\Delta H^{\ddagger}$, $\Delta S^{\ddagger}$ and $\Delta G^{\ddagger}$) were calculated.

Keywords: Kinetics; Mechanism; UV Spectroscopy, phthalimide

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The effect of ultrasonic irradiation, time and concentration on morphology of novel nano Hg (II) metal-organic coordination polymer

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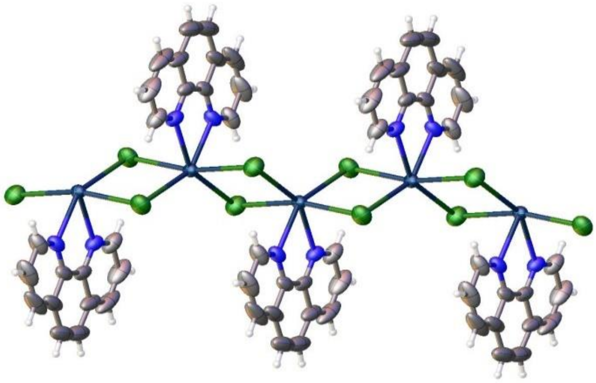
Coordination compounds or metal-organic hybrid materials remarkably have attracted huge and unabated attention because of their properties[1-3] .A sonochemical method was used to prepare nano-rods of a novel mercury(II) metal-organic coordination polymer, $[Hg(1,10\text{-}phen)Cl_2]_n$ (**1**) (1,10-phen = 1,10-phenanthroline). The effect of the synthesis parameters such as time, concentrations and irradiation power has been studied and optimized. Nano rods and nano flowers morphologies were obtained by applying diverse sonication time, power and concentration. The compounds were characterized by scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), elemental analysis, IR spectroscopy, X-ray powder diffraction (XRD), and single crystal X-ray analysis. The X-ray structure analysis revealed that the Hg (II) atom is coordinated by two nitrogen atoms of the “1,10-phen” ligand and four chloride bridging atoms with a HgN_2Cl_4 donor set with symmetrical octahedral geometry. The crystal forms a one-dimensional zig-zag polymer. The adjacent chains connected by π—π of adjacent aromatic rings of “1, 10-phen” and other weak interactions. Hence, the weak interactions also allow the 1D zig-zag structure to form a 3D metal-organic coordination polymer. HgO nanoparticles were prepared by thermolysis of compound **1** at 180 °C with oleic acid as a surfactant. The morphology and size of the as-synthesized HgO nanoparticles were further examined using SEM.



Fragment of the coordination polymer showing the 1D arrangement

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Sonication-assisted synthesis of some new mercury complexes with a tetradentate Schiff base ligand: Antimicrobial and thermal behaviors

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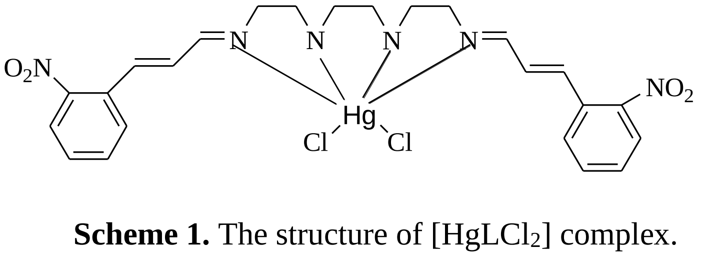
Among different ligands used for synthesis of new coordination compounds in inorganic chemistry, Schiff base ligands are still on top because of their easy preparation, various properties and coordinating ability toward different metals ions [1]. Schiff base ligands based on the number of donor sites are classified to monodentate, bidentate, tridentate and so on. Their complexes have been extensively studied in the past few years for antibacterial and anticancer activities, catalysts, models of metalloenzymes and luminescent properties [2, 3].
In this work, a new N_4-Schiff base ligand obtained from condensation of 2-nitrocinnamaldehyde and triethylenetetraamine has been successfully synthesized and its mercury complexes were characterized by FT-IR, ^{1}H NMR, UV–Vis spectra and molar conductance measurements. Based on spectral data, the general formula of $HgLX_2$ ($X = Cl^-$, I^-, N_3 and SCN^-) was proposed for the mercury complexes. The mercury compounds in nano-structure size were also prepared by sonochemical method. The nano-structure compounds were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). Furthermore, the antimicrobial activity of the ligand and its mercury complexes against four gram positive and gram negative bacteria and also two fungi was assessed by the disk diffusion method. Also, DNA cleavage potential of all compounds was investigated by agarose gel electrophoresis method. Finally, thermal behaviors of all compounds were studied by TG/DTG/DTA analyses data.



