

CHEM 07 2018

Book of Abstracts 7th Biannual Conference on Chemistry

Organizing Committee CHEM 07
CHEMISTRY DEPARTMENT – FACULTY OF SCIENCE –
CAIRO UNIVERSITY – GIZA-EGYPT.



Preface

In 2000, the Department of chemistry launched its very first scientific conference Chem01. When we first thought about it we set a goal to have these conferences more than just a scientific meetings; an event that involve not only faculty staff members but also graduate and post-graduate students too. Chem0x series of conferences kept this goal along the way from Chem01 to Chem06 in 2010. In Chem0x we tried our best to invite distinguished speakers from all over the world. This enriched the scientific discussions, kept us connected with the latest in chemistry and allowed us to make new friends. Along the scientific meetings and lectures we were able to launch several different workshops aimed at our students. Every one of the 6 Chem0x conferences had its own taste, advantages and memories which will never be forgotten.

Egypt went through a lot since our last conference Chem06 in 2010. But now it is the time to re-gain the momentum and start looking at the future. Chem07 come with a lot of expectations. We start organizing it from scratch. I tried to put together our old team ; three only accepted, *Profs. Hamed Ead, Faten Nour El-Dein* and *Azza Shoukry*. For whom I am really deeply indebted. A group of the younger generation having great enthusiasm and courage joined us, *Rabab El Sherif , Sahar Fadl Allah, Rasha El Nashare, Riham Rashad, Shymaa Medany* and *Randa Abdlahmeed*. Along the way, we got more momentum when *Profs. Hamdi Hassanen* and *Abdelgawad Fahmi* Joined us. Now we have a wonderful team which dedicates itself for Chem07.

Chem07 will witness a lot of events. Three general lectures and more than 40 invited lectures and keynotes will bring to us the latest in all disciplines of chemistry. Chem07 is really international, thus in addition to the 50 Egyptian participants; colleagues from 11 different countries are joining us. Chem07 will start a new tradition, for the first time, it will organize tribute sessions dedicated to men and women who served and enriched our department and left us with their great Heritage. In Chem07 we will



pay tribute to three great scientists, *Prof. Schomberge, Prof. Ahmed Sami* and *Prof. Waheed Badawy*.

A nanochemistry and technology workshop will be organized. It will visit the nanotechnology center of Cairo University in 6th October City where participants will have the chance to see and hear from scientists about the latest instruments and research conducted and its applications.

On the social side, we always try to allow our guests to taste the Egyptian civilization; ancient, old and modern. Several site seeing tours and visits will be organized just after or along the conference days.

We really hope that Chem07 come as we would like it to be and more. A real addition to the department. We hope to boost a new spirit of cooperation, respect and love among us in our department.

On behalf of the organizing committee

Rifaat Hilal

Conference Coordinator

Cairo Feb. 24th, 2018



CHEM 07 Committee

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HALL (A)

SESSIONS OF:

- Electrochemistry.
- Computational Chemistry.
- Catalysis.
- Nanochemistry and Technology.



Multifunctional Nanoparticles: Morphology and Size Control

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ABSTRACT

With the current fast growth of technological understanding in nanoscience, researchers have intended to familiarize this knowledge to various technical issues within engineering and applied science. Extraordinary advances in nanomaterials manifest a new era in all aspects and applications with the expectation that they would have huge contributions to healthcare and industry. We presented here a survey on some nanomaterials existing in the form of products. We tried to illustrate in some recent research work how morphology transition and/or size dependence could affect the physico-chemical properties. Additionally, we present tailoring nanomaterial design to achieve optimized properties for a specific application.



Photodegradation of Eosin Y Using Silver-Doped Magnetic Nanoparticles

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ABSTRACT

The purification of industrial wastewater from dyes is becoming increasingly important since they are toxic or carcinogenic to human beings. Nanomaterials have been receiving significant attention due to their unique physical and chemical properties compared with their larger-size counterparts. The aim of the present investigation was to fabricate magnetic nanoparticles (MNPs) using a coprecipitation method, followed by coating with silver (Ag) in order to enhance the photocatalytic activity of the MNPs by loading metal onto them. The fabricated magnetic nanoparticles coated with Ag were characterised using different instruments such as a scanning electron microscope (SEM), transmission electron microscopy (TEM), energy-dispersive X-ray (EDAX) spectroscopy, and X-ray diffraction (XRD) analysis. The average size of the magnetic nanoparticles had a mean diameter of about 48 nm, and the average particle size changed to 55 nm after doping. The fabricated Ag-doped magnetic nanoparticles were used for the degradation of eosin Y under UV-lamp irradiation. The experimental results revealed that the use of fabricated magnetic nanoparticles coated with Ag can be considered as reliable methods for the removal of eosin Y since the slope of evaluation of pseudo-first-order rate constant from the slope of the plot between $\ln(C_0/C)$ and the irradiation time was found to be linear. Ag-Fe₃O₄ nanoparticles would be considered an efficient photocatalyst to degrade textile dyes avoiding the tedious filtration step.



Silver Nanoparticles Immobilized on The Activated Carbon As Efficient Adsorbent For Removal of Malachite Green Dye From Aqueous Solution

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ABSTRACT

The focus of the present work is on exploiting the excellent structural properties of the nanomaterials. More specifically, it is demonstrated that Ag nanoparticles (AgNPs) chemically immobilised onto activated carbon (AC-AgNPs) can act as an effective solid sorbent for removal and/ or minimisation of selected malachite green (MG) dye from aqueous solutions by conducting experiments on water samples. Spectroscopic tools such as FTIR, SEM, TEM and XRD were used in the characterisation of the adsorbent before and after adsorption. The adsorbent dose, pH, contact time, rotation velocity, initial concentration of adsorbate and the temperature effects were examined to evaluate their role in the percentage elimination of malachite green. malachite green uptake was favourable in alkaline media at pH =8.0. Freundlich adsorption model and pseudo second-order model fitted the data well and the thermodynamic parameters (ΔH , ΔS , and ΔG) of MG retention revealed that the uptake is endothermic and spontaneous in nature. When AC-AgNPs was utilised, it removed a greater MG percentage from aqueous solution relative to AC. The mechanism of adsorption was explored using the intra-particle diffusion model and the liquid-film model. Desorption studies were made to elucidate recovery of the adsorbate and adsorbent for the economic competitiveness of the removal system. The AC-AgNPs was successfully recycled for eight successive adsorption-desorption cycles indicating its high reusability.



Improved Electro-Oxidation of Formic Acid on a Palladium and Manganese Oxide Binary Nanoelectrocatalyst

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ABSTRACT

The current investigation introduces a novel binary catalyst for formic acid electro-oxidation (FAO); the essential anodic reaction in direct formic acid fuel cells (DFAFCs). The catalyst is prepared by the sequential electrodeposition of Pd (nano-Pd), and manganese oxide (nano-MnOx) nanoparticles onto the surface of a glassy carbon (GC) electrode. The deposition strategy of the catalyst was properly adjusted to eventually improve both of the electrocatalytic activity and stability toward FAO. The highest catalytic activity and stability are obtained at the Pd-MnOx/GC electrode (for which nano-Pd and nano-MnOx were simultaneously deposited onto the GC electrode). Several techniques including cyclic voltammetry, chronoamperometry, electrochemical impedance spectroscopy, field-emission scanning electron microscopy, energy dispersive X-ray spectroscopy, and X-ray diffraction were employed to evaluate and analyze the catalyst's activity and stability in addition to report its morphology, composition, and crystal structure. The enhancement was believed to originate from facilitating the direct oxidation of FA and/or minimizing the adsorption of poisoning species at the electrode surface.



Fabrication of Simultaneously Co-electrodeposited Platinum-Manganese Oxide Binary Nanocatalyst for Efficient Formic Acid Electro-Oxidation

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ABSTRACT

A new synthetic methodology replacing the typical sequential “layer-by-layer” immobilization and employing instead a “simultaneous co-electrodeposition” protocol has been proven eminent for assembling efficient nanoelectrocatalysts for formic acid (FA) electro-oxidation (FAO). This strategy was successful to integrate homogeneously Pt nanoparticles (nano-Pt; the essential component for FA adsorption/oxidation) with manganese oxide nanowires (nano-MnOx; a CO poisoning alleviator) in a single blend surpassing the ideal catalytic activity of Pd substrates and realizing a minute negligible CO poisoning level. The molar ratio of the catalyst's ingredients (Pt/Mn) in the deposition bath was critical in identifying the catalytic activity of the catalyst where a molar ratio of (1:8) was optimum yielding the lowest required overpotential (– 475 mV shift in onset potential of direct FAO), highest catalytic activity (ca. 15 times enhancement) and least CO poisoning level during FAO. Several techniques including cyclic voltammetry, chronoamperometry, electrochemical impedance spectroscopy, field-emission scanning electron microscopy, high-resolution transmission electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffraction were all combined to report the catalyst's activity evaluating its morphology, composition, and structure. It is believed that adjusting the catalyst's composition could preferably act against the adsorption of poisoning CO intermediate and/or support electronically the desired (low overpotential) direct dehydrogenation pathway of FAO.



Novel Hydroxyapatite/Graphene Nanocomposite for the Effective Removal of water pollutants

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ABSTRACT

A novel hydroxyapatite/graphene(HAp/G) nanocomposite was found to be an excellent sorbent for the removal of heavy metals (Pb, Cd), organic dyes (methylene blue, MB), mineral metals (Fe, Mn) and industrial emulsified oil via a batch adsorption experiment. High-resolution transmission electron microscopy (HR-TEM), energy dispersive X-ray analysis (EDX), X-ray diffraction (XRD), Fourier transform infrared (FTIR)spectrophotometry, particle size distribution, and zeta potential measurements were performed to reveal the morphology, composition, crystal structure, functionality and stability of the prepared sorbent. The equilibrium concentration of pollutants was identified according to standard methods. The kinetics of the sorption process were investigated together with the influence of the initial pollutants concentration, sorbent dosage and solution pH on the sorption capacity. The sorption process followed pseudo-second-order kinetics, and 30 min was quite enough to attain equilibrium. The data were correlated using two adsorption isotherm models (Freundlich and Langmuir) to understand the adsorption mechanism.



Development of n-Type Anodized Nanoporous Stainless Steel 316L For Enhanced Photoelectrochemical Water Splitting

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ABSTRACT

The urgency to secure alternative resources for fossil fuels along with the advanced revolution in nanoscience have stimulated a significant motivation in the sector of energy to develop nanostructured materials for several electrochemical and photoelectrochemical applications. Of these applications, the hydrogen production, storage, and oxidation received exceptional attention in renewable energy plants. Actually, most of renewable plants perform efficiently under certain circumstances (e.g., the daytime for solar cells). Therefore, a storage/restoring system is required to save excess electricity from the time of plenty to the time of delay. So far, the applications of water splitting experience a lack of materials ensuring enhanced efficiency and reasonable stability. We herein propose a procedure to develop metal oxide nanostructured-based material for solar energy conversion. We herein suggest a propitious photoanode prepared by the anodization strategy for water splitting. This novel photoanode is composed of nanoporous arrays of stainless steel 316L films. The anodization parameters (potential, time, temperature, electrolyte, pH, etc) were tuned to improve the catalytic properties towards visible-light-driven water splitting. The morphology, composition, and crystal structure of as-prepared photoanodes were investigated using the *state-of-art* instrumentations as the field-emission scanning electron microscope, the energy dispersive X-ray spectrometer and the X-ray photon electron spectroscopy (XPS). The optical properties of the anodized sample was investigated using UV-Vis spectroscopy. The current-potential measurements were carried out in a three-electrode electrochemical cell and a scanning potentiostat was employed to measure the dark and illuminated currents.



Efficient Electrooxidation of Formic Acid at Bimetallic Nanoparticle-Based Pani-Modified Anodes

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ABSTRACT

Research is moving rapidly to sustain convenient energy resources fulfilling the global climate legislations. Herein, a group of novel catalysts of platinum (PtNPs), palladium (PdNPs) binary catalysts dispersed onto polyaniline (PANi) is recommended for formic acid electro-oxidation (FAO). The catalyst's preparation scheme allows a sequential electrodeposition of fibril PANi and spherical PtNPs, PdNPs on a glassy carbon (GC) substrate and permits a precise control over the deposition sequence and loading. Interestingly, incorporation of PANi into the catalyst's ingredients improves the catalytic activity of the catalysts towards FAO by shifting the mechanism towards the desirable dehydrogenation pathway and mitigating the undesirable poisoning dehydration pathway. Several techniques (CV, SEM, XRD and TEM) are employed to confirm the successful deposition of the catalysts and to evaluate its morphology, composition, crystal structure and catalytic activity. While PtNPs and PdNPs are essential for FA adsorption, PANi improves their dispersion and thus facilitates the charge transfer and mitigate CO poisoning. A promising catalytic stability is achieved in a long continuous electrolysis experiment.



Polyoxometalate Ionic Liquid as Anticorrosion Coating of Steel In Acidic Solution

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ABSTRACT

Metal corrosion is a global problem of worldwide significance affecting many industries. Many studies have shown that the annual direct cost of this inevitable problem to an industrial economy is approximately 3.1% of the country's Gross National Product (GNP). In order to avoid severe corrosion and metal lost, many approaches are used to protect the metallic surface such as, electrochemical methods, inhibitors and coating. In this research we focus on the use of polyoxometalate ionic liquid hybrid materials as coating anticorrosion protection of steel alloy surfaces. For this purpose $((C_8H_{17})_4N)_6[PW_{11}O_{39}Cu(H_2O)]$ has been synthesized and characterized by FT-IR, UV/Vis, ^{31}P , ^{13}C , 1H NMR spectroscopies. The effect of hydrophobic mixed metal kegging polyoxometalate ionic liquid $((C_8H_{17})_4N)_6[PW_{11}O_{39}Cu(H_2O)]$ as anticorrosion coating of steel surface was investigated in H_2SO_4 acidic aqueous solution with different concentrations ranging from 0.25 to 1.0 M at room temperature ($25\text{ }^\circ\text{C} \pm 1$) by means of electrochemical experiments which are electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP). The obtained results reveal that POM-ILs exhibit surface active properties and showed that this coating has fairly good inhibition properties against corrosion of steel in different concentrations of H_2SO_4 solutions, with efficiency $\geq 99.00\%$ (at optimum coating of inhibitor, temperature at $25\text{ }^\circ\text{C} \pm 1$ and time of 1.0 h).



Selectivity Toward Propylene Over Partially Crystalline H-ZSM-5 in Methanol-to-Olefin Reaction

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ABSTRACT

Partially crystalline mesoporous ZSM-5 material (P-ZSM-5) was successfully synthesized with the ratio of Si/Al= 45, the MFI structure was confirmed using XRD and Solid State-NMR. The morphology and textural properties of the sample were investigated by SEM, TEM and N₂-physisorption measurements. Further, the acidic property of synthesized material was studied by TPD-NH₃ and FTIR spectrometer of probe molecule CO adsorption. The P-ZSM-5 was tested in the methanol-to-olefin reaction at 500°C using operando UV-Vis spectroscopy and on-line gas chromatography. The MFI of synthesized sample show very selective toward propylene formation in comparison to commercial crystalline H-ZSM-5 with Si/Al=40. The P-ZSM-5 showed a selectivity ratio of C₃=/C₂= 12, while it is around 2 for the commercial H-ZSM-5 sample. The UV-Vis spectra for all studied materials reveal the nature of active and deactivated species within MFI structure.



Influence of Loading Amount of NiO Nanoparticles Supported on Graphite Planes as an Electrocatalyst for Urea Electro-Oxidation Reaction in Alkaline Medium

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ABSTRACT

Nickel oxide nanoparticles are fabricated onto graphite planes [NiO/Gt] by chemical precipitation of $\text{Ni}(\text{OH})_2$ particles with consecutive calcination at 400°C . The formed electrocatalysts are characterized using X-ray diffraction (XRD) and Transmission electron microscopy (TEM). TEM images demonstrate the deposition of NiO nanoparticles on graphite surface through their crystallite lattice fringes with spacing values of 2.45 \AA (111), 2.10 \AA (200) and 1.48 \AA (220). The electrocatalytic activity of NiO/Gt electrocatalyst is examined towards urea electro-oxidation in NaOH solution using cyclic voltammetry, chronoamperometry and electrochemical impedance spectroscopy. Urea oxidation peak current density is observed at NiO/Gt electrocatalyst containing 15 wt.%NiO [NiO/Gt-15] at a potential value of +640 mV (Ag/AgCl) with a current density value of 17.63 mA cm^{-2} . The loading amount of NiO in the prepared electrocatalyst significantly affects its electrocatalytic performance. NiO/Gt-15 exhibits the highest urea oxidation current density with the desired stability. The lower Tafel slope, charge transfer resistance and the higher exchange current density and diffusion coefficient values of urea molecules at NiO/Gt-15 surface elect its application as a promising electrocatalyst material during urea oxidation reaction in fuel cells.