Scheme 1. The structure of [$HgLCl_2$] complex.

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Synthesis, characterization, theoretical calculation and antimicrobial properties of some new cadmium halide complexes

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The scientific field of Schiff bases and their complexes is interesting in inorganic chemistry points of view. These compounds have a variety of structures and applications depending on the aldehyde and amine used in their synthesis. These ligands and their metal complexes have different applications in bioinorganic chemistry, material science, catalysis, separation and encapsulation processes, hydrometallurgy, formation of compounds with unusual properties and metal–metal interactions. Many biologically active Schiff bases have been reported in the literature that show antimicrobial, antibacterial, antifungal, anti-inflammatory, anticonvulsant, antitumor and anti HIV activities[١-٣]. In this work, we present synthesis and characterization of some cadmium halide complexes with formula of $CdLX_٢$ (($X= Cl^-$, Br^-, I^- and L= a new ligand formed via condensation of bromobenzaldehyde and bis(٢-aminoethyl)amine). The ligand and its complexes were characterized by physical and spectral data. After characterization, the ligand and its complexes have been subjected to biological standard tests for their antimicrobial activities. Finally, the compound structures were optimized and then some structural parameters and vibrational frequencies were calculated at the B٣LYP/LANL٢DZ level of theory.

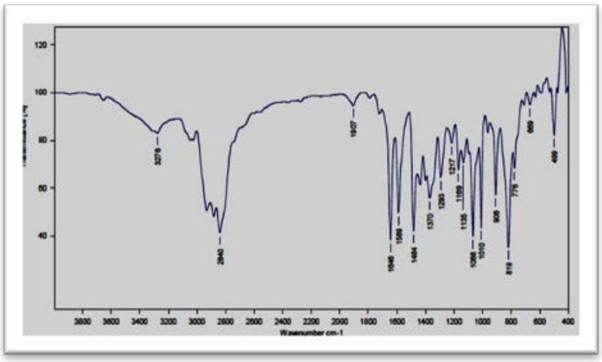

Figure ١-The FT/IR of ligand.

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Synthesis and identification of the nickel dimethylformamide and thiocyanate $[Ni(SCN)_2(DMF)_4]$ complex by hydrothermal method

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In this paper, we synthesized $[Ni(SCN)_2(DMF)_4]$ complex (DMF= N, N-dimethylformamide and SCN= thiocyanate) by hydrothermal method [1]. This complex characterized by single-crystal X-ray analysis (X-Ray), Fourier Transfer infrared (FT-IR) and UV-vis spectroscopy. The results of infrared spectroscopic studies showed stretching vibration of CN bond in the NCS ligand in the 2063 cm^{-1} region. Absorption spectra of complexes showed transitions in the UV-Vis region, which are related to the SCN and dimethylformamide (DMF) ligands. Low-intensity absorbing bands in the 400-800 area that are attributed to d-d metal doped metal ions in the complex. These delicate bands are the result of multiple to multiple transitions in d orbital. The d → d transfers of nickel are seen in the region of 800nm. The electron transfer in this region corresponds to $^3A_2g \rightarrow {}^3T_2g$. Ni also contains $^3A_2g \rightarrow {}^3T_1g$ (F) and $^3A_2g \rightarrow {}^3T_1g$ (P) transfers [2]. The ORTEP diagram of the complex is shown in Figure 1.

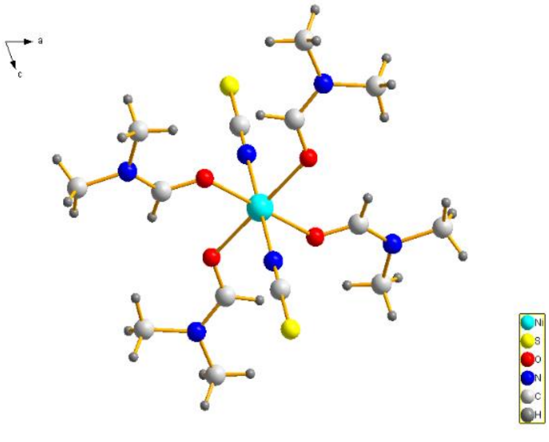

Figure1. ORTEP of the complex

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2- . N. Raman[a,*], S. Sobha [a], L. MituDesign [b], synthesis, DNA binding ability, chemical nuclease activity and antimicrobial evaluation of Cu(II), Co(II), Ni(II) and Zn(II) metal complexes containing tridentate Schiff base. *Journal of Saudi Chemical Society*.

Some new nanostructure cadmium imidazolidine Schiff base complexes: Thermal behavior, antimicrobial, and DNA cleavage potential

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Schiff bases are very popular ligands for inorganic chemists because of their easy synthesis, structural variety and high coordinating ability for different metal ions [1]. these compounds and their metal complexes form important class of materials in medicinal chemistry with various biological activities including urease inhibitory, antitumour, antifungal, antibacterial, antiproliferative, anti-inflammatory, antiviral and insulin-enhancing activities [2].
In this study, a new series of cadmium halide/pseudohalide complexes with a novel Schiff base ligand containing imidazolidine ring has been successfully synthesized. Schiff base ligand and its complexes were characterized by FT-IR, ^{1}H, ^{13}C NMR, UV–Vis spectra, thermal analyses and molar conductance measurements. based on spectral data, the general formula of $CdLX_2$ ($X = Cl^-$, Br^-, I^- and SCN^-, N_3^-, NO_3^-) was proposed for the cadmium complexes. CdO nanoparticles were prepared by direct calcination process of cadmium bromide complex at 600°C under air atmosphere. the cadmium compounds in nano-structure size were also prepared by sonochemical method. the nano-structure compounds were characterized by Xray diffraction (XRD) and scanning electron microscopy (SEM). furthermore, antibacterial activities of compounds have been screened against various bacteria and fungi by disk diffusion method. finally DNA cleavage potential of the compounds was investigated by agarose gel method.

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$Ce_{0.25}Sr_{1.75}NiO_{3.75}$ Assisting with Pd and Co Nanoparticles: Synthesize, Characterization and Catalytic Potentiality for Ethylene Glycol Electrooxidation

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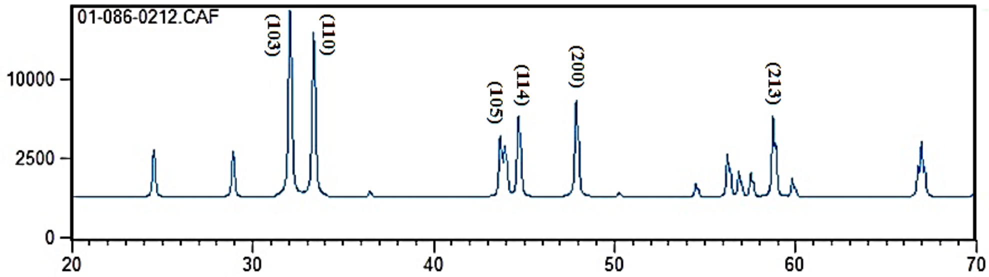
A fuel cell is an electrochemical' device operating at the different temperatures that convert the chemical energy of a fuel (e.g., alcohol) and an oxidant in the presence of a catalyst to the water, CO_2, heat, and electricity [1]. Lately, the metal oxide composites have attracted significant attention as electrocatalysts owing to their low cost, easy preparation, and stable structure [2]. Ethylene glycol can be introduced as a suitable fuel for the fuel cells, due to its low vapor pressure, lower price, easier storage and lower flammability compared to other organic compounds [3]. In this work, the $Ce_{0.25}Sr_{1.75}NiO_{3.75}$ mixed metal oxide was synthesized in nano-size (~ 24 nm) by the co-precipitation method in the presence of oleic acid as surfactant and characterized *via* spectroscopy and microscopy techniques. Then, Pd and Co nanoparticles were chemically reduced on as-prepared $Ce_{0.25}Sr_{1.75}NiO_{3.75}$ in chitosan matrix. The physicochemical characteristics and electrochemical behavior were determined for Pd-Co-$Ce_{0.25}Sr_{1.75}NiO_{3.75}$. The electro-catalytic ability of $Ce_{0.25}Sr_{1.75}NiO_{3.75}$, Pd, Pd-Co, and Pd-Co-$Ce_{0.25}Sr_{1.75}NiO_{3.75}$ toward ethylene glycol oxidation was compared *via* the electrochemical studies in alkaline media. The results showed that the incorporation of as-prepared mixed oxide to Pd-Co was efficient to improve the current density and the transferred charge during the electrooxidation of ethylene glycol.