Electrochemical Growth Approach to High –Quality Titanium Nano Oxide Thin Films for Medical and Industrial Applications

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ABSTRACT

Owing to the wide characteristics, passive thin films and their stability on a metal surface play an important role in a recent and future research. Efforts have been applied to study these thin films to improve their properties for a variety of applications. Manufacturing high-quality thin, porous film is made from the metal atoms. The properties of these thin films depend on how the atoms are arranged. The basic information introduced here is to create metal oxide thin films with small grain size by using electrochemical techniques, which are considered a low cost and simple techniques and can form good adhesion thin film layers. Based on electrochemical methods, can easily load small nanoparticles on the thin film matrix to develop their features, quality, performance and to broad their applications range. The top applications that depended on the high –quality nano metal oxide films include bio-materials, semiconductors, sensors, supercapacitors and multi-functional coatings. Here we briefly demonstrate the fabrication methods, properties, modification and extensive uses of thin oxide films in medical and industrial fields, focus on highly ordered titanium oxide nanostructure thin films fabricated and investigated *via* electrochemical techniques.



Electroless Coating of Copper with a Composite of Iron/Nickel/Phosphorus

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ABSTRACT

Iron/nickel/phosphorus with different ratios –composite had been deposited on a mechanically polished copper surface for different purposes. Different baths compositions have been tested. Thickness, composition, present phases, hardness, morphology of the composite layer were specified with relevant techniques. The corrosion behavior of the composite layer has been studied in 3.0% aqueous sodium chloride solution by the potentiodynamic polarization method. Furthermore, the effect of annealing on the characteristics of the deposit has been made to optimize its properties.

- 1- Part of the M.Sc. of Mr. Mostafa S.A. Sayed.
- 2- Ministry of Military Production.
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Enhancement of Methanol and Ethanol Fuel Cells Efficiency Using Ni-MgO/C Nano-Composite Anodes

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ABSTRACT

Ni-MgO nano-composites were prepared on carbon anodes by electro-deposition from a nickel Watts bath in the presence of fine MgO reinforcement particles. Their performance as electro-catalysts for the oxidation of methanol and ethanol in alkaline medium was investigated and compared with that of carbon coated pure Ni (Ni/C). The chemical composition, phase structure, and surface morphology of the deposited nano-composites were studied by energy dispersive X-ray spectroscopy, X-ray diffractometry, and scanning electron microscopy, respectively. Different electrochemical techniques were used to estimate the catalytic activity of the prepared electro-catalyst anodes, including cyclic voltammetry (CV), chronoamperometry, and electrochemical impedance spectroscopy (EIS). The Ni/C electro-catalyst alone exhibited remarkably low catalytic activity and poor stability toward the electro-oxidation process. The inclusion of MgO significantly promoted the catalytic activity of the Ni catalyst for the alcohol electro-oxidation and enhanced its poisoning resistance. The EIS results confirmed those of CV and revealed a lower charge transfer resistance and enhanced roughness for the Ni-MgO/C nano-composite electrodes compared with those of Ni/C.



Carbon Supported Pd-metal Oxide Electrocatalysts for Ethanol Electro-Oxidation in Alkaline Medium

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ABSTRACT

Various Pd-metal oxide/C electrocatalysts were fabricated using ethylene glycol as a reducing agent in modified microwave-assisted polyol process. The crystal structure and surface morphology were studied using X-ray diffraction and transmission electron microscopy. All prepared Pd-metal oxide/C electrocatalysts exhibited a shift of Pd diffraction planes in the positive direction in relation to that of Pd/C. Highly dispersed palladium nanoparticles were formed on different metal oxide/C supports. The electrocatalytic performance of these electrocatalysts for ethanol oxidation was examined in NaOH solution using cyclic voltammetry, chronoamperometry and electrochemical impedance spectroscopy. An improvement in electrochemical parameters including onset potential, oxidation current density and I_a/I_b values was recorded at different Pd-metal oxide/C electrocatalysts, especially Pd-NiO/C. Three folds increment in steady state oxidation current density value was also displayed by investigated Pd-metal oxide/C electrocatalysts when contrasted to that of Pd/C to reflect their enhanced stability behavior.



Theoretical Insights into Dehydrogenative Chemisorption of Alkylaromatics on Pt(100) and Ni(100)

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ABSTRACT

This study reports on the relevance of alkyl substituents on the chemisorption of alkylaromatics on metal surfaces, namely Pt(100) and Ni(100). Density functional theory (DFT) calculations are used to calculate the chemisorption energies of benzene, toluene, xylene, mesitylene, and ethylbenzene on Pt and Ni. Removal of hydrogens from the adsorbed benzene substantially reduces the stability of the adsorbed species on both Pt(100) and Ni(100) surfaces. Methyl substituents on the benzene ring, i.e., toluene, xylenes and mesitylene, result in exothermic dissociation of a C-H bond from each methyl substituent on both Pt and Ni surfaces. This leads to formation of CH₂ groups connected to the aromatic ring, resulting in a π -conjugated system stacked over the metal surface, and expanding over the entire molecule. The energy gain associated with dehydrogenation of each of the methyl groups cumulates, so that complete dehydrogenation of the methyl groups of xylenes and mesitylene should be expected. Further removal of hydrogen from aromatic rings of the π -conjugated system is always endothermic on both surfaces. The study is extended to ethylbenzene on the same surface, and results suggest that dehydrogenation of methylene group followed by dehydrogenation of the methyl group, leading to formation of adsorbed styrene is favored. These results may justify more explicitly the essential role of cofed (or recycled) hydrogen to produce alkylaromatics in practical applications, enabling to recover sp³ alkyl substituents to desorb the products. Although the actual catalysis involves more complexities on other types of metal sites, such as edges and kinks, the current study already demonstrates one significant aspect of the hydrogenation-dehydrogenation catalysis on metal surfaces.



DFT/PCM-TD-DFT Investigation and Molecular Docking Study of Thiouracil-Based Indenopyridopyrimidine Derivatives

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ABSTRACT

UV-Visible absorption spectra of thiouracil based in indenopyridopyrimidine and its derivatives were measured in different solvents. A benchmark evaluation against experimental results on the accuracy of different DFT functionals in predicting reliable ground state geometries is carried out. The benchmark of the geometric structure indicated hybrid functionals are found to be the most satisfied functionals and the best agreement with x-ray data is achieved by using the B3lyp functional. The di-keto forms of the indenopyridopyrimidine isomers of the studied compounds are found to be the most stable tautomers. The assignment of the absorption bands of the studied compounds has been confirmed on its π - π^* nature. The CT lengths (Δr), dipole moment change ($\Delta\mu_{CT}$) and natural transition orbitals (NTO's) indices showed that the charge transfer character of the electronic transitions is directly proportional to the electron-releasing strength of substituted phenyl ring. Molecular docking study is carried out to calculate the binding energy between these molecules and relevant proteins.



HALL (B)

SESSIONS OF :

- Organic Synthesis.
- Polymer.
- Organic and Organometallic.
- liquid crystals.
- Biochemistry and Bioanalytical techniques.



Synthesis of Novel Biodegradable Antibacterial Grafted Xanthan Gum

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ABSTRACT

Xanthan gum (XG) is natural polysaccharides used in food industries as stabilizers and thickener agents. The problem is that some food products are found to be contaminated by pathogenic bacteria such as *Escherichia coli* (*E. coli*) and *Staphylococcus aureus* (*S. aureus*) that reduce their shelf life. This research aims to synthesize biodegradable antibacterial XG-grafted-poly(*N*-vinyl imidazole) PVI and the effect of reaction parameters were studied on grafting yield (G), grafting efficiency (GE), total conversion (TC) and homopolymer (H) %. XG-g-PVI was characterized via various analysis tools. Thermal analysis showed that grafted XG was more thermally stable than unmodified XG and their stability increased with increasing PVI%. XG-g-PVI was acting as antibacterial agent against (*E. coli* and *S. aureus*) bacteria that cause food borne diseases. Their activity increases with increasing grafting yield%. Surface morphology showed change from irregular lobules shape in XG to smooth surface in its graft with PVI.



Nucleosides 10 [1]: Synthesis of New Derivatives of Pyrimidine and Fused Pyrimidine Nucleosides of Expected Biological Activity

Mosselhi Abdel nabi Mosselhi Mohamed, Laila M. Break Abu – Alola & Ohoud Aaide Awaad Al-Thubaiti

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ABSTRACT

Many serious attempts have been reported to synthesize N-Azine nucleosides, especially N-pyrimidine nucleosides, which showed activity against tumors during the last thirty years [2]. The recently adopted attempts to prepare the way Hilbert-Johnson, which includes coupling between dialkoxypyrimidines and halosugars that have been protected, and in a way that either heat or through the use of mercury as a catalyst or by using the silylation method. The nucleosides which contain different types of heterocyclic compounds represent a new era of bioorganic molecules[2]. Pyrimidines, such as uracils and fused pyrimidines, such as thienopyrimidines reacted with 1-O-acetyl-2,3,5-tri-O-benzoyl- β -D-ribofuranose, followed by reaction with methanolic sodium methoxide to get new derivatives of the corresponding N-nucleosides. The new nucleosides formed were tested for biological activity against some of microorganism (some fungi and bacteria species). Some of the tested products showed moderate activity and the results were reported.

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Chimerically Designed Multitarget Anticancers: Investigation of 4-Substituted-5-substitute Diaminopyrimidines as Dual Inhibitors of Tyrosine Kinase and HDAC

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ABSTRACT

The development of novel anticancer agents green protocol possessing enhanced activity, better selectivity and overcoming emerging resistance are needed in combating cancer diseases. The multitarget drugs approach enables the design of molecules having more multiple mechanisms of action, offering opportunities achieve better efficiency and minimizing side effects and resistance. We suggest chimeric molecules capable of inhibiting both of tyrosine kinase receptor and histone deacetylases as potential anticancer agents. As of novelty of proposed designed scaffold, patent could be claimed to protect intellectual property rights of inventors. According to elicited level biological activity, selectivity and safety.



Production of Fuel by Pyrolysis of Low Density Polyethylene (LDPE)

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ABSTRACT

The hazards of plastic waste are well known to us. The conversion of oil from plastic has dual benefits. First of all the oil produced can be used as a fuel for domestic purposes and also in vehicles and industries when further refined. Secondly the various types of pollution caused due to waste plastics can be minimized. Plastic in the first place is manufactured from natural gas specifically from ethane which is a constituent of natural gas. Therefore the waste plastic can be converted back into it. For the process of conversion a machine can be used which will heat the plastic to a high temperature so that it pyrolyzed and does not burns at a temperature range (480-5800c). The furnace and reactor have been designed in order to do pyrolysis process in absence of oxygen to produce fuel from plastic (LDPE). Reaction was carried out with and without using natural bentonite and kaoline catalysts. Upon Comparison between fuel obtained with and without catalysts, it is observed that in absence of catalyst, process gives about 61.6% yield, with bentonite catalyst yield is 67.7 %. From this result, it can be concluded that the oil produced in the catalytic pyrolysis can be used as a substitute of petro fuels. Catalyst is used to give higher yield (67%). The products that obtained showed that the efficiency of that process with high yield and good properties, all the other fuel properties of the oil obtained is almost similar and comparable to petroleum fractions. Moreover, it has high calorific of 49.2 MJ/kg value. Analysis of oil samples showed presence of gasoline, kerosene and diesel fractions (C5-C20) with other high molecular weight fractions for all systems. Scaling up of the present method would contribute to solve some of fuel lacking problem.



Photo-Stabilizers for Rigid Poly (Vinyl Chloride) Based on Polytoluidine

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ABSTRACT

Polytoluidines (*ortho*, *Meta* and *para*) were prepared by chemical oxidation process using ammonium peroxy disulfate as initiator. Prepared polytoluidines were characterized by spectral and thermal analyses. Their electrical conductivities were measured and poly (*para*-toluidine) showed the highest value. The prepared polytoluidines were examined as UV-stabilizers for rigid poly(vinyl chloride) (PVC) films as compared with the blank PVC and PVC stabilized by the commercial UV-stabilizer (chimasorbs). The prepared PVC films were exposed to UV lamp with definite power and wavelength for 30 days. Consequently, the changing of color and weight for irradiated films were followed at definite time intervals. The obtained results showed the high efficiency of polytoluidines as photo stabilizers for PVC Film.



Dianionic Oxy-Cope Rearrangement with Benzil Derivatives: *meso*-Selective 3,3-Coupling of Two Tetrahydrofuran Moieties

Amr Mohamed Abdelmoniem, Ismail Abdelshafy Abdelhamid, Jörg Fohrer, Iris Bardenhorst, Rudolf Wartchow, and Holger Butenschön

ABSTRACT

Benzil and its derivatives naphthyl and pyridyl have been found to undergo a dianionic oxy-Cope rearrangement upon reaction with 2-lithio-4,5-dihydrofuran to give 3,3'-octahydrobifuranyls selectively as the *meso* diastereomers. The diastereo selectivity is explained based on the reaction mechanism and the conformation of the starting material. 4,4'-Di-*tert*-butylbenzil gave the respective intramolecular aldol adduct, whose relative configuration was determined by NOE experiments.



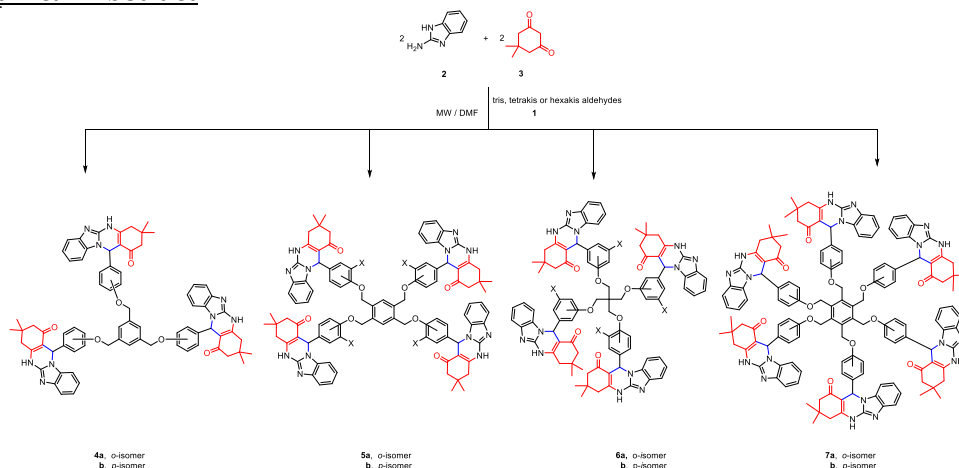
Regioselective Synthesis of Tris-, Tertakis- and Hexakis(tetrahydrobenzo[4,5]imidazo[2,1-*b*]quinazolin-1(2*H*)-one) Using Begenelli Like Reaction

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ABSTRACT

In continuation to our ongoing research work on bis-heterocycles^[1-3] as well as on the synthesis of heterocycles utilizing C-C bond formation reactions^[1-4], a new series of tris, tetrakis and hexakis (3,3-dimethyl-3,4,5,12-tetrahydrobenzo[4,5]imidazo[2,1-*b*]quinazolin-1(2*H*)-one) were synthesized in good yields using a one-pot cyclocondensation reaction of the appropriate poly(aldehydes) with dimedone and 2-aminobenzimidazole in DMF as solvent. The structures of the newly synthesized compounds are well established based on spectral data.

Graphical Abstract



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Mirror-Symmetry Breaking in Photosensitive Bent-Core Mesogens

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ABSTRACT

The observation of spontaneous development of chirality in liquid crystalline (LC) phases of achiral molecules is a contemporary research topic for fundamental scientific research and technological applications. Dark conglomerate phases (DC phases) composed of conglomerates of macroscopic chiral domains and formed by some achiral bent-core mesogens, represent such a case. Recently, we have found that the azobenzene unit is a very useful building block for designing bent-core molecules (BCLCs) exhibiting different subtypes of DC phases with crystalline local structure.¹⁻⁵ Here we report new BCLCs forming new types of DC phases or conventional liquid crystalline phases depending on the molecular design (Figure 1). These BCLCs are derived from 4-substituted resorcinol central core connected to azobenzene-based side arms with additional peripheral fluorine substitution. The number and position of fluorine atoms was changed systematically. All materials were characterized by DSC, polarizing microscopy, electro-optical studies and XRD. The results indicate the formation of amorphous solids composed of helical nano-crystallites with short coherence length (HNC phases) which is considered as a third major type of DC phases, distinct from the well known sponge phases and the HNF phases.