XRD pattern of as-prepared $Ce_{0.25}Sr_{1.75}NiO_{3.75}$ nano-particles

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Preparation and Characterization of $SrCeCuO_3$ and its Application Assisting with Pd and Co as Nano-Catalyst for Electrooxidation of Ethylene Glycol

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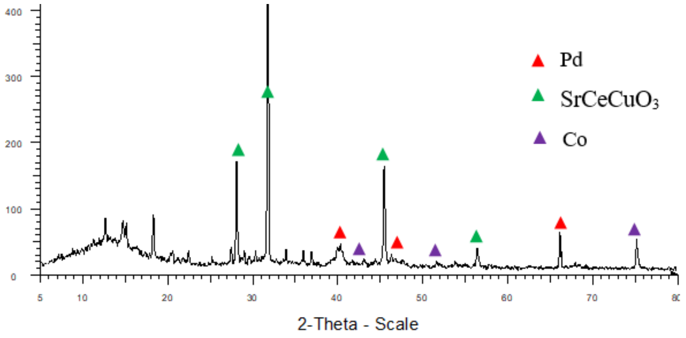
Recently, the electrooxidation of organic compounds (e.g., alcohols) is considered in the connection with the progress of fuel cells [1, 2]. It is an electrocatalytic reaction proceeding over the electron transfers and is intricated *via* the molecule adsorption on the surface of the heterogeneous catalyst and creation of poisoning intermediate. In the present study, a facile sol-gel assisted with the ultrasonic method for the synthesis of well-dispersed $SrCeCuO_3$ nanocrystals (~ 50 nm) was developed in the presence of oleic acid as the surfactant. The product was characterized with using Fourier transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy, and energy dispersive X-ray spectrometer. Afterward, it was focused on the chemical reduction of Pd and Co nano-particles on $SrCeCuO_3$ nanocrystals. The morphology and status of Pd-Co-$SrCeCuO_3$ nano-composite were determined by using a field emission electron microscope. The catalytic activity of $SrCeCuO_3$, Pd, Pd-Co, and Pd-Co-$SrCeCuO_3$ for the electrooxidation of ethylene glycol was compared by the electrochemical techniques in alkali. The results presented that the integration of $SrCeCuO_3$ mixed metal oxide to Pd-Co was effective to increasing the current density and transferred charge during the ethylene glycol electrooxidation reaction.



XRD pattern of as-prepared Pd-Co-$Ce_{0.25}Sr_{1.75}NiO_{3.75}$ nano-particles

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Synthesis and characterization of Fe_3O_4@MoO_3 nanoparticles

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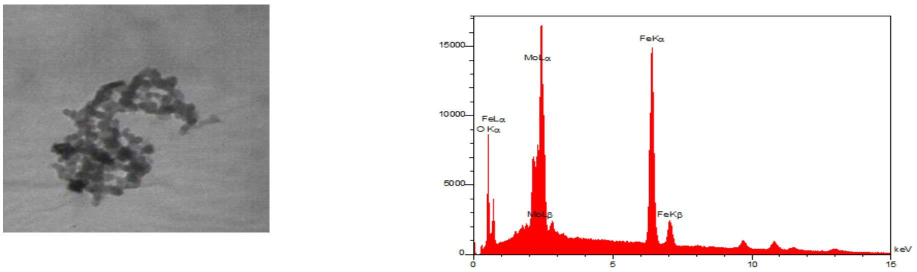
Magnetic particles play an important role in biomedical applications, for instance, nanoprobes [1-2]. In this study, we demonstrated the synthesis of a new core-shell nanoparticle (Fe_3O_4@MoO_3) by using Fe_3O_4 nanoparticles and ammonium heptamolybdate and characterization of its structure by some spectroscopic methods like FT-IR, scanning electron microscopy (SEM), Transmission Electron Microscopy (TEM), X-ray powder diffraction patterns (XRD) and MAP analysis. In this work we prepared new core-shell nanoparticles (Fe_3O_4@MoO_3) by reflux of Fe_3O_4 and ammonium heptamolybdate in ethylene glycol with a rapid method [3]. Firstly, Fe_3O_4 nanoparticles were synthesized by a solvothermal method. Then 100 mg of Fe3O4 nanoparticles were dispersed in a round bottom flask containing 50 mL ethylene glycol. Then a solution of 617 mg of ammonium heptamolybdate in 10 mL deionized water was added to the flask and the mixture was refluxed at 160 °C for 12 hours. The obtained black products were filtered out and washed with absolute ethanol and distilled water several times to remove impurities and dried in an oven 60 °C for 4 hours.