Synthesis of Novel Heterocycles Incorporating Antipyrine Moiety as Potential Anti-breast agents

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ABSTRACT

Reaction of 1-[4-(1,2-dihydro-1,5-dimethyl-2-phenyl-3-oxo-3H-pyrazol-4-yl)-2-phenylsulfonyl-1-ethanone (1) with phenyl isothiocyanate, in DMF/ followed by treatment with dilute hydrochloric acid afforded the corresponding 4-(3-mercapto-3-(phenylamino)-2-(phenylsulfonyl)acryloyl)-1,5-dimethyl-2-phenyl-1H-pyrazol-3(2H)-one (2). Treatment of compound 2 with hydrazonoyl chlorides 3a-h afforded the corresponding 1,3,4-thiadiazole derivatives 5a-h. Cyclocondensation reaction of compound 2 with the appropriate α -halo-compounds 6, 8, 10, 12a,b or 14 (ethyl 2-chloroacetate, chloroacetonitrile, 1-chloropropan-2-one, 2-bromo-1-phenylethanone, 2-bromo-1-p-tolyethanone and 2-bromoacetyl-3H-benzo[f]chromen-3-one, afforded the corresponding 1,3-thiazole 7, 9, 11, 13a,b and 15, respectively. Coupling of the ketosulphone 1 with the appropriate diazotized heterocyclic amines, namely, 4H-1,2,4-triazol-3-amine (16) or 2-aminobenzimidazole (19) afforded the corresponding 1,5-dimethyl-2-phenyl-4-(4-(phenylsulfonyl)-[1,2,4]triazolo[5,1-c][1,2,4]triazin-3-yl)-1H-pyrazol-3(2H)-one (18). 1,5-Dimethyl-2-phenyl-4-(4-(phenylsulfonyl)benzo[4,5]imidazo[2,1-c][1,2,4]triazin-3-yl)-1H-pyrazol-3(2H)-one (21), respectively. The synthesized compounds were confirmed on the basis of their elemental analysis and spectral data and evaluated as potential anticancer agents.



Ultrasound one Pot Synthesis of Fused Quinazolinones and Quinazolinediones, *in vitro* Screening and Molecular Modeling Study as Phosphodiesterase 7A1 Inhibitors.

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ABSTRACT

A new series of 3-substituted 6-aryl-dihydroisoindolo[2,1-a]quinazoline-5,11-diones (4-13) were synthesized using ultrasound one pot methodology. The synthesized compounds were inspected for their *in vitro* PDE7A1 inhibitory activity. Compounds 14-21 were synthesized using ultrasound and seven of them were assayed for their *in vitro* inhibitory activity for enzyme PDE7A1. Compounds 6, 9, 12, 17 and 18 showed effective inhibitory activity of enzyme PDE7A1 with half maximal inhibitor concentration (IC₅₀μM) of 0.005, 0.0073, 0.004, 0.007 and 0.008 μM respectively indicating high inhibitory activity for the enzyme. All the synthesized compounds were docked into the enzyme PDE7A1 binding site to study their mode of interaction compounds 6, 9, 12 exhibited good interaction at the PDE7A1 binding site.



Synthesis, Cytotoxicity, Antimicrobial and Docking Simulation of Novel Pyrazolo[3,4-*d*]Pyrimidine and Pyrazolo[4,3-*e*][1,2,4]Triazolo[3,4-*c*]Pyrimidine Derivatives

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ABSTRACT

Treatment of isobutyrohydrazonoyl bromide **1** with malononitrile in sodium ethoxide solution afforded 5-amino-4-cyanopyrazole derivative **2**, which converted to formidate derivative **3** upon refluxing with TEOF in acetic anhydride. The reaction of the latter product with hydrazine hydrate afforded imino-amine derivative **4**, which was converted to hydrazino derivative **5** by refluxing with hydrazine hydrate. Hydrazino as well as imino amino derivatives undergo condensation and cyclization reactions to give pyrazolo[3,4-*d*]pyrimidine and pyrazolo[4,3-*e*][1,2,4]triazolo[3,4-*c*]pyrimidine derivatives, respectively. Antimicrobial studies are performed using two-gram positive bacteria, *Bacillus subtilis* and *Staphylococcus aureus*, as well as two-gram negative bacteria, *Escherichia coli* and *Pseudomonas aeruginosa*. Data revealed that compounds **5**, **6b**, **9a** and **10d** explore high antibacterial effect against all tested strains. Compound **9a** is the most promising antibacterial agent with high efficiency (low MIC value). Unfortunately, all compounds have no antifungal activity against the selected fungal strains. Regarding cytotoxic assay, compound **8c** is the most potent and promising drug against hepatocellular carcinoma with IC₅₀ value (3.79 µg/ml). In attempts to detect the molecular action of **8c**, molecular docking simulation was run using DHFR PDB:ID (1DLS). This modeling study revealed that compound **8c** is good inhibitor for DHFR enzyme.



An Efficient Sonochemical Synthesis, Molecular docking of 2-Phenyl-1, 8-Naphthyridine derivatives and their Cytotoxic Activity Against HepG2 Cell Lines

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ABSTRACT

The availability and wide acceptance of several 1,8-naphthyridine derivatives as chemotherapeutic agent especially as antimicrobial and anticancer agent, encouraged us to synthesize some new series of type of compounds such incorporated into another nitrogen, heterocycles, mannich bases, styryl compound hoping that the resulting target products would possess cytotoxic activity. Some of the newly synthesized compounds were selected to evaluate their in vitro growth inhibitory activities against humancultured liver carcinoma cell lines (HEPG2) some of the tested derivatives showed makeable activity towards such study.



Evaluating the Production of the Neurotoxic Amino Acids β -N-Methylamino-L-Alanine (BMAA) and 2,4-Diamino-Butyric Acid (DAB) in Cyanobacteria, Using LC/ESI-MSn

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ABSTRACT

The neurotoxic non-protein amino acid β -N-methylamino-L-alanine (BMAA) has been found to be produced by different strains of cyanobacteria. BMAA has controversially been suggested as the possible cause of neurodegenerative disorder Amyotrophic Lateral Sclerosis/Parkinsonism Dementia Complex (ALS/PDC). Various methods of detection of BMAA in cyanobacteria have been developed some involving derivatization of the amino acid while others were devoid of amino acid derivatization. In this study, a solid phase extraction was applied for sample clean-up prior to HPLC-ESI-MSn analysis using Thermo Scientific Hyper Sep Verify TM -CX SPE column. Both derivatized and underivatized sample analysis were employed. BMAA and DAB (derivatized) were detected in axenic laboratory cultures of *Synechocystis* NPLB 2 and *Nostoc* MAC PCC 8009 while only BMAA (underivatized) was detected in axenic laboratory cultures of *Synechocystis* NPLB 2 and *Nostoc* MAC PCC 8009 by the application of high performance liquid chromatographic separation coupled with electrospray ionization ion trap mass spectrometry detection (HPLC-ESI-MSn). BMAA and DAB were analysed as total BMAA/DAB in cyanobacteria not as free or protein-bound. This study appears to be the first to detect BMAA/DAB in cyanobacteria using HPLC-ESI-MSn. Our results suggest further that BMAA and DAB are produced by cyanobacteria.



Development of Porous Metal Organic FrameWork Nanocarriers for Drug Delivery and Biomedical Imaing

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ABSTRACT

Despite the outstanding achievement made in understanding the fundamental science behind many diseases, researches into comparable progress in the treatment of these diseases are yet to be fully explored. Current therapeutic drugs are limited by their nonspecific distribution throughout the body leading to high doses, rapid clearance, poor pharmacokinetics, and unwanted side effects. Polymeric nanoparticles (NPs), micelles NPs, dendrimers and liposomes, nanocrystals, among others, have been proposed as drug delivery systems (DDS). These above nano materials show poor drug loading and rapid release of the proportion of the drug that is attached to the external surface of the nanocarrier. Metal-Organic Frameworks are new substitutes which are well suited to serve as nanocarriers for delivery and biomedical imaging because of their tunable structures, high porosity for better drug interactions and high loadings. Furthermore, MOFs can be non-toxic (i.e. iron carboxylates) and might include within their framework biologically active moieties (BioMOFs), which facilitate their use in theranostic nanomedicine. Therefore, this review article explored the emerging research progress related to metal-organic frameworks (MOFs) with focus on synthesis strategies and drug delivery, molecular imaging, and theranostic applications. The future prospects of MOFs are also elaborated in the context of post-synthetic modifications with the view to enhanced there nanomedicine application. More effort is necessary to develop clinically adaptable MOFs for various applications in nanomedicine.



Bioassay Guided Isolation of N-Butanol Fraction of *Mormodica Balsamina* Against *Salmonella Typhimurium* and *Staphylococcus Aureus*

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ABSTRACT

The purpose of this study was to isolate and evaluate the antibacterial activity of n-butanol fractions of *Mormodicabalsamina* against *Salmonellatyphimurium* and *Staphylococcus aureus*. Fraction was isolated using Column Chromatography and six different (A, B, C, D, E and F) fractions of *M.balsamina* were tested for antibacterial activity using agar well diffusion method against *Salmonellatyphimurium* and *Staphylococcus aureus*. Fourier Transform Infra-red Spectroscopy (FTIR) was used to detect the characteristic peak values and their functional groups present in the specific fraction that exhibited potent antibacterial activity. The results highlighted that the fractions showed higher zone against all isolates, the highest inhibitory zone (31.00 ± 1.41 mm) was observed on fraction C against *Salmonella typhimurium*. Further assessment of minimum inhibitory concentration and minimum bactericidal concentration ranged between 3.125 to 50 mg/ml respectively. Fourier Transform Infra-red (FTIR) Spectra of fraction C revealed the presence of different functional groups ranging from carboxylic (R-C (O)-OH), alkanes (C-H), aldehydes (R-CH=O) and alkenes (RCH=CH₂), Amides (R-C(O)-NH₂), Alkyl halides (R-F), Alcohol (Ar-OH), Ethers (Ar-o-R), and Aromatic (C-H) respectively. Low Minimum Inhibitory Concentration and low Minimum Bactericidal Concentration may justify the traditional uses of the leaves of *M.balsamina* for therapeutic purposes. FTIR graphs provided characteristic peaks which represented the components responsible for antibacterial activity.



HALL (C)

SESSIONS OF:

- Sensors and Analytical Techniques.
- Material science.
- Bio-inorganic.
- Inorganic Chemistry
- Environmental analysis



Determination of Fluoride and Some Heavy Metals in Water, Blood and Urine Samples Among Some Inhabitants of Gashu, Bade local Government Area, Yobe State, Nigeria

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ABSTRACT

The research area was in Gashua, Bade Local Government Area, Yobe State, Nigeria. The levels of fluoride, cadmium, arsenic, lead, iron and nickel were determined in sachet and borehole water samples. The levels of fluoride, cadmium, arsenic, lead, iron and nickel were also determined in blood and urine samples with respect to age groups and gender. Sample collection and preparations were carried out using standard procedures. The concentrations of all the studied metals were determined using atomic absorption spectroscopy (A.A.S). The concentration of fluoride was observed to be higher in the male subjects when compared to the female subjects. It was also observed that the concentration of fluoride was significantly higher in the urine samples when compared to the blood samples. From the present study the concentration of iron ranged from 0.11 to 2.13 mg/L, 0.01 to 1.42 mg/L arsenic, 0.01 to 2.13 mg/L cadmium, 0.01 to 1.77 mg/L nickel and 0.02 to 2.13 mg/L lead. Results from the present study showed that the mean concentrations of arsenic in the borehole water samples from the different wards in Gashua ranged from 0.87 to 2.98 mg/L; 0.44 to 0.77 mg/L lead, 1.04 to 2.13 mg/L nickel, 0.12 to 0.35 mg/L cadmium and 2.56 to 5.56 mg/L iron. The values obtained from the borehole water samples were higher than the WHO standard value of 0.05 mg/L arsenic, 1.0 mg/L iron, 0.01 mg/L lead, 0.07 mg/L nickel and 0.005 mg/L cadmium for drinking water. Information from this research showed the possible factors that may result in gender metal accumulation. The concentrations of all the study metals in the urine and blood samples were significantly higher than the WHO limits. Data obtained from borehole water samples showed that, the borehole water might be a contributing factor to blood/urine metal accumulation. Information from this research also showed the possible factors that may result to higher concentrations of all the metals in urine (both recent and past exposure) when compared to blood (only recent exposure). Data obtained from the present research indicate that the concentrations of all the metals in the blood and urine samples increased with increase in age group. This fact could be explained by the tendency of heavy metals to accumulate in the human body (bioaccumulation of heavy metals) with time, indicating that metal accumulation is age dependent.



Physico-Chemical Determination of Pozzolanic Properties of Arachishypogaea L shells (Groundnut) as Cement Replacement in Concretes

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ABSTRACT

As biomass power production becomes more main stream, problems with waste disposal arise. Arachishypogaea l. shells (groundnut) ash, a by-product of Groundnuts production, has beneficial strength and durability properties when used as a cement replacement material. This study examined strength and durability characteristics of mortar and concrete samples containing Arachishypogaea l. shells ash (groundnut) Lowe,(2012).The chemical and mineralogical compositions of the ash were determined using X-ray fluorescence (XRF), X-ray diffraction (XRD), and energy dispersive X-ray spectroscopy (EDS). The compositions met the requirements outlined by the ASTM C618 specification, the Standard Specification for Arachis hypogaea Ash and Raw of Calcined Natural Pozzolana Use in Concrete, with the silica being the most abundant compound.The measured loss on ignition was greater than that allowed by the ASTM C618 specifications. The microstructure of the ash was observed using a scanning electron microscope (SEM). As-received, the AHS ash had a high carbon content and required further processing. To determine the optimal method of processing the ash, mortars were created using different ash replacement levels, varying the temperatures at which the ash was fired, and varying the grinding regime. Compressive strength tests and thermogravimetric analyses (TGA) were used to compare the samples. It was found that a 20 percent replacement level and a 30 minute grinding time produced the most favorable results. Further studies are required to determine the optimal firing temperature. The TGA showed only a slight reduction in Ca(OH)_2 indicating minimal pozzolanic reactivity. This means the compressive strength results could be the result of the filler effect rather than pozzolanic reactivity. Reducing the firing time may improve the pozzolanic reactivity of the Arachis hypogaea ash. Concrete properties were measured using compressive strength tests and rapid chloride permeability tests. Concrete cylinders were cast using a AHS ash replacement level of 10 percent, grinding the ash at 250 rpm for 20 minutes and firing the ash at 950 oC for one hour. The samples containing AHS ash produced a compressive strength of 77 percent than that of the control. 4.3The XRD analysis result. The XRD analysis result indicate the qualitative presence of crystalline minerals in AHS ash (figure 3.4).XRD analysis was conducted twice to ensure accuracy. XRD diffraction patterns detected at various peaks in Figure 3.4 indicate many crystalline phases. The oxide composition of the AHS ash is as follows: CaO 10.91%,SiO₂ 33.36%, Al₂O₃ 6.73%, MgO 4.72%, SO₃ 6.40% k₂O+Na₂O 5.28% and CO₂36.40%.



Optimal Design and Operation of Multivessel Batch Distillation for Binary Mixture Separation

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ABSTRACT

In the literature reviews and in the past work on the Multivessel Batch Distillation Column, only multicomponent distillation is considered. No consideration was given to binary distillation and off-cut production for MultiVBD column. In this work, the MultiVBD column with binary distillation and with off-cut production is considered and discussed. In this study, one scenario is considered. In this scenario a fixed batch time, optimal design and operating policy are determined with strict product specifications. For a binary mixture, the performance of the MultiVBD column is also evaluated against that of a conventional batch distillation column. It was found that the vapour load for the MultiVBD column is about 24.1% lower compared to CBD column and the operating cost (an indirect measure of the energy cost and environmental impact) is more than 23.9% lower for MultiVBD column. Finally, the overall profit realised by MultiVBD column is about 25.6% more than by CBD column. Thus, for a given separation task, MultiVBD column is more environment friendly.



Functional Colloidal Magnetic Dispersions for Metal Remediation

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ABSTRACT

Among the organic and inorganic pollutants, heavy metals are considered as the most hazardous even at trace levels due to their persistent character.¹ They are non-biodegradables, cannot be metabolized by the body and are accumulate in the living organisms causing various diseases and disorders as cancers, organ damages, nervous system damages, and in extreme cases, death. The contamination is usually associated with intensive industry activities, mining smelting, agriculture, factory farms, roadways and automobiles and others activities like fracking.²⁻³ We report in this presentation some of our results on the design of efficient, easily accessible, sensitive and reusable magnetic nano-adsorbents based on 1,2,3-triazole functionalized iron oxide nanoparticles (MNPs).⁴⁻⁵ These adsorbents have the advantage to be superparamagnetic and could be easily recovered or manipulated with an external magnetic field after metal remediation without the degradation of the active sites. Their adsorption and regeneration behaviors were investigated for several heavy metal ions as Pb(II), Cu(II) and Zn(II). These nanoparticles have been also used to prepare polyHIPE monolith adsorbents with open cellular architecture of large pores and interconnected small pores.

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Recycling of Used Engine Oil Using Extraction by Single Solvent and Glacial Acetic Acid Treatment

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ABSTRACT

Optimizing the recycle of used oil is an important goal toward improving the sustainable and reducing the environmental impact of our needs. Used oil can contain hazardous wastes due to its high concentration of heavy metals, organic substance. In Libya thousands tones of vehicle waste oil is generated every year, most of this oil is wasted because no suitable disposal route exists and does not have companies for treatment and recycling of used oil. In this study, two different methods have been used by solvent extraction and acid treatment. The performance of the solvent extraction method is evaluated against that of acid treatment. The yield of base oil of the solvent extraction is 55.0-55.3% more compared to those of acid treatment. Thus, for a given separation task, solvent extraction is more environment / friendly.