TEM images and EDX analysis data for Fe_3O_4@MoO_3

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Synthesis and characterization of magnetite Fe_3O_4 nanoparticles by a rapid method

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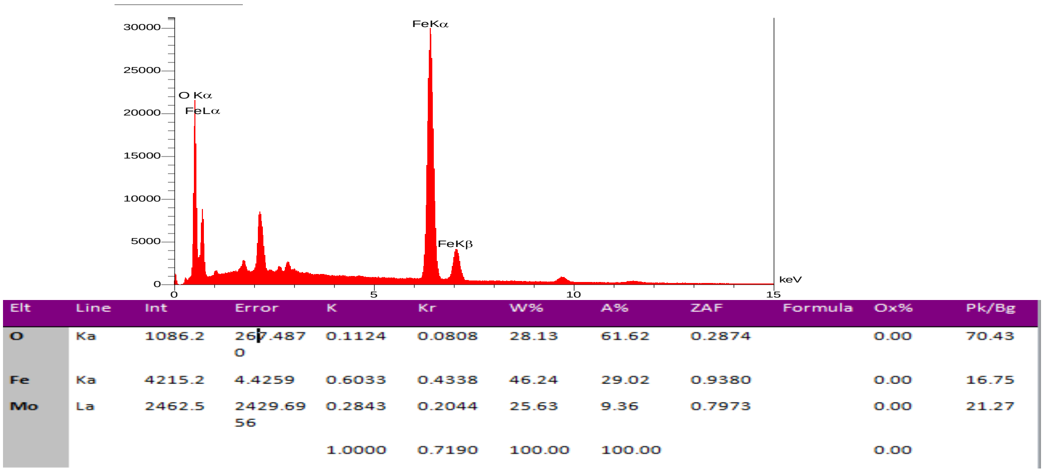
The magnetic properties of iron oxides have been studied in various ranges of applications including magnetic recording media, catalysts and Ferro fluids [1-3]. So in this work we synthesis of a nano sized Fe_3O_4 by a simple method and characterized by some methods, X-ray Diffraction (XRD); Infra-red Spectroscopy (IR), Scanning Electron Microscope (SEM) and Energy Dispersive Spectroscopy (EDS). A Fe (II) solution was prepared by using 5 g of $FeSO_4.7H_2O$ and dissolved in 35 ml of distilled water in a 50 ml round bottom flask under nitrogen gas. In a separate flask 0.40 g of KNO_3 and 2.80 g of KOH were dissolved in 15 ml distilled water (solution b) at 90˚C in an oil bath. Solution b was added drop wise for 5 minutes into the Fe(II) under nitrogen gas yielding a black solution. The solution was maintained in the bath at 90˚C for an hour to ensure homogeneity of the solution, and was left overnight at the same temperature. After 15 hours the nanoparticles were separated magnetically and washed with 30 ml water for six times and dried in an oven 95 °C for 2 hours.



Elt	Line	Int	Error	K	Kr	W%	A%	ZAF	Formula	Ox%	Pk/Bg
O	Ka	1086.2	267.4870	0.1124	0.0808	28.13	61.62	0.2874		0.00	70.43
Fe	Ka	4215.2	4.4259	0.6033	0.4338	46.24	29.02	0.9380		0.00	16.75
Mo	La	2462.5	2429.6956	0.2843	0.2044	25.63	9.36	0.7973		0.00	21.27
				1.0000	0.7190	100.00	100.00			0.00	

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Ultrasonic-Assisted Synthesis and Crystal Structure of a New Di-nuclear Copper (II) Complex

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Recently have been reported that metal-organic complexes based on copper, ruthenium and rhodium with N,N'-donor ligands such as 2,2',-bipyridine or 1,10-phenanthroline acts as an anticancer agent more effective than cis-platinum[1, 2]. The complexation of transition metal ions such as Cu(II) with pyrazolone derivatives, causes them to be used as active agents in biological, pharmacological and clinical. In this study, a dinuclear copper (II) complex with a formula of $[Cu_2(pydc)_2(inta)_2(H_2O)_2]$ $.3H_2O$ (Fig.1) have been synthesized under ultrasound irradiation and characterized using various techniques such as (SC- XRD), FT-IR spectroscopy, UV–Visible spectroscopy and thermal analysis methods (TGA and DSC). The two Cu(II) centers have different coordination number and geometry. One of the centers is six-coordinate with a distorted octahedral geometry and another one is penta-coordinate with a distorted square pyramidal. The two centers of copper are coordinated to each other through one μ-carboxylate oxygen of pydc ligand.