Synthesis and Equilibrium Investigation of the Interaction of Model Antitumour Palladium (II) Complex With Biorelevant Ligands. DNA Binding Studies and Biological Activity

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ABSTRACT

With the purpose of the search of new antitumor metal complexes and evaluating the ability of Pd(II) complex to interact with DNA molecule as the main biological target, the complex-formation reactions of model Pd(II) diamine complexes, $[\text{Pd}(\text{diamine})(\text{H}_2\text{O})_2]^{2+}$, (where diamine is 2,2'-dipyridylamine / and or 2,2'-bipyridine) with some selected biorelevant ligands containing different functional groups and occurring in vivo as, amino acids, amides, dicarboxylic acids and DNA unit constituents, will be investigated at 25°C and at constant 0.1 mol.dm⁻³ ionic strength. The stoichiometry and stability constants of the complexes formed in solution will be evaluated and the binding centers of the ligands will be assigned in details. The effect of chelate ring size of the dicarboxylic acid complexes on their stability constants will be examined. Structural effects of the amide on the amide deprotonation will be investigated. In order to allow extrapolating the investigation to some biological micro-environment of low polarity, as active sites of enzymes and side chain proteins, the complex formation equilibria will also be studied in media of low polarity as in dioxane-water mixture of different composition. The concentration distribution diagrams of the various species formed in solution will be evaluated. Further investigation of the binding properties of the diaqua palladium (II) complexes with calf thymus DNA (CT-DNA) will be investigated by UV-vis spectroscopy. The intrinsic binding constants (K_b) will be calculated from the UV-vis absorption studies. The mode of binding of the diaqua complexes with CT-DNA will be investigated using different physico-chemical tools as (cyclic voltametry, viscosity measurements and thermal denaturation DNA cleavage studies. The biological activity of the synthesized palladium (II) complexes will also be tested against some cancer cell lines, some bacteria and fungi.



Synthesis and Characterization of Substituted Mo and W Carbonyl Complexes Containing Isoniazid Dimethyl Glyoxime

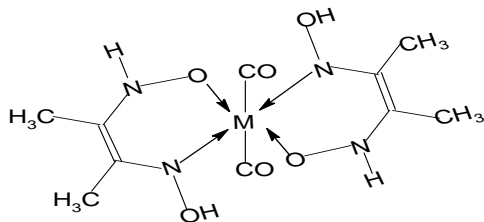
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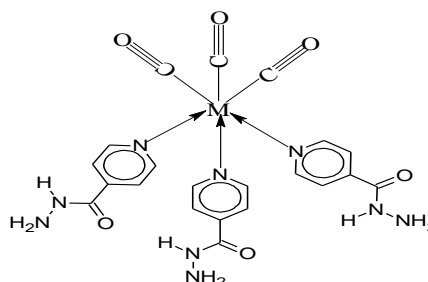
ABSTRACT

Substituted metal carbonyls with biologically relevant ancillary ligands are reported to systematically release CO and non-harmful substrates in vivo promising to be useful candidates as CO-releasing molecules (CO-RMs).¹ In a one pot synthesis, we prepared substituted carbonyl complexes of dimethylglyoxime (DMG) and isoniazid using manipulated Schlenk technique under N₂ in THF. The decarbonylation and substitution of the Mo & W hexacarbonyls were successfully carried out by stirring the mixtures at room temperature for 24 h and 36 h respectively in the presence of trimethylamine N-oxide.² The compounds were characterized using ¹H NMR, FTIR, and CHN analyses. Results reveal dicarbonyl and tricarbonyl species **I** and **II**, where two DMG and three isoniazid moieties were coordinated to the central metal atoms.



M = Mo, W

I



II

The resulting complexes with CO ligands of decreased bond strength promises to be good candidates for CO release studies in biological system with the use of appropriate CO release activating agent, thus offering some hope for their use as CO-releasing molecules.

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Synthesis of a Simply Modified Electrochemical Nicotine Sensor Based on Nanoparticles

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ABSTRACT

Innovative electrochemical nicotine (NIC) modified sensor was created. Different electrochemical techniques were used in both aqueous and micellar media. Surface characterization was performed using scanning electron microscope (SEM) and energy dispersive x-ray analysis (EDX) techniques. NIC measurements were investigated in Britton–Robinson (B–R) buffer solutions with a pH range (2.0–8.0) containing (1.0 mM) sodium dodecyl sulfate (SDS). The electrode based NIC sensor exhibited a good sensitivity and detection limit. The proposed sensor is capable of detecting trace levels of NIC in real urine samples and different brands of commercial cigarettes.



Crystal Growth Study of a Guest-Free Microporous Metal-Organic Framework Zinc 5-tert-butyl Isophthalate (Zn(tbip)) by Atomic Force Microscopy

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ABSTRACT

Zn(tbip) is a novel guest-free Microporous metal-organic framework (GFMMOF) composed of Zn-based secondary building units (SBUs), [Zn(NO₃).6H₂O], and 5-tert-butyl isophthalate (tbip²⁻) ligands has been synthesised and characterised structurally robust with an extraordinary thermal stability. The Powdered X-ray diffraction pattern of the sample indicated that a monophasic sample had been prepared, which is very similar to the theoretical pattern of Zn(tbip). The scanning electron microscopy (SEM) revealed that the crystals have elongated hexagonal prism morphology with crystals sizes ranging from 700 μm to 1 nm. Thermogravimetric analysis (TGA) showed that the crystal is thermally stable up to 450 °C and is guest molecule free. Solid-state NMR also proved that the crystals are guest-free. Single crystals were determined by single crystal X-ray diffraction (SXRD). *Ex-situ* atomic force microscopy (AFM) investigation on the elongated hexagonal prism of Zn(tbip) surface provided information concerning the crystal growth mechanism of the material. Multilayer anisotropic growth features were observed in the AFM micrographs, indicating much more rapid growth of the crystals in the direction parallel to the channel system than perpendicular to it. The cross-sectional analyses of the height images reveal that most of the growth steps are within the 45 – 50 nm and indicated that the extended structural units are stabilised on the crystal surfaces. This work demonstrates the use of AFM to provide new information on the crystal growth a non-cubic MOF, Zn(tbip).



Facile Synthesis of High Thermally Stable Au/TiO₂ Nano-Photocatalyst

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ABSTRACT

This work describes a new and straightforward approach for the synthesis of high-temperature stable hybrid Au/TiO₂ nanocomposites (NCs). This novel approach allows one to produce Au cores decorated with titanium dioxide (TiO₂) nanoparticles owing to a modified solvothermal process that makes use of gold salt HAuCl₄ and Titanium (IV) butoxide as the gold and titanium precursors, and Dimethyl Sulfoxide (DMSO) as a solvent. The structure and morphology of the Au/TiO₂ nanocomposites were characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM), Energy Dispersive X-ray Fluorescence (EDXRF), high-resolution transmission electron microscopy (HRTEM), Raman and photoluminescence spectroscopies. Based on FTIR and TDA/TGA measurements, a proposed mechanism for the formation of Au/TiO₂ NCs in DMSO (without adding of any other reagents) is discussed in this contribution. Optical absorption measurement showed that the Au/TiO₂ NCs exhibit a UV significant absorption peak clearly blue-shifted with respect to that of bulk TiO₂. The produced nanocomposites consist of monodisperse quasi-spherical AuNPs core decorated with TiO₂ anatase phase (average size of 11nm). The hybrid Au/TiO₂ NCs show a high photocatalytic performance in the degradation of diuron pesticide (C₉H₁₀Cl₂N₂O) under illumination by UV light. The high crystalline quality, together with the easy synthesis process, makes the Au/TiO₂ NCs a promising candidate for many applications such as optoelectronics and water photolysis for hydrogen production.



Synthesis, X-ray, Biological Activity and Equilibrium Studies of Palladium(II) Complexes as a Model of Antitumour Agents Incorporating Dicarboxylic Acids.

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ABSTRACT

The stoichiometry and stability constants of the complexes formed between $[\text{Pd}(\text{MAMP})(\text{H}_2\text{O})_2]^{2+}$, (MAMP = 2-methylaminomethyl-pyridine) with some dicarboxylic acids were investigated at 0.1 mol.dm^{-3} ionic strength. Equilibria are readily achieved with Pd(II) and the results serve as a reference for slowly reacting Pt(II). The concentration distribution of the various complex species was evaluated as a function of pH. The effect of chelate ring size of the dicarboxylic acid complexes on their stability constants was examined. Formation of the metal complexes has been found to be spontaneous, exothermic and entropically favorable. The thermodynamic parameters calculated from the temperature dependence of the equilibrium constants were investigated. Crystal structure of $[\text{Pd}(\text{MAMP})\text{Ox}]\cdot 2\text{H}_2\text{O}$ shows that Pd(II) cation displays a distorted square planar geometry, 2-methylaminomethyl-pyridine (MAMP) acts as a bidentate ligand bonded to the Pd(II) ion through the deprotonated nitrogen of pyridine and secondary NH groups and oxalic acid (Ox) is coordinated by the oxygen atoms of carboxylate groups. The complex crystallizes in the space group $P2_1/c$, $a = 6.8441(9) \text{ \AA}$, $b = 9.8915(10) \text{ \AA}$, $c = 18.779(2) \text{ \AA}$, $\alpha = 90.00^\circ$, $\beta = 94.317(6)^\circ$, $\gamma = 90.00^\circ$, $V = 1267.7(3) \text{ \AA}^3$, $Z = 4$ (i.e. four molecules per unit cell). The isolated Pd(II)-complexes were screened for their antimicrobial and cytotoxic activities. The results are expected to contribute to the chemistry of tumor therapy.



Kinetics and Thermodynamic Behavior of Cadmium(II) Uptake From Aqueous Iodide Media on to Polyurethane Foam Physically Immobilized With Some Basic Dyes

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ABSTRACT

Clay minerals represents the most efficient and low cost solid phase extractors (SPE) among various solid sorbent and/or adsorbent for removal and/or minimization of heavy metal pollutants in water treatment. Thus, the present article reports the influence of various analytical parameters that control mercury(II) uptake from water onto 1-(2-pyridylazo)-2-naphthol (PAN) treated clay. The overall rate constant of mercury(II) uptake was found equal $0.182 \pm 0.043 \text{ min}^{-1}$ and the retention step was fitted well with pseudo first order equation. The R_d values were found 0.91 and 1.1 $\text{mol.g}^{-1}.\text{min}^{-1/2}$ for PAN immobilized clay in the first (up to 4.0 min of agitation time) and second stages of agitation time, respectively. The thermodynamic parameters (ΔG , ΔH , ΔS) were determined using Vant Hof equation with excellent correlation factor of 0.998 of the linear plot. Thus, retention of Hg ions was exothermic process and spontaneous. The negative value of ΔS provides indication of moderate sorption of $[\text{Hg}(\text{PAN})\text{I}_2]$ complex and ordering of the ionic charges without compensatory disordering of the sorbed species onto the sorbent. Solid phase extractor was successfully packed in column for chromatographic separation of the analyte from the test aqueous iodide solution by the proposed solid phase extractor.



Molecularly Imprinted Polymers Electrochemical Sensors: From Macro to Micro Molecules detection

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ABSTRACT

Molecularly imprinted polymers (MIPs) are synthetic materials with so many applications as recognition elements in many types of electrochemical sensors due to their very unique properties including: high thermal stability, longer shelf stability, reusability besides higher selectivity that is comparable to natural biological receptors. For a chemical sensor to work, two mechanisms are required: recognition and transduction. MIPs play a wonderful role as recognition receptors in combination with a transducer that transforms the concentration of substrate or the product of interaction of the target material in the electrode matrix into electrical signal that is amplified and further processed. Molecularly imprinted polymers (MIPs) can be easily Incorporated either on polymeric membrane or within solid matrix to form the active electrode surface allowing the design of electrochemical sensors with very fixable analytical characteristics. Also, Magnetic Molecularly imprinted polymers (MMIP) can be utilized to improve properties of the sensor by offering a simple and fast elution of the template molecules from MMIPs by simply using an external magnetic field. Many other materials were also combined with MIP to give electrodes of improved analytical performance to fit in different applications, such as nanomaterials such as gold and silver nanoparticles (AuNPs and AgNPs), single-walled and multiwalled carbon nanotubes (SWCNTs and MWCNTs). Also, different types of MIPs were applied including, bulk, surface imprinted, hydrogels. The recent advances in application of MIP as recognition receptors will be discussed in this presentation.



PVC-Based Miptode for The Determination of Pharmaceutical Preparation

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ABSTRACT

molecularly imprinted polymer (MIP)-PVC-based optode, miptode, for the determination of phenylephrine hydrochloride in the physiological fluids as spiked serum and urine was prepared Preparation of MIP and non-imprinted polymers (NIP), using phenylephrine hydrochloride as template. Using of MIP and NIP particles as selective ionophores for the determination of phenylephrine hydrochloride. buffer was prepared and used for preparation of the drug and interfering ions. Using methacrylic acid (monomer), ethylene glycol dimethacrylate (cross linker), benzoyl peroxide (initiator), with or without phenylephrine hydrochloride (template) for preparation of MIP or NIP, respectively. The mechanism of the proposed miptode is the same for the conventional PVC-optodes which responds to simple cations with concomitant deprotonation of the chromoionophore ETH5294 leading to absorbance increase at 650 nm. pH must be controlled at certain value because we used pH-dependent chromoionophores. The optode showed very promising selectivity results over most lipophilic species in comparison to NIP-based optode. The sensor could be applied for the determination of the drug in physiological fluids with reliable recovery values.



Earth-Abundant Nanostructured Materials for Efficient Solar Energy Conversion

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ABSTRACT

If solar energy is to become a practical alternative to fossil fuels, we must have efficient ways to convert photons into electricity, fuel, and heat. To this end, direct solar energy conversion to storable fuels offers a promising route toward less reliance on fossil fuels. The development of a successful solar-fuel-generation technology would require the invention of new photoactive materials that accomplish the combined tasks of light harvesting, charge separation, and compartmentalized chemical transformations. One of the most critical issues is the development of a suitable semiconductor photoanode with high efficiency and long-term durability in aqueous environments. In addition, the lack of effective oxidation and reduction catalysts is among the most serious obstacles preventing the development of an efficient and scalable artificial fuel generator. In this regard, nanoscience can make a difference. This talk will cover the assembly and development of new semiconductor nanoarchitectures as well as interface control for the purpose of solar energy conversion in general and direct solar-to-chemical energy conversion in particular.



Effect of Fly Ash and Superplasticiser on the Hardening Properties of Self Compacting-Concrete

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ABSTRACT

The self-compacting concrete is a relatively innovative type of concrete that differs from the conventional vibrated concrete in that it contains a novel superplasticiser, Fly ash which contributes significantly to increasing the ease and rate of its flow and another advantage is that the novel superplasticiser is very cheap and available compared with the conventional one because it originated from waste material. It was first introduced in late 1980s in Japan when the researcher realized that poor compaction was the major contribution to the decline of quality construction work. Since then various research investigations have been carried out for establishing rational mix design methods in order to be self-compactable. The fresh concrete must show high fluidity beside good cohesiveness to make self-compacting concrete a standard concrete. This research presents the result of an experimental programme that has been carried out, aimed at investigating of fresh properties of SCC contain fly ash and novel superplasticiser. The fresh state properties of the concrete were evaluated. Finally, some hardened state properties of the concrete were assessed. Portland cement was partially replaced with 30%, 50%, 70% and 90% fly ash the water cement ratio was maintained 0.5 for all the mixes. Properties included workability, compressive strength, all were evaluated. The result indicated that the medium volume content of fly ash can be used in SCC to produce good strength concrete with this type of superplasticiser that originated from waste material. High absorption values are obtained with increasing amount of fly ash however almost all the specimen exhibits absorption of less than 5%. The concrete mixes contained 3 different dosage of a novel super plasticiser based on the carboxylic with and without fly ash. the percentage of dosage of superplasticiser is 0.25%, 1%, and 2% respectively. The increase in superplasticiser dosage from 0.25% to 2% the workability increase so the required slump flow meet the criteria of EFNARC also the result of mechanical properties compressive strength for 0.25%, 1% and 2% have shown significant performance compared with the control mixes. The workability test utilised in this research were the slump flow, L-box and j-ring, which can be used to assess the passing ability of self-compacting concrete. based upon the experimental result there are some linear relationship between fresh properties and each of the workability tests achieved.



K-M Reactor, New Technology for Core Shell Materials

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ABSTRACT

In this study, Nano iron-copper core shell was produced by using K-M Micro Mixer. The reaction between nano pure iron with copper sulphate pentahydrate ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$) beside ethylene diamine tetraacetic acid (EDTA) as stabilizer and ascorbic acid in K-M micro mixer reactor gives many advantages in comparison with traditional chemical method for production of nano iron-Copper core shell in batch reactor. Many factors were investigated for its effect on the process performance such as initial concentrations of nano iron, copper sulphate pentahydrate, EDTA and solution flow rate. Different techniques were used for investigation and characterization of the produced nano iron particles such as SEM, XRD, UV-Vis, XPS, TEM and PSD. The produced Nano iron-copper core shell particle using micro mixer showed better characteristics than those produced using batch reactor in different aspects such as homogeneity of the produced particles, particle size distribution and size, as core diameter 10nm particle size were obtained. The results showed that 10 nm core diameter were obtained using Micro mixer as compared to 80 nm core diameter in one fourth the time required by using traditional batch reactor and high thickness of copper shell and good stability.



Green Hybrid Biocomposites: Effect of Modification of Fiber and Polymer on Material Properties

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ABSTRACT

In the present work, borax (BX)- treated oil palm mesocarp fiber (OPMF) and kenaf core fiber (KCF) were hybridized manually and reinforced into maleic anhydride (MA)-modified poly(lactic acid) (PLA) through melt-blending and compression-molding techniques, aiming at a synergistically improved mechanical, physical, morphological, thermogravimetric and dynamic mechanical properties of their resulting hybrid biocomposites. The BX-treated fibers showed considerable increase in cellulose and decrease in hemicellulose, while lignin partially decreased as confirmed by chemical analysis, Fourier transformed infrared spectroscopy, X-ray diffraction analysis, bulk density and scanning electron microscopy. The best material performances were exhibited by the hybrid system i.e. BX(OPMF-KCF)-MAPLA, which involved BX-treated hybrid fiber reinforced MA-modified PLA, consequent of the synergistically enhanced interface adhesion provided by the BX treatment of the fibers and the compatibilization potential of MA-modified PLA. The optimum hybrid system exhibited promising application performances to be employed as an alternative to medium density fiberboard.



Development of Composite Catalyst and its Catalytic Performance in FCC Cracking

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ABSTRACT

This study presents development of composite catalyst and its catalytic performance in fluid catalytic cracking (FCC). FCC composite catalyst was formulated using as-synthesized zeolite Y and ZSM-5 anchored on support matrix made of activated alumina, metakaolin and silica sol. The catalyst was characterized using Brunauer-Emmett-Teller (BET) texture analysis, scanning electron microscopy (SEM) and Differential/thermogravimetric (DTG/TG) analysis. The BET analysis showed that the zeolite Y, ZSM-5 and FCC catalysts formulated were microporous. Incorporation of ZSM-5 reduced the specific surface area and pore volume of the catalyst by 28 and 30% respectively. DTG/TG analysis of both the zeolite Y and ZSM-5 catalysts showed that they were thermally stable. Catalytic cracking of n-hexadecane yielded 40.7%, 59.5% and 60.0% gasoline at 400, 500 and 500°C respectively. The corresponding gasoline selectivity were 76.5%, 81.3% and 67.5% respectively.



Potential Role of L-Arginine and Vitamin E Against Bone Loss

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ABSTRACT

The purpose of this study was to illustrate the effects of zinc oxide Q1 nanoparticles (ZnO-NPs) administration on bone turnover and bone resorbing agents in rats and how L-arginine (L-arg) or vitamin E (vit E) coadministrations might affect them. Fasting rats were randomly divided into four groups (n = 10): G₁—normal healthy animals; G₂—ZnONPs-exposed rats (600 mg/kg⁻¹/day⁻¹); G₃—ZnO-NPs-exposed rats co-administrated L-arg (200 mg/kg⁻¹/day⁻¹); G₄—ZnO-NPs-exposed rats co-administrated vit E (200 mg/kg⁻¹/day⁻¹). The ingredients were Q2 orally administered by guava daily. The body weight and food consumption of rats were recorded during the administration period and the experiment continued for three consecutive weeks. The results demonstrated that ZnO-NPs administration induced bone loss in rats as manifested by reduced activity of bone alkaline phosphatase (B-ALP) and increased level of C-terminal peptide type I collagen (CTx). The increase of inflammatory markers, tumor necrosis factor-alpha (TNF-α) and interleukin-6 (IL-6) by ZnO-NPs suggests that deleterious effects of ZnO-NPs on bone turnover were, in part, due to inflammation. Confirming this suggestion, both L-arg and vit E evidenced from elevated day reduced TNF-α and IL-6 levels and consequently decreased Q3 bone resorption as indicated by reduced serum CTx level. This study proved that ZnO-NPs can induce bone turnover, which may be reduced by L-arg or vit. E co-administration, partly by anti-inflammatory mechanism.



A New Template-Directed Triazole Ligand Strategy for The Synthesis of Silver Nanoparticles

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4.

ABSTRACT

The ability to prepare silver nanoparticles (AgNPs) in a size- and shape-controlled fashion is a vital component for their use in optoelectronic diagnostic and nanomedical devices. Current preparative methods for the synthesis of AgNPs have mainly focused on a select few reactions that require elevated temperatures or strong reducing agents. In this study, a mild one-pot, template-directed process of AgNP synthesis using sugar triazole ligands (1-3, Figure1) and the Tollens' reagent will be presented, with a focus on how the structure of the triazole ligands influences the size, shape and colloidal stability of AgNPs [1]. Furthermore, the synthesis of sugar triazole ligands bearing short ethyleneglycol chains (4-6, Figure 1) will be presented as a new biosensing platform using SERS [2].

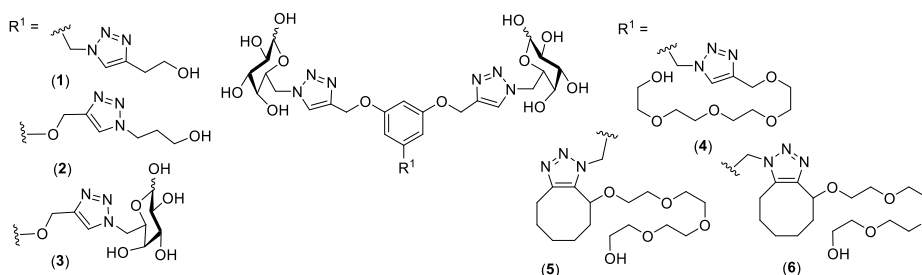


Figure 1: Structures of sugar triazole ligands (1-6) prepared in this study.

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Utilization of Date Stone for The Heterogeneous Catalytic Conversion of Cyclohexane

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ABSTRACT

The kinetics of heterogeneous catalytic conversion of cyclohexane over Cu supported active carbon of date stone catalysts at 280-380 °C and time of contact 13.63-6.52 min were studied in flow system under normal pressure . The solids were prepared by impregnation of active carbon of date stone and Cu acetate solution by different ratio 5,10 and 15% producing CuACSI ,CuACSII and CuACSIII respectively. The prepared solids were characterized by TG A, D TA, X-ray diffraction pattern and BET surface area measurements. The Heterogeneous Catalytic conversion of cyclohexane at temperature ranging from 280-380° C was studied by flow system technique. The liquid and gaseous products were analyzed by gas liquid chromatography. The catalytic activity and selectivity toward benzene formation were investigated.



POSTER SESSIONS



Olea Europaeasubsp.Cuspidate Wood Tar Oil From Saudi Arabia (Albaha district) as Anticorrosion for Metals in Aqueous Media

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ABSTRACT

The most practical methods for protection against corrosion is the use of inhibitors to prevent unexpected metal dissolution and acid consumption. Different organic and inorganic compounds have been studied as inhibitors to protect metals from corrosion attack especially in acidic solutions. The known hazardous effects of most synthetic organic inhibitors and restrictive environmental regulations have now made researchers to focus on the need to develop cheap and environmentally benign natural products as corrosion inhibitors. The efficiency of an aqueous extract of the bark of *Olea europaeasubsp. cuspidata* as corrosion inhibitor for mild steel in 1 M sulphuric acid was carried out using the electrochemical (PDP and ESI) methods. The results showed that the extract of *Olea europaeasubsp. Cuspidate* acts as good inhibitor and the performance of the inhibitor was varied with concentrations. Surface analysis (SEM) was also carried out to establish the corrosion inhibitive property of *Olea europaeasubsp. cuspidata* in 1 M H₂SO₄ solution. It has surprisingly been discovered that *Olea europaea subsp. Cuspidate* extract work as corrosion inhibitor for steel in acidic solutions, e.g. used as anticorrosion for metals in acidic media. This corrosion inhibitor is cheap, safe, friendly and readily available in large quantities.



Physicochemical Studying for Catalytic Conversion of Iso-propanol over Palladium Supported Nano-Particles.

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ABSTRACT

Nano palladium supported catalyst solid samples was prepared by reduction method, using hydrazine hydrate as reducing agent. The physicochemical studies for solid samples were investigated using transimission electron microscope, Textural Characteristics (BET), X-ray powder diffraction, Thermo Gravimetric Analysis (TGA) and Differential Thermal Analysis (DTA). The catalytic activity was studying for conversion of isopropanol at 100-180°C using flow system technique, the liquid products analyzed by gas liquid chromatography. Nano palladium supported solid catalysts investigated behaved as dehydrogenated and dehydration catalyst. The environmental applications were investigated for solid samples using eosin Y, methylene blue and saffranindyes.



Biodegradable Polymers Based on PLA and Organoclay Fillers Containing Gemini Surfactants

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ABSTRACT

In recent years biopolymers, and more particularly polylactic acid, have attracted much interest for industrial application as eco-friendly, biocompatible and biodegradable materials for the substitution of conventional polymers.¹⁻
²PLA shows however some limitations which limit its use on a larger scale as a reduced impact resistance and melt strength and poor thermal properties and barrier performance for small molecules (water and oxygen). Therefore, research efforts were devoted to the improvement of PLA performance, mainly by means of blending with other biopolymers or the use of nanofillers.³

In this work, we present the synthesis and the characterization of novel nanofillers based on organo modified clays with gemini-quaternary ammonium surfactants bearing different spacer and hydrophobic chain lengths. These organoclays were used to prepare PLA-clay nanocomposites by melt processing method. Substantial improvement of their thermal stability, mechanical, rheological and morphological properties was obtained in comparison with pristine PLA.

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Ni-MgAl-Layered Double Hydroxide for Suzuki C-C Coupling

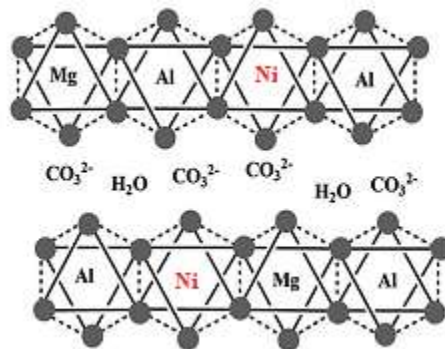
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ABSTRACT

Suzuki cross-coupling reaction has become one of the most effectual approaches for the synthesis of biaryls or substituted aromatic moieties from aryl halides and arylboronic acids with a palladium-catalyst in the past two era's. Compounds comprising biaryl assemblies are significant building blocks for polymers, natural products such as alkaloids, and several agrochemicals and biologically active pharmaceuticals. In the present study, we introduce Pd-free layered double hydroxide containing nickel catalyst as an efficient alternative to the classical Pd-containing catalysts. The classical organic synthesis as well as the Ball-mill techniques were applied to synthesis various biaryls. High yield/selectivity for the desired products was obtained. The sustainability of both catalyst and the catalytic process should encourage forthcoming in C-C coupling reactions.



Scheme 1. Schematic of NiLDH structure.



Corrosion Inhibition of Metals in Acidic Medium by Eco-friendly Extracts Capped with Metallic Oxides Nanocomposite

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ABSTRACT

Corrosion of metals in the presence of water or aqueous solutions is a common problem across many industries. Corrosion costs manifest in the form of premature deterioration or failure necessitating maintenance, repairs and replacement of damaged parts. Recently, there has been metal corrosion is an inevitable and can be controlled and managed. There are direct and indirect expenses due to corrosion control. Every year billions of dollars are used for corrosion control. Therefore, corrosion control is very important to protect the environment and economy. The development of nontoxic (green) effective corrosion inhibitors for metallic substrates is an issue of great importance for protection of metal alloys and components. In modern science Nanotechnology is a ablaze field for the researchers. Semiconductor metal oxides, in particular, have been widely used as photocatalysts for the decomposition of organic pollutants and air contaminants because of their high stabilities, redox capacities, low toxicities, and photophysical properties. The natural product was used as capping agent to produce highly dispersed coated oxide nanoparticles. The greensynthesis was done by using the aqueous solution of plant extract and metaloxide. The nanoparticles were synthesized and characterized by UV-vi's Spectrophotometer, FTIR, DLS, Zeta Analysis, XRD, TEM and SEM analysis to examine the surface properties of the produced oxide nanoparticles. The corrosion inhibition efficiencies of aqueous solutions of natural product (Merrah) capped with zinc oxidenanoparticals for steel in acidic solution have been investigated at different concentrations of the inhibitor using potentiodynamic polarization and electrochemical impedance spectroscopy measurements.

Objective of the study

The study aims at preparing of Zinc oxide (ZnO) nanoparticales and capped the inhibitor with it and to explore the anti-corrosion protection of naturalproduct (Merrah) caped with ZnO nanoparticals for steel in sulphuric acid.



Heavy Metals in Lipstick Products Marketed in Saudi Arabia

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ABSTRACT

This study was undertaken in order to determine heavy metal content in twenty-two ($n = 22$) lipstick products, both imported and locally manufactured, that were marketed at AlbaldSouj, Jeddah, Saudi Arabia. An analytical test was performed for fourteen metals in lipstick products using an Inductivity coupled **plasma** – Optical emission spectrophotometer (ICP-OES). The overall mean ($n = 22$) concentration for each heavy metal was analyzed as follows: Al, Fe, Ti, Ag, As, Ba, Cd, Co, Cr, Cu, Mn, Ni, Pb, and Zn were 3131.18 ± 0.09 , 9642.92 ± 0.079 , 46.59 ± 0.109 , 0.545 ± 0.009 , 2.041 ± 0.024 , 1371.439 ± 0.085 , 0.134 ± 0.008 , 4.242 ± 0.02 , ND, 3.934 ± 0.03 , 19.712 ± 0.012 , 20.196 ± 0.056 , 0.725 ± 0.012 , and $858.666 \pm 0.083 \mu\text{g/g}$, respectively. The correction coefficient of the results is up to 0.9995, showing an excellent linear relationship between metal concentrations in samples and detection by ICP-OES. The results of the study reveal that the total concentrations of toxic metals in various samples ranged from 1201.35 to 60800.36 $\mu\text{g/g}$. The dark-colored lipstick samples 1B, 2B, 3B, 4B, 5B, 7B, B8, 9B, and 10B showed the highest value of total toxic metals compared with the light-colored lipstick samples 1A, 2A, 3A, 4A, 4C, 5A, 7A, 8A, 9A, and 10A. The concentrations of Al, Fe, Ba, and Zn in the samples within each class under investigation were relatively higher, while the concentrations of Ag, As, Cd, Co, Cu, and Pb were the lowest; Ti, Mn, and Ni concentrations were below $100 \mu\text{g/g}$. Chromium was not detected in any sample. Since no safe limits for most of these metals relating to cosmetic products are available in Saudi Arabia, it is hard to ascertain whether the values obtained in this study are relatively high or low. Prolonged use of products containing these elements may pose a threat to human health and could damage the environment.



Photocatalytic Removal of Congo Red Dye Using MCM-48/Ni₂O₃ Composite Synthesized Based on Silica gel Extracted from Rice Husk Ash; Fabrication and Application

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ABSTRACT

MCM-48 mesoporous silica was successfully synthesized from silica gel extracted from rice husk ash and loaded by nickel oxide (Ni₂O₃). The resulted composite was characterized using X-ray diffraction, scanning electron microscope, and UV-vis spectrophotometer. The role of MCM-48 as catalyst support in enhancing the photocatalytic properties of nickel oxide was evaluated through the photocatalytic degradation of Congo red dye under visible light source. MCM-48 as catalyst support for Ni₂O₃ shows considerable enhancement in the adsorption capacity by 17% and 29% higher than the adsorption capacity of MCM-48 and Ni₂O₃, respectively. Additionally, the photocatalytic degradation percentage increased by about 64% relative to the degradation percentage using Ni₂O₃ as a single component. The adsorption mechanism of MCM-48/Ni₂O₃ is chemisorption process of multilayer form. The using of MCM-48 as catalyst support for Ni₂O₃ enhanced the adsorption capacity and the photocatalytic degradation through increasing the surface area and prevents the nickel oxide particles from agglomeration. This was done through fixing nickel oxide particles throughout the porous structure which providing more exposed active adsorption sites and active photocatalyst sites for the incident photons. Based on the obtained results, supporting of nickel oxide particles onto MCM-48 are promising active centers for the degradation of Congo red dye molecules.



Layer-by-Layer Electrochemical Assembly of Propitious FeOx/Pt-Modified Nanocatalysts for Formic Acid Electro-oxidation

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ABSTRACT

The direct formic acid fuel cells (DFAFCs) have recently appeared attractive for providing clean electricity for various stationary and portable power applications[1, 2]. However, before moving into a real commercialization, the DFAFCs should be subjected to a critical improvement for the overall cell performance that is typically deteriorated upon poisoning the anodic catalyst (typically Pt) with CO produced *non-faradaically* during formic acid electro-oxidation (FAO). In this investigation, a novel catalyst composed of Pt nanoparticles (nano-Pt) and iron oxide nanostructures (nano-FeOx) is suggested for efficient FAO. The deposition protocol of the catalyst's ingredients adopted the layer-by-layer electrochemical assembly. The loading level and sequence of the catalyst's ingredients impacted intensively both of the catalytic activity and stability of the as-prepared catalyst toward FAO. Several materials and electrochemical characterization techniques were employed to evaluate the catalyst's morphology, composition and structure in addition to revealing and interpreting its catalytic activity and stability. Interestingly, at this catalyst, CO poisoning that is typically appear at Pt-based catalyst disappeared with a significant enhancement in FAO. We believe the modification of Pt with nano-FeOx could successfully enrich the surface with activated hydroxyl groups to inspire an enhanced removal of CO at low potentials (bi-functionality). The existence of FeOx at the catalyst's surface could also stimulate an enhanced charge transfer during FAO, as the impedance measurements accounted.