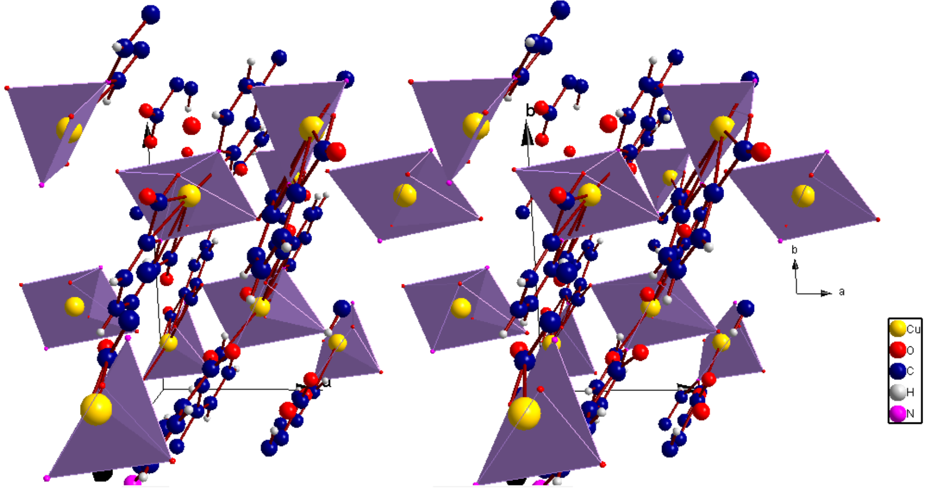

Fig.1. A polyhedral geometry around centers of copper.

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Synthesis, Characterization and Magnetic Behavior of A Metal-Organic Frameworks Based on Lanthanum(III)

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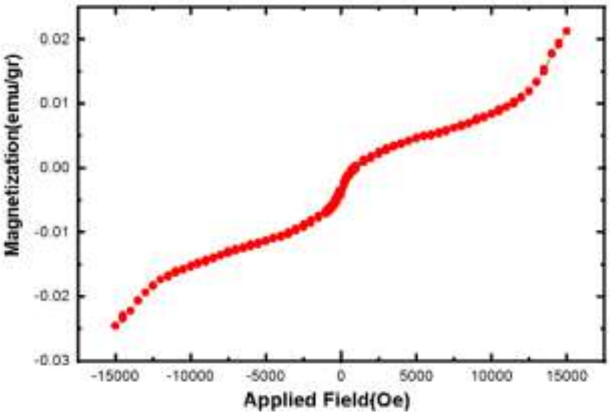
Lanthanide complexes have unique physicochemical properties, especially their magnetic and luminescent properties [1, 2]. Many chemists reported the synthesize of MOFs based on lanthanides with a lot of different carboxylic acids, such as pyridine- 2,6-dicarboxylic acid with beautiful and interesting structures[3]. In the present work, a new polymer formulated as $[([La(Pydc)_2(H_2O)_3].4H_2O)_n$ (**1**) that Pydc = pyridine-2,6-dicaboxylic acid was synthesized by a sonochemical process. The results of crystallography confirmed that complex revealed a monoclinic space group P21/c. The La (III) ion is nonacoordinated in collaboration with two dipicolinate ligand as tridentate chelating ligands and three oxygen atoms of water molecules. The remanent magnetization (M_r) and the coercive field (H_c) for complex are 0.016emu/g and 1164.67Oe, respectively. However, the saturation magnetization was not observed even in 15kOe of applied magnetic fields and magnetization increases linearly with increasing applied field.



Magnetization as a function of magnetic field at room temperatures of complex **1**.