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Harvesting Clean Electricity from Liquid Fuel Cells: Advances and Challenges

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ABSTRACT

This study is aimed at the development of efficient and stable nano structured anodes for the electro-oxidation of methanol (MO), formic acid (FAO), and ethylene glycol (EGO) for their respective potential applications in the direct methanol (DMFCs), formic acid (DFAFCs) and ethylene glycol (DEGFCs) fuel cells. The motivation of this work is inspired from the promising future of DMFCs, DFAFCs, and DEGFCs as potential alternatives to the traditional hydrogen fuel cells (HFCs) in harvesting clean electricity for several portable and stationary applications. While HFCs experience troubles with the H₂ use, storage and transportation, the DMFCs represented a reasonable convenience employing a small liquid fuel and offering a high theoretical energy density (4690 WhL⁻¹). On the other hand, the DFAFCs enabled the direct use of liquid fuels without a reformer (a reactor for H₂ production) and offered the potential for enhanced cell performance by lowering the fuel crossover. Owing to the impressive hydrogen content and high boiling point of ethylene glycol, the DEGFCs were also promising, particularly with their high volumetric energy density (5900 WhL⁻¹). However, unfortunately, the catalytic activity of platinum (that typically represents the anodic catalyst in DMFCs, DFAFCs, and DEGFCs) deteriorates rapidly due to the accumulation of different poisoning intermediates. This consumes the active Pt sites, which are supposed to participate in the corresponding anodic reactions; lowering significantly the overall cell efficiency. Before moving into real marketing of DMFCs, DFAFCs, and DEGFCs, their efficiency and durability have to be improved by developing efficient and stable anodes. The current investigation suggests a synthetic methodology to mitigate the poisoning by several modifications for Pt nanoparticles with gold nanoparticles (nano-Au), polyaniline (PANi) and transition metal oxide nanostructures. The modification is targeting the poisoning mitigation and/or improvement of the anodic reaction's kinetics. The catalytic enhancement was analyzed with the assistance of *state-of-the-art* characterization tools and the results were promising to sustain a future prosperity.

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Enhancement of the Photocatalytic Degradation of Organic Pollutants by Graphene Nanoplatelets Doped Zinc Oxide Photocatalyst

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ABSTRACT

Nanocrystalline zinc oxide decorated with different molar ratio graphene nanoplatelets (1, 2, 4 and 8%) photocatalysts were successfully prepared via microwave irradiation technique to enhance the photocatalytic activity of the ZnO in organic pollutants degradation. The prepared photocatalysts were calcined at different calcination temperatures (ca. 300, 400, 500 and 600°C) and characterized using X-ray diffraction analysis (XRD), Surface area measurements (BET) , Fourier transform infra-red spectroscopy (FT-IR) , Diffuse reflectance UV-Vis spectroscopy (DR-UV-Vis), Raman spectroscopy and scanning electron microscopy (SEM). The calcined catalysts were tested for the decolorization of different types of organic dyes. The characterization results confirmed the presence of only pure ZnO phase with particle size ranged between 27 to 36 nm as well as an effective interactions between graphene and zinc oxide. Doping of graphene nanoplatelets led to an increase in a specific surface area, thus increases the number of active sites and subsequently, improve the degradation efficiency as well as the photogenerated electron-hole pair separation rate as shown by the UV-vis diffuse reflectance spectroscopy measurements. The nature of microporosity and/or mesoporosity were due to the needle like structure morphology for the prepared photocatalyst, with band gap ranged between 3.14 and 3.35 eV. Zinc oxide photocatalyst exhibited less decolonization efficiency compared with the graphene doped zinc oxide samples (99% of degradation) in a short reaction time (60-120 min) under both ultraviolet and visible light irradiation. Reusability results showed a negligible loss of activity after reusing 5 times. Effect of the calcination temperatures on the physicochemical and photocatalytic activity of the prepared catalysts has been conducted to explore the new class of photocatalyst materials with potential uses in the remediation of polluted water.



Developing A Novel SZ Photodegradation System Catalyzed by using p-benzoquinones and Picric acid: Application to Charge Transfer Complexes.

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and Ahmed M. Mansour

ABSTRACT

The antibiotic drugs are series of persistent organic pollutants and their effective control has become a research hotspot, specially, the antibiotic drug sulfadiazine (SZ) is one of the challenging problems in the field of environmental chemistry. In this work, the concentration of SZ was determined by a rapid and accurate method and then find a suitable method to degrade the assayed products into harmless chemicals. The color of the charge transfer (CT) complexes developed from the reaction of SZ with 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), chloranilic acid (CHL) and picric acid (PA) was used to determine the concentration of SZ at 528, 510 and 410 nm, respectively. The Lambert-Beer & #039;s law is obeyed in the ranges of 6.80–68.06, 13.61–136.12 and 6.80–27.22 mg mL⁻¹ for DDQ, CHL and PA complexes. The addition of sodium nitrite into SA/DDQ photodegradation system remarkably enhanced the degradation Efficiency of SZ to 80.0% within 45 min compared with the control experiments. The degradation efficiency of SA in of SZ / DDQ system followed first-order kinetics, with rate constant values ranging from 0.0055 min⁻¹ to 0.0103 min⁻¹ depending on the operating parameters, such as the amount of energy and catalysts(oxalic acid, sodium nitrite , and hematite nano particles). This was simply spectrophotometrically followed by a decrease in the intensity of the CT band. The effect of some additives such as oxalic acid, and hematite nano particles was studied. For comparison, other p-acceptor reagents such as CHL and PA were used. About 80% of SZ is degraded in 45 min upon the illumination of SZ / DDQ at 256 nm, whereas 90 min is required in the case of CHL and PA to attain the same degradation limit.



Solution Equilibria of Binary and Ternary Complexes Involving Zinc(II) with 2,6-Diaminopyridine and Various Biologically Relevant Ligands

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ABSTRACT

The complexing properties of 2,6-diaminopyridine (DAP) with zinc(II) were investigated pH-metrically at 25°C and at ionic strength of 0.1 mol_{dm}⁻³ (NaNO₃). Binary and ternary complexes of Zn(II) involving DAP and various biologically relevant ligands containing different functional groups are investigated. The ligands used (L) are amino acids, dicarboxylic acids, amides and DNA unit constituents. The ternary complexes are formed by simultaneous reactions. The results showed the formation of Zn(DAP)(L) complexes with amino acids and dicarboxylic acids. Amides form both Zn(DAP)(L) complexes and the corresponding deprotonated amide species Zn(DAP)(LH-1). The concentration distributions of the various complex species formed in solution were also evaluated as a function of pH. The effect of dioxane as a solvent on the protonation constant of DAP and the formation constants of Zn(II)–DAP complexes were discussed. The effect of ionic strength on the protonation constants of DAP is also evaluated.



Understanding the Photochemical Mechanism and Polar Reaction of Bisphenol A: DFT Study

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ABSTRACT

Bisphenol-A (BPA) is particularly considered as one of the most suspicious disruptors. Exposure to BPA may bring about possible human toxicities, such as cancerous tumor, birth defects and neoteny. Furthermore, BPA is an emerging contaminant widely used in manufacturing of epoxy, unsaturated polyester-styrene, polycarbonate resins, and flame retardants. BPA is released into the environment through industrial and municipal wastewater discharges; its degradation products are probably more dangerous than BPA itself. Motivated by these finding and the fact that there is no systematic study of the electronic structure, bonding characteristics and degradation pathways for BPA, we propose the present research project to investigate the ground state electronic structure of BPA, our efforts to investigate and compare the acid-base properties of BPA will be detailed. Thus, the optimized geometries and the energies of various forms of BPA are computed at a high level of theory. Proton affinities and deprotonation enthalpies are computed and discussed. To gain much deeper insight into the protonation processes, DFT-based molecular dynamics simulation will be carried out and energy profiles will be analyzed and discussed. Bonding characteristics are investigated within the natural bond-orbital (NBO) and quantum theory of atom in molecule (QTAIM) frameworks. Furthermore, BPA degradation products were identified and density functional theory simulations were used to determine the most probable reaction pathways.



Soft X-ray Spectroscopy of $[\text{Co}(\text{H}_2\text{O})_6]$: a Theoretical Perspective

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ABSTRACT

X-ray spectroscopy is one of the most powerful tools to access structure and properties of matter in different states of aggregation. X-ray spectroscopic techniques probe the local electronic structure of a particular atom in its environment.^{1,2} This is in contrast to UV/vis spectroscopy, where transitions generally occur between delocalized molecular orbitals. The combination of different absorption, emission (scattering) as well as photo- and autoionization X-ray methods allows addressing various aspects of ultrafast dynamics and identification of short-lived intermediates of catalytic reactions.¹ However, interpretation of complex experimental spectra and verification of experimental hypotheses is a non-trivial task and a powerful first principles theoretical approach that allows for a systematic investigation of a broad class of compounds is needed.^{1,3} An additional complexity stems from strong electron correlation and spin-orbit coupling in the core-excited electronic states. X-ray absorption (XAS) and resonant inelastic scattering (RIXS) of $[\text{Co}(\text{H}_2\text{O})_6]$ complex with special care to the effect of basis set studied theoretically using the RASSCF/RASSI approach. This enables us to quantify the L-edge excitations of electrons from the 2p core to unoccupied MOs which containing information on the nature of metal-ligand interaction. For comparing purpose, the spectra were calculated with the relativistic atomic natural orbitals basis sets (ANO-RCC-VDZ, ANO-RCC-VTZ, ANO-RCC-VQZ). Specific findings deduced from the analysis of the shape of the L-edge excitations and RIXS spectra concern the efficiency of the theoretical methodology under investigation. The notably different patterns of spectroscopic features in basis set develops an efficient and versatile theoretical methodology for the treatment of soft X-ray spectra of $[\text{Co}(\text{H}_2\text{O})_6]$ complex based on the multiconfigurational self-consistent field electronic structure theory combined with a perturbative LS-coupling scheme for spin-orbit coupling.

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Experimental and Theoretical Study of Donor- π -Acceptor Compounds Based on Malononitrile

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ABSTRACT

A set of different donor- π -acceptor compounds having dicyanovinyl as the acceptor and aryl moieties as donors were synthesized by Knoevenagel condensation. The UV-visible absorption and fluorescence spectra were investigated in different solvents. The optical band gap energy (E_g) was linearly correlated with the Hammett resonance effect of the donor to reveal that the higher the value of Hammett resonance effect of a donor, the lower the E_g of the molecule. The photophysical data revealed that compounds 4-6 are typical molecular rotors with fluorescence due to twisted intramolecular charge transfer (TICT). Compound 5 revealed the largest Stokes shift (11089 cm^{-1}) making it a useful fluorescent sensor for the changes of microenvironment. The effect of substituents on the optical properties donor- π -acceptor compounds having dicyanovinyl are studied using density functional theory and time-dependent density functional theory (DFT/TD-DFT). The optical transitions are thoroughly examined. Geometrical structures, molecular orbitals, absorption and emission spectra of these dicyanovinyl compounds have been discussed. We have found that substitution of the dicyanovinyl skeleton affects both the absorption and emission spectrum, mainly through the modification of the structure of the excited. The theoretical results have shown that TD-DFT calculations, with a hybrid exchange-correlation and the long-range corrected density functional PBEPBE with a 6-311++G** basis set, was reasonably capable of predicting the excitation energies, the absorption and the emission spectra of these molecules.



Synthesis, Characterization and Biological Activity of Cu(II) and Ni(II) with Novel Hydrazones

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ABSTRACT

Novel hydrazone 2-(2-((1*E*,2*E*)-2-(2-phenylhydrazineylidene)propylidene)hydrazineyl)pyridine and its Nickel(II) and copper(II) complexes have been synthesized and characterized. The ligand (H₂PGL) was prepared by the condensation reaction of 1-(2-phenylhydrazineylidene)propan-2-one and 2-hydrazinopyridine. The crystal structure of Ni(II) complex was determined. In both Ni(II) and Cu(II) complexes, H₂PGL act as a neutral tridentate ligand forming two fused five-membered chelation rings through NNN set of donor atoms. Octahedral geometry is proposed for both complexes based on magnetic, spectroscopic studies. ESR spectroscopy was performed for Cu(II) complex which exhibited a considerable Cu–Cu interaction and harmonize directly with measured magnetic moment. The molecular modeling structures were optimized and showed the bond length, bond angle, chemical reactivity, MEP, Mulliken atomic charges, and binding energy (kcal/mol) for all the title compounds. Theoretical infrared intensities and ¹H NMR of H₂PGL was calculated using DFT method. A comparison of the experimental and theoretical spectra can be very useful in making correct assignments and understanding the basic chemical shift. Biological activity of the synthesized compounds was investigated versus some Gram positive, Gram negative bacteria and some fungal strains. Also, the antitumor activity was investigated.



Designing Schiff Base Ligands for Photophysically-Active Cyclometallated Iridium (III) and Platinum (II) Complexes

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ABSTRACT

Non linear optical (NLO) active and luminescent organometallic chromophores are of considerable interest as photofunctional materials. When compared to organic chromophores, they possess more design flexibility due in part to the possibility of varying the metal, oxidation state and co-ligands. Among the variant organometallic classes, cyclometallated complexes of platinum (II) and iridium (III) have been under special attention. The early reports of Watts and Gudel highlighted iridium (III) cyclometalated complexes with fascinating conversion of electric energy to photons with internal quantum efficiencies around 100%. The employment of such findings in designing light emitting diodes (LEDs) devices allowed the most optimal electroluminescence to be achieved. Such studies motivated extensive efforts in developing variant iridium (III) complexes, establishing the structure-property relationships to improve the phosphorescence efficiencies further and to cover emissions with variant light domains [Figure 1]. The thermal and chemical stabilities of this class of organometallic complexes along with ability to reuse several times. These properties are useful for fulfilling the efficient conversion of the long-lived triplet excited state energy into many applications such as photosensitizers in photocatalyzed water splitting and in photovoltaic cells. Interesting outcomes have been observed for platinum (II) cyclometalated complexes of general formula $Pt(C^{\wedge}N)(dione)$ [Figure 1].

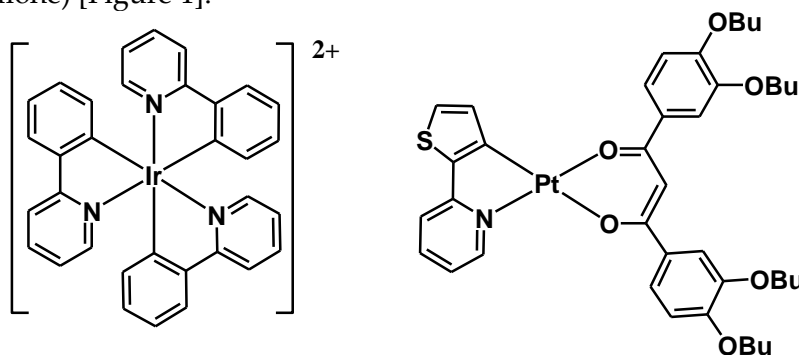


Figure 1. Examples of cyclometalated complexes with interesting photophysical properties



The Agriculture Waste Productive Use of Palm Tree Fiber as Adsorbent for Methylene Blue Dye from Wastewater

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ABSTRACT

Palm Tree Fiber (PTF) residue of date farms and industry was successfully used as bio-sorbent for Methylene blue (MB) dye from contaminated water. The chemical composition and surface morphology of the bio sorbent was critically studies using ICP-OES, FT-IR, RDX, and FESEM. In batch separation mode, the effect of various analytical parameters (adsorbent dose, ion strength, contact time, pH, and temperature) on MB uptake by the used bio sorbent was studied. The kinetic data were also subjected to pseudo-first order, pseudo- second order, and intra-particle diffusion mathematical models. The pseudo-second order was more predominant for MB uptake. The adsorption equilibrium data of MB retention were subjected to Langmuir and Freundlich to assign the most probable retention mechanism. Langmuir and Freundlich isotherm models indicated an adsorption in mono- and multi-layers. The application study showed that 99% of MB was removed from the environmental water samples and a good removal percentage on the 2-time recycling was achieved. PTF has a potential to uptake MB from waste water.



Determination the Accumulation of Heavy Metals in the Soil, Water and Plants in Farm from Jeddah City

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ABSTRACT

Heavy metals are found in nature and their measurement in environment is necessary to develop health management strategies. This work investigates the concentration of heavy metals (chromium, copper, nickel, lead, iron, and zinc) in the soil, irrigation water, and edible vegetables on a selected farm nearby the city of Jeddah, Saudi Arabia from May to October 2016. Samples were taken from soil and water, totally 11, and 4 vegetable samples were collected which is coriander (*Coriandrum sativum*), dill (*Anethum graveolens*), parsley (*Petroselinum crispum*) and arugula (*Eruca sativa*). The acid digestion was applied for digesting the samples and the concentrations of heavy metals were determined by inductively coupled plasma optical emission spectrometry (ICP-OM). The spatial surfaces of heavy metals were created using geospatial information system. The order of heavy metals in soil were $Fe > Cr > Zn > Pb > Ni > Cu$, while in water were $Pb > Fe > Cu > Zn > Ni = Cr$. Moreover, the order of heavy metals in vegetables was $Fe > Zn > Cu > Cr > Ni > Pb$. The concentrations of Fe mg/kg, Cr mg/kg and Pb mg/kg in the soil were more than the maximum allowable limits of the Food and Agriculture Organization (FAO) and the World Health Organization (WHO). In summary, the concentrations of heavy metals in water and vegetables samples were below FAO and the WHO standards, however, the soil was still contaminated by Fe, Cr and Pb.



Kinetics, Isotherm and Thermodynamic Characteristics of Chromium(VI) Sorption from Water using Non Modified Coffee Husk

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ABSTRACT

A fast and selective method has been developed for chromium (VI) removal from water by untreated coffee husk (CH) sorbent as a solid phase extractor (SPE). The method was based upon formation of halochromate (CrOCl_2^-) in the test 3 aqueous HCl solution and subsequent extraction by untreated sorbent. The sorption of (CrOCl_2^-) ions by the used 3 aq biosorbent was subjected to kinetics and sorption models. The (CrOCl_2^-) retention followed second order rate equation 3 aq with an overall rate constant of $0.132 \pm 0.033 \text{ min}^{-1}$. The values of ΔH and ΔS were $-11.54 \pm 0.9 \text{ Jmol}^{-1}$ and $-66.58 \pm 3.1 \text{ Jmol}^{-1} \text{ K}^{-1}$, respectively. The thermodynamic parameters (ΔH , ΔS and ΔG) suggest that the sorption was spontaneous and exothermic process. The negative value of ΔS provides indication of moderate sorption of (CrOCl_2^-) complex ion 3 aq associate and ordering of the ionic charges without compensatory disordering of the sorbed species onto the sorbent. Sorption of (CrOCl_2^-) is mainly dominated by 3 aq absorption related to "solvent extraction" and an added component for "surface adsorption".



K-M Reactor, New Technology for Core shell Materials

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ABSTRACT

In this study, Nano iron-copper core shell was produced by using K-M Micro Mixer. The reaction between nano pure iron with copper sulphate pentahydrate ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$) beside ethylene diamine tetraacetic acid (EDTA) as stabilizer and ascorbic acid in K-M micro mixer reactor gives many advantages in comparison with traditional chemical method for production of nano iron-Copper core shell in batch reactor. Many factors were investigated for its effect on the process performance such as initial concentrations of nano iron, copper sulphate pentahydrate, EDTA and solution flow rate. Different techniques were used for investigation and characterization of the produced nano iron particles such as SEM, XRD, UV-Vis, XPS, TEM and PSD. The produced Nano iron-copper core shell particle using micro mixer showed better characteristics than those produced using batch reactor in different aspects such as homogeneity of the produced particles, particle size distribution and size, as core diameter 10nm particle size were obtained. The results showed that 10 nm core diameter were obtained using Micro mixer as compared to 80 nm core diameter in one fourth the time required by using traditional batch reactor and high thickness of copper shell and good stability.



Mesoporous Nano-sized Copper Oxide Ex-hydrotalcite Catalysts for Henry Reaction

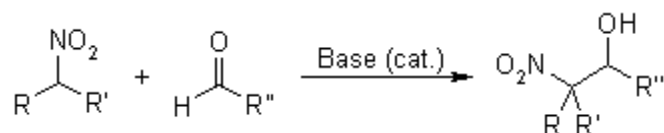
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ABSTRACT

Great progress has been made in mesoporous solid bases in the last decade [1]. They are extremely desirable in green catalytic processes, due to their advantages including accelerated mass transport, negligible corrosion, and easy separation. In addition to their wide applications in the catalytic synthesis of organics and fine chemicals, mesoporous solid bases have also been used in the field of energy and environmental catalysis [2]. Nano-sized metal oxides behave efficiently as they have unique features in their specific surface area, electric conductivity, and thermal stability. The utilization of such solid base mesoporous nano-sized catalysts is one of the alternative pathways to the classical environmentally unfavorable homogeneous catalysts. The current proposal deals with the classical Henry nitro aldol condensation utilizing solid mesoporous nano-sized copper oxide form copper-hydrotalcite-like material synthesized post-treated under hydrothermal autogenous pressure. We introduce here a simple, facile and one-pot synthesis for Henry nitro aldol condensation than usual time-consuming synthesis routes.



Scheme 1.

References

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TD-DFT Calculations, Electronic Structure, Biological Activity, NBO , NLO Analysis and Electronic Absorption Spectra of Some Novel 3-formyl Chromone Derivatives

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ABSTRACT

The electronic structure and spectra of 3-formyl Chromone and some of its derivatives are investigated using TD-DFT/B3LYB/6-311G (d, p) level of theory. The results of calculations show that all the studied compounds **1-6** are planar, as indicated from the dihedral angles. The electronic absorption spectra of the studied compounds are recorded in the UV-VIS region, in both ethanol (as polar solvent) and dioxane (as non-polar solvent). The observed vertical electronic transitions assignments are facilitated via time-dependent density functional theory TD-DFT. Solvent dependence of the band maxima (λ_{max}) and intensities of the observed spectra are explained in terms of blue and red shifts. Electronic configurations contributing to each excited state are identified and the relevant MOs are characterized. The theoretical spectra computed at CAM-B3LYP/6-311G (d, p) in gas phase, ethanol and dioxane nicely reproduce the observed spectra. The natural bond orbital (NBO) analysis were discussed in terms of the extent of delocalization, intermolecular charge transfer and second order perturbation interactions between donor and acceptor MOs. The calculated E_{HOMO} and E_{LUMO} energies of the studied compounds can be used to explain the extent of charge transfer in the molecule and to calculate the global properties; the chemical hardness (η), global softness (S), electrophilicity (ω), and electronegativity (χ). The effect of substituent's of different strengths on the geometry, energetic and nonlinear optical properties are analyzed and discussed. The choice of these substituent's in the studied compounds aims at creating a push-pull system on the 3-formyl Chromone basic structure which pave the way to understand their nonlinear optical properties. The calculated nonlinear optical parameters (NLO); polarizability (α), anisotropy of the polarizability ($\Delta\alpha$) and first order hyperpolarizability (β) of the studied compounds have been calculated at the same level of theory and compared with the prototype Para-Nitro-Aniline (PNA), show promising optical properties. 3D-plots of the molecular electrostatic potential (MEP) for some of the studied compounds are investigated and analyzed showing the distribution of electronic density of orbital's describing the electrophilic and nucleophilic sites of the selected molecules. The biological activity of the studied compounds was tested against gram positive, gram negative and Fungi. A correlation between energetic, global properties and biological activity were investigated and discussed. **Key words:** UV spectra; TD-DFT; solvent and substituent effects; NBO and NLO analysis; biological activity ; 3-formyl Chromone derivatives



Development of Metal Oxide Nanoparticle-based Catalysts for Efficient Biodiesel Production

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ABSTRACT

Biodiesel is an important alternative fuel in energy production to meet the growing needs for energy in developing and developed countries. Biodiesel is an environmentally friendly fuel that can be used directly in diesel engine, offering high efficiency. Esterification and Transesterification are by far the most frequently used methods for the transformation of Fatty acids or triglycerides feed stocks to biodiesel. The rate of esterification (transesterification) reaction is accelerated using a catalytic material (e.g. NaOH and H₂SO₄). The use of heterogeneous catalysts is proposed instead of the use homogeneous catalysts to overcome the drawbacks of the latter in terms of separation and soap formation which hinder the overall process. In this study, the use of mixed metal oxide nanoparticles as heterogeneous catalysts for the transesterification (esterification) of oil (Fatty acid) into biodiesel is proposed. The effects of various experimental parameters; including methanol: oil (Fatty acid) molar ratio, catalyst loading level, reaction temperature and time of the reaction on the biodiesel yield are investigated.



Analytical Studies and Biocontrol of Ochratoxin A Contamination *in-vitro* and in Stored Wheat

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ABSTRACT

The health risk associated with the presence of Ochratoxin A (OTA) in cereals requires selective and sensitive techniques for determination. In this study a comparison of two validated methods for determination of OTA in wheat samples was conducted using Immunoaffinity (IAC) and C18 cleanup columns followed by HPLC-FLD. The method performance resulted in recoveries (89-97% and 80-91%) and limit of detection (0.12-0.5 µg/kg), respectively. The study has concluded the efficiency and selectivity of IAC for OTA determination in wheat samples. Five organisms were examined for activities against OTA producing *Aspergillus Steynii*. *Trichoderma harzianum*, *Trichoderma viride* and *Bacillus mycodis* had no antifungal effect on the studied *A. steynii*, whereas, there were significant reductions in colony area (>30%) using *B. subtilis* and *P. aeruginosa*. The metabolites of both strains were extracted with different solvents. Chloroform extract showed in vitro inhibition for the fungal growth at 1000 ppm recording 42.5 and 55.7% inhibition using *B. subtilis* and *P. aeruginosa* respectively. Interestingly, the inhibition effect was obviously clear on OTA production (75 and 94%, respectively). Higher concentrations of both extracts (500, 1000, 2000 and 5000 ppm) were tested against fungal activity and OTA production in stored wheat. The inhibition effect of 30-46% by *B. subtilis* was noticeable at 1000, 2000 and 5000 ppm. It is also detected that the OTA production was decreased by 36% and 50% at 500 and 5000 ppm respectively upon using *P. aeruginosa*, where the concentration of 1000 and 2000 ppm had no effect on its production. In conclusion, OTA production was easily controlled in vitro in contrast with the case of stored wheat that required higher concentration of bacterial extracts.



Analytical Methods for Determination of Quality and Direct Adulteration of Honey.

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ABSTRACT

Honey is a sweet, viscous food substance that produced naturally. Direct adulteration and quality of honey can be detected by analysis of sugar contents; especially its sucrose level. As a result of improper storage, Hydroxy methyl furfural (HMF) is formed due to break-down of fructose. HMF is reported as potential carcinogen to human. During this study, a method was developed and validated based on Ion Chromatography coupled with Pulsed Amperometric Detection (IC-PAD) to determine glucose, fructose, sucrose and maltose in honey samples. The average recoveries from several different levels varied between 75 % and 120 %. The method showed good linearity of 1-250 µg/ml range. The limits of quantization (LOQ) were 5% for glucose and fructose and 0.5 % for sucrose and maltose. The limits of detection (LOD) were less than 3 % for glucose and sucrose and less than 0.2 % for sucrose and maltose. The measurement uncertainty in terms of expanded uncertainty that expressed as relative standard deviation is in the range of $\pm 27\%$ (at 95 % confidence level, and coverage factor $k = 2$). For determination of HMF in honey, this study proposed a validated method based on HPLC coupled with diode array detector (HPLC-DAD) as a detection technique. The average recovery of HMF in honey sample from several different levels varied between 73 % and 102 %. The limit of quantization was 5 mg/Kg, while the method showed good linearity over the studied range of 0.1-10 mg/Kg. The measurement uncertainty is in the range of $\pm 29\%$. These validated methods were applied to monitor the quality and adulteration levels of local honey samples.



New Sensors for Determination of Aluminum in Real Samples using Aluminium- Dicloxacillin Ion-Associate

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ABSTRACT

Three new poly vinyl chloride (PVC), modified carbon paste (MCP), and coated graphite (CG) based electrodes using aluminum dicloxacillin $\text{Al}(\text{DX})_3$ ion-associates were constructed and utilized as $\text{Al}(\text{III})$ sensors. The developed sensors showed good sensitivities towards $\text{Al}(\text{III})$ with slopes 20.0, 19.3 and 16.7 mV/concentration decade and detection limits 1.99×10^{-6} , 3.16×10^{-7} and 4.04×10^{-4} mol L^{-1} for MCP, PVC and CG based $\text{Al}(\text{III})$ sensors. The electrodes exhibit fast response time reaching 10, 20 and 15 seconds for MCP, PVC, and CG based $\text{Al}(\text{III})$ sensors. The developed sensors are pH independent in the range 4.5-6.5, 3.9-7.5 and 2.6-4.5 for MCP, PVC and CG based electrodes. The electrodes were successfully applied for determination of $\text{Al}(\text{III})$ in real samples and as indicator in the potentiometric titration of $\text{Al}(\text{III})$ with disodium hydrogen phosphate.



Chromatographic Separation of Some Inorganic Pollutants from Aqueous Media using Nano sized Solid Phase Extractor

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ABSTRACT

Concern for human health and animals. Thus, the overall goals of the present study were Focused on: Studying the retention profile, kinetics, thermodynamic and sorption isotherms of a i- Series of chromium ions from aqueous media by Polyurethane foams (PUFs) Chemically impregnated with Nano sized copper oxide as a low cost and effective Solid adsorbent for chromium ions in aqueous solutions ii- Developing of an excellent ion spectrophotometric method for precise Determination of trace and ultra-trace concentrations of chromium ions from water Using Nano sized copper oxide treated flexible PUFs sorbent packed column. Iii -Developing a simple, selective and low cost extractive spectrophotometric method For determination of trace concentrations of tungsten (VI) in water by using liquid-Liquid extraction process.



Electrochemical Oxidation of Alomotriptan Maleate, Sumatriptan Succinate and Zolmitriptan in Bulk and Pharmaceutical Dosage Forms at Pencil graphite Electrode and Carbon Past Electrode

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ABSTRACT

A sensitive electrochemical procedure based on oxidation of Alomotriptanmaleate (alomo), Sumatriptan succinate (suma) and Zolmitriptan (zolmi) at two different electrode ; carbon paste (CPE) and pencil graphite (PGE). Inbritton-robinson (BR) buffer solutions using cyclic, differential pulse and square wave voltammetric techniques. The oxidation process was shown to be irreversible over the pH range (2.0-9.0) and was diffusion controlled. The analytical method was developed for determination of the cited drugs in BR buffer solution at pH 5 as supporting electrolyte. Linear calibration plots were obtained over the concentration ranges of (0.94-12) $\mu\text{g mL}^{-1}$ for alomo, (0.83-12.4) $\mu\text{g mL}^{-1}$ for suma and (0.958-9.85) $\mu\text{g mL}^{-1}$ for zolmi at CPE and (0.94-16.6) $\mu\text{g mL}^{-1}$ for alomo, (1.37-19.3) $\mu\text{g mL}^{-1}$ for suma and (0.-958.19) $\mu\text{g mL}^{-1}$ for zolmi at PGE. The limits of detection (LOD) were found to be 0.48 for alomo, 1.55 for suma and 0.52 for zolmi and limits of quantification (LOQ) were found to be 1.49 for alomo, 1.55 for suma and 0.85 for zolmi at CPE .while AT PGE The limits of detection (LOD) were found to be 0.3 for alomo, 1.34 for suma and 4 for zolmi and limits of quantification (LOQ) were found to be 0.92 for alomo, 4 for suma and 6.16 for zolmi .Validation parameter such as sensitivity, accuracy, precision and recovery were evaluated The method was applied for the determination of the cited drugs both in raw materials and in pharmaceutical dosage forms .the results were compared with those obtained by the reported methods showing higher sensitivity of our proposed method.



A Theoretical Study on Adsorption of Some Toxic Heavy Metals on graphene and graphene Quantum Dots

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ABSTRACT

The adsorption of three heavy metals (HMs) (Pb, Cd, Cr) and their cations (Pb²⁺, Cd²⁺, Cr⁶⁺) on graphene surface has been studied by applying first principles density functional theory (DFT). The interaction of these HM atoms on periodic graphene supercells and graphene quantum dots (GQDs) was investigated using the B3LYP functional in combination with different basis sets. All calculations were performed using CRYSTAL14 and GAUSSIAN09 software packages. Different adsorption sites were studied: B-site (bridge), H-site (Hollow) and T-site (Top). The B-site was found to be more energetically favorable adsorption site for Pb, while that for Cd and Cr was the H-site. However, the more favorable adsorption sites were altered for Pb²⁺ and Cd²⁺ cations: from B to H-site for Pb²⁺, and from H to B-site for Cd²⁺. We also found that the adsorption energies for the studied HM cations are relatively large as compared to those for the corresponding HM atoms. Moreover, the energy barriers between different sites are quite small (< 50 meV). This implies that the adatoms are susceptible to diffuse along the surface. Based on our findings, graphene can be used as a good adsorbent for toxic HMs, and hence it can be employed in wide applications like water treatment.



Electrocatalytic Urea Oxidation on Nickel Oxide Nanoparticles Modified glassy Carbon Electrode

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ABSTRACT

Electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) are used here to investigate the electrochemical characteristics of the urea oxidation on nickel oxide (NiO_x) nanoparticles modified glassy carbon (GC) electrode from alkaline 0.5 M NaOH solution. The effects of NiO_x loading and urea concentration on urea electrocatalytic oxidation are discussed in the light of the EIS data. The Nyquist plots show semicircles with fitting parameters that are dependent on the applied conditions. Lower charge transfer resistance is found in presence of urea due to higher rates of urea electrooxidation. CV helps to investigate the catalytic properties of urea oxidation on the GC/NiO_x. The results indicate a diffusion-controlled irreversible process. Optimization of the loading extent of NiO_x and interpretation of the effect of urea concentration is enabled from the CVs, EIS and equivalent circuit parameters.