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Polymeric Schiff Base Zinc(II) Complex Based on N,N-bipyridinium: Synthesis, characterization and thermal study

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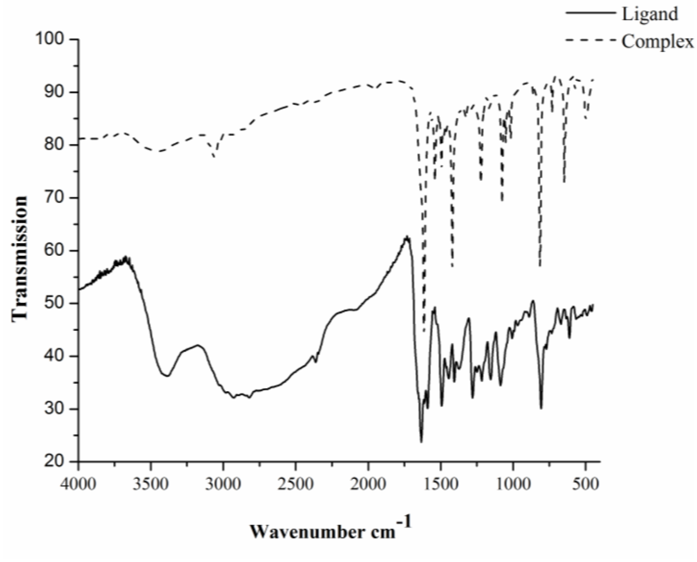
Polymeric Schiff bases are an important class of coordination polymers with multidentate donor sites, known to form polychelates with transition metal ions. The essential properties of polymeric Schiff base are due to the azomethine linkage in polymeric backbone [1-2]. In this study, it is described the synthesis and characterization of a new polymeric Schiff base ligand derived from diethylene triamine and bipyridinium bis(methyl salicylaldehyde) and its zinc(II) polymeric Schiff baes complex. Ligand and ionic zinc-Schiff base complex were characterized by different methods: FT- IR, ^{1}H-NMR and CHN. The thermal properties of polymer were evaluated by differential thermal analysis (DTA) and thermogravimetric (TG) analyses. The results of C, H and N analysis agree with the expected values. In the FT-IR spectrum of the polymer metal complex the stretching vibration band of OH group appears as a weak band. Also the azomethine band shifted to 1608 cm^{-1}. These observations indicating the coordination of the ligand to metal ion. The analyses of the thermal curves of the polymer metal complex show higher thermal stability than the polymeric Schiff base ligand.



FT-IR spectra of ligand and zinc complex

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Synthesis and spectroscopic properties of one mixed metal salophen complex with azide bridge ligands

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Dinuclear transition metal complexes have been extensively investigated in molecule-based magnetism and catalysis [1].The complexes have been shown interesting properties depending on metal ions, bridging ligands and anions [2]. In particular, an azide ion as bridging ligand have been used for constructing a variety of structures and developing molecule-based magnetic materials, due to its binding modes such as end-on, end-to-end, and terminal [3]. Here we report the syntheses, characterization and spectroscopic properties of one dinuclear Co(II) and Cu(II) complex with salophen-type and azide ligands. The salophen ligand is prepared from condensation reaction between 4-chloro-1,2-diaminobenzene and salicylaldehyde in ethanol. The complex is obtained from the reaction between one equivalent salophen with $Cu(CH_3COO)_2.H_2O$ and $Co(CH_3COO)_2.4H_2O$ and two equiv. of NaN_3 in methanol.

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Synthesis and characterization of NiO-CuO nanocomposite by thermal decomposition method

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Mixed metal oxides have found increasing research focus and applications in physics, chemistry, materials science and engineering. The combination of two or more metals in an oxide matrix can produce materials with novel physical and chemical properties leading to relatively higher performance in various technological applications [1]. CuO is a p-type low-band gap (1.2 eV) semiconductor used as high T_c superconductor, for magnetic storage media, gas sensing, photocatalysis, photovoltaics and battery applications [2]. NiO is p-type with a wide band gap of 3.6 - 4.0 eV and has wide applications in drug delivery, gas sensing, battery electrodes, photoelectrodes and electrochromic windows [3]. In this work, the NiO-CuO nanocomposite is obtained from pyrolysis of Cu(II) complex with N,N-bis(salicylidene)4-bromo-1,2-phenylendiamine at 550 ºC for 24h in nickel crucible. The synthesized nanocomposite is characterized and studied with several techniques such as FT-IR spectroscopy, X-ray powder diffraction (XRD) and scanning electron microscopy (SEM).

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