A New Rapid and Economic Liquid Chromatographic Method for Simultaneous Determination of Meglitinides with Metformin :Application in the Presence of Metformin and Repaglinide Impurities and Related Compounds

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ABSTRACT

A new liquid chromatographic method was developed for simultaneous determination of the widely used oral antidiabetic, metformin hydrochloride with antidiabetics comprising the meglitinides class in bulk, laboratory- prepared mixtures and pharmaceutical products. It was applied in the presence of metformin-reported impurity (1-cyanoguanidine). It was also applied for the determination of repaglinide in the presence of its related compounds. Chromatographic separation was achieved with isocratic elution mode using a mobile phase of acetonitrile: 0.01 M sodium dihydrogen phosphate (pH: 2.8) (67:33; v/v) flowing through a Li Chrospher NH₂ (amino) Agilent® column (250 × 4.6 mm—5 µm) at a rate of 0.8 mL/min at ambient temperature in a run time of 4 min. UVdetection was carried out at 220 nm. The method was validated according to International Conference on Harmonization guidelines. Linearity, accuracy and precision were satisfactory over concentration ranges (µg/mL): 3.5–350 for metformin hydrochloride, 14–140 for nateglinide, 1–100 for mitiglinide calcium and 0.1–100 for repaglinide. Coefficients of determination were >0.99 for all analytes. Limits of quantification were found (in µg/mL): 0.06, 0.08, 0.198 and 0.029 for metformin hydrochloride nateglinide, mitiglinide calcium and repaglinide, respectively. The present method was found to be rapid, selective, economic and simple in operation satisfying the chromatographers' needs for quality assessment of pharmaceutical products.



Cytotoxicity, Molecular Modeling, Cell Cycle Arrest, and Apoptotic Induction Induced by Novel Chalcones Derivatives

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ABSTRACT

Novel Chalcones derivatives were synthesized and their structures were confirmed by different spectral tools. Cytotoxicity test revealed that all compounds exhibited strong to moderate effect against different cancer cell lines (MCF7, A549, HCT116, and Hepg2). Breast carcinoma revealed higher sensitivity toward all derivatives especially compounds 5 and 8 which offered the lowest IC₅₀ values (50.05, and 27.15 µg/ml) respectively, relative to the positive control 5-flourouralic (5-FU) (IC₅₀ = 178 µg/ml). In addition, the two compounds exhibited less toxic effect toward normal melanocytes (HFB4). Several theoretical and experimental studies were done to reveal the molecular mechanisms that control breast carcinoma metastasis using the two promising novels 5 and 8. Docking simulation studies against the two proteins EGFR and DHFR demonstrate that compound 8 showed higher binding affinity toward the two proteins more than compound 5, suggesting that trimethoxy groups may be responsible for this higher activity through the formation of five hydrogen bonding with the active domain (4r3r) and other four interactions with the active domain (1dls). Real time PCR assay illustrates that the two compounds up regulated BAX, p53, caspase-3 genes and down regulated BCL2, MMP1, CDK4 ones. In addition, it was noted that compound 8 was more effective in gene regulation and apoptotic induction than compound 5. Also, flow cytometer analysis demonstrates that both compounds 5 and 8 induced cell growth arrest at G1 phase and thus inhibit G1/S transition and cell cycle progression. In addition, both compounds stimulate apoptotic death of breast cells significantly to reach 8.72%, and 17.28% respectively, compared to their control (0.55%). Apoptotic induction of breast cells was enhanced effectively through activation of caspase-3 by compound 8 using Elisa assay.



An Efficient Stereoselective Synthesis of a Sulfur-bridged Analogue of Bosse Opentaenoic Acid as a Potential Antioxidant Agent

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ABSTRACT

An efficient approach to the stereoselective synthesis of a novel sulfur-bridged analogue of bosseopentaenoic acid (BPA) by employing the Z-selective modified Boland semi-reduction procedure as the key step is described. The free radical scavenging potential of the thiophene analogue of bosseopentaenoic acid is studied. The results showed that the thiophene ring led to increased antioxidant activity.



Spectral Characteristics, Laser Parameters and Excitation Energy Transfer of 1,4-Bis[β -(2-naphthothiazolyl)vinyl]benzene. A New Candidate Laser Dye

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ABSTRACT

The optical parameters like electronic absorption spectra of $S_0 \rightarrow S_1$, extinction coefficient (ϵ), transition dipole moment (μ_{12}), oscillator strength (f), excited state lifetime (τ_f), emission spectra and fluorescence quantum yield (ϕ_f) for 1,4-Bis[β -(2-naphthothiazolyl)vinyl]benzene (BNTVB) were detected in different organic solvents. The electronic absorption is less sensitive to polarity of the medium. A red shift was noticed in fluorescence spectra (ca. 40 nm) when the solvent polarity increases, indicating that the polarity of BNTVB increases upon excitation. The change in dipole moment value ($\Delta\mu$) was calculated using the variation of Stokes shift with solvent polarizability (Δf) (Lippert – Mataga plot) and from the plot of normalized transition energy E_T^N versus the Stokes shift. The dipole moment of ground state (μ_g) and the excited singlet state dipole moment (μ_e) are determined from Bakshiev and Kawski – Chamma – Viallet equations using the variation of Stokes shift with solvent polarity function of ϵ (dielectric constant) and n (refractive index) of the solvent. The result was found to be 0.019D and 5.13D for ground and excited state, respectively. DFT/TD-DFT methods were used to study the geometric and electronic structures of BNTVB in different solvents. A good agreement was found between the experimental and theoretical results. The photochemical quantum yield (Φ_c) of BNTVB was calculated in different organic solvents such as Dioxane, CHCl_3 , EtOH and MeOH at room temperature. The values of ϕ_c were calculated as 2.3×10^{-4} , 3.3×10^{-3} , 9.7×10^{-5} and 6.2×10^{-5} in Dioxane, CHCl_3 , EtOH and MeOH, respectively. The dye solutions ($2 \times 10^{-4}\text{M}$) in DMF, MeOH and EtOH give laser emission in the blue - green region upon excitation by a 337.1 nm nitrogen pulse. The tuning range, gain coefficient (α) and emission cross - section (σ_e) of laser emission have been determined. Excitation energy transfer from BNTVB to rhodamine 6G and N,N-bis(2,6-dimethylphenyl)-3,4,9,10-perylenebis-(dicarboximide) (BDP) was studied in EtOH to increase the output of laser emission from R6G and BDP when excited by nitrogen laser. The energy transfer dye laser system (ETDL) obeys a Forster resonance energy transfer mechanism (FERT) with a critical transfer distance, R_0 of 40 and 32 Å and k_{ET} equal 2.6×10^{13} and $1.06 \times 10^{13} \text{ M}^{-1}\text{s}^{-1}$ for BNTVB / R6G and BNTVB / BDP pair, respectively.



Regioselective Synthesis and Antifungal Activities of bis(tetrahydrobenzo[4,5]imidazo[2,1-*b*]quinazolin-1(2*H*)-one)

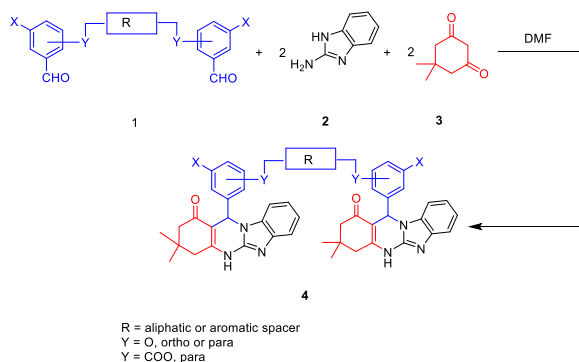
Mohammed A. Enaya, Ahmed H. M. Elwahy and Ismail A. Abdelhamid

Chemistry Department, Faculty of Science, Cairo University, Giza, Egypt.

ABSTRACT

In continuation to our research interest on the synthesis of heterocyclic utilizing C-C bond formation reactions¹⁻¹⁰ as well as on the synthesis of bis-heterocycles¹⁻⁸, a novel series of bis((3,3-dimethyl-3,4,5,12-tetrahydrobenzo[4,5]imidazo[2,1-*b*]quinazolin-1(2*H*)-one)) were prepared *via* the three component reaction of bis-aldehydes with 2-aminobenzimidazole and dimedone. The reaction mechanism was studied. The structures of the newly synthesized compounds are well established based on spectral data. The synthesized compounds were tested for their antifungal activity against some species of toxigenic fungi *Aspergillus* such as *Aspergillus Flavus*, *Aspergillus Parasitica*, *Aspergillus Westerdijskiae* and *Aspergillus Carbonarius*.

Graphical Abstract



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New reactive Ketenaminal: Synthesis, Reaction, Tautomeric Study and Antimicrobial Evaluation of the products

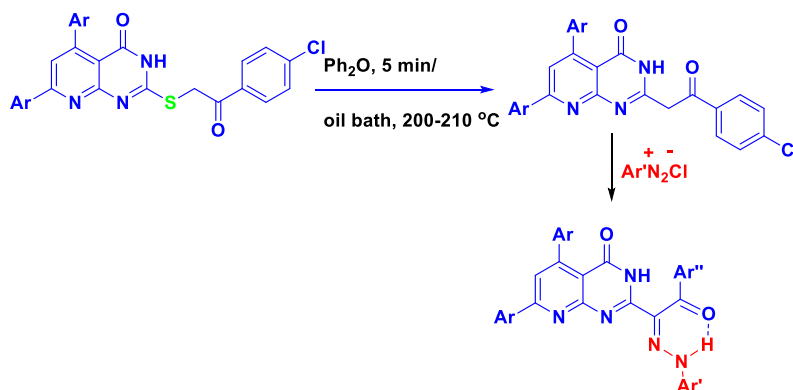
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ABSTRACT

One of the most successful reagents used in the synthesis of the reactive enaminone is DMF-DMA, but it is very expensive with high harmful effect for the human health and reacts with special compounds to generate the enaminone such as acetyl group and activemethylene centers. In this article we interested to synthesis a new ketenaminal by simple method with inexpensive reagents with starting compounds free from acetyl or activemethylene centers. Thus, a novel reactive ketenaminal (enaminone) was synthesized from the desulfurization of 2-((2-(4-chlorophenyl)-2-oxoethyl)thio)-5,7-bis(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(3*H*)-one with dipheny lether. The starting keteneaminal was coupled with diazotized anilines *via* the known coupling conditions to give a new series of 2-(4-chlorophenyl)-1-(2-(arylhydrazono)-2-oxoethyl)-5,7-bis(4-methoxyphenyl)pyrido[2,3-d]pyrimidin-4(1*H*)-ones. Moreover, the potency of these compounds as antimicrobial agents has been evaluated. The results showed that some of the products have high activity nearly equal to that of the used standard antibiotic. The structure of the new compounds was elucidated based on their IR, ¹H-NMR, ¹³CNMR, and mass spectra.





Preparation and Characterization of Pd-ZnO/MWCNT Nanocomposites for the Photocatalytic Degradation of Methylene Blue Dye

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ABSTRACT

Pd-ZnO/MWCNT nanocomposites were prepared by a hydrothermal method. Many tools were used to describe the synthesized nanocomposites. The XRD results reveal that only a single phase for ZnO is observed for undoped or doped ZnO samples. There are no characteristics peaks for palladium or palladium oxide because the dispersion of palladium above the indium oxide surface is high. XPS results reveal that the state of palladium is metallic. The values of band gap energy for ZnO can be controlled by controlling the weight percentage of palladium and MWCNT. The photocatalytic performance of Pd-ZnO/MWCNT nanocomposites was studied by measuring Methylene blue dye photocatalytic degradation under visible light. Parameters of photocatalytic reactions, such as palladium weight percentage and dose of nano composites, were measured. The Pd-ZnO/MWCNT nanocomposites had photocatalytic activity higher than that of ZnO because the addition of Pd and MWCNT to ZnO decreases the recombination rate of the electron-hole; furthermore, the absorption of ZnO was shifted to a high wavelength.



Benzothiazole-Based Monomethine Cyanine Dyes: Synthesize and Characterization

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ABSTRACT

Cyanines dyes are unique in their structure in that they have two nitrogen containing heterocycles moieties connected via conjugated methine groups. One moiety is quaternary ammonium salt and acts as the electron acceptor and the other is tertiary amine containing heterocycle and acts as the electron donor. This structural feature allows delocalization of electrons via the conjugated system with the property of high molar extinction coefficient. It was envisioned that having different monomethine cyanine dyes based on benzothiazole would furnish new dyes of optical interest amenable in sensing application. Thus, different heterocyclic quaternary ammonium salts derived from 2-methylquinoline, 2-methylquinoline and 2-methylbenzothiazole have been synthesized and characterized. These heterocyclic salts were used for the synthesis of monomethine cyanine dyes. The dyes obtained were characterized by ¹H and ¹³C NMR, FTIR, UV-visible and fluorescence spectroscopy.



Organic Electronics Based on N-(4-Methoxyphenyl) Imidazole Derivative as Electron Acceptor: Synthesis, Characterization and Optoelectronic Properties

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ABSTRACT

Organic electronics are semiconductors in which the valence band is the π molecular orbital (HOMO) and the conduction band is the π^* molecular orbital (LUMO). Organic hole transport materials (HTMs) are of prime importance for perovskite solar cells (PSCs). The pre-requisite for HTMs is to have a tuned HOMO-LUMO energy suitable for PSCs. On the other hand, organic light emitting diode (OLED) that are of growing interest for electronic display panel applications for example, is also one of organic electronic semiconductors, which have similar feature of HOMO-LUMO band gap energy correlation with those of HTMs. Therefore it was hypothesized that designing a novel organic electronics based on N-(4-methoxyphenyl) imidazole derivative moiety as electron acceptor in conjunction with different heterocyclic donors would furnish new organic electronics, which might find applications as OLED or as HTMs in PSCs. For this purpose, different N-octyl heterocycles derived from carbazole, phenothiazine and phenoxazine were synthesized and fully characterized. Vilsmeier formylation of these N-octyl heterocycles afforded the corresponding mono-formyl derivatives at the para-position to the N-octyl group. Then, the formyl derivatives underwent Radziszewski reaction to afford the corresponding donor- π -acceptor organic electronics and their chemical structures as well as their optoelectronic properties were fully characterized. UV-visible, fluorescence spectra and cyclic voltametry were measured and the HOMO-LUMO energy levels were estimated.



Synthesis of Novel N, N'-Diphenyl-1,3-Benzene-bis-Carbohydrazonoyl Bromide and its Utility in Facile Synthesis of new 1,3-Phenylene Bridged bis-Heterocycles

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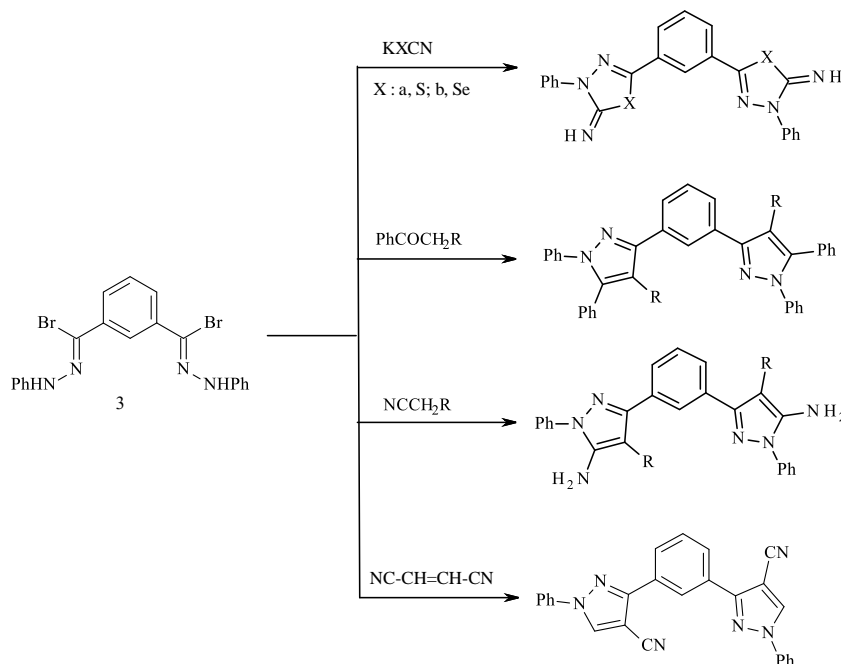
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ABSTRACT

Reaction of N,N'-diphenyl-1,3-benzene-*bis*-carbohydrazonoyl bromide **3** with potassium thiocyanate, potassium selenocyanate, active methylene compounds and dipolarophilic alkenes were studied. Structures of the products were established on analytical and spectral data as well as chemical transformations. The results indicated that compound **3** is useful precursor for synthesis of a wide variety of 1,3-phenylene-bis-heterocycles.





Synthesis and Reactions of 3-Amino-4-iminopyrazolo[3,4-*d*]pyrimidines and Biological activity of the Isolated products.

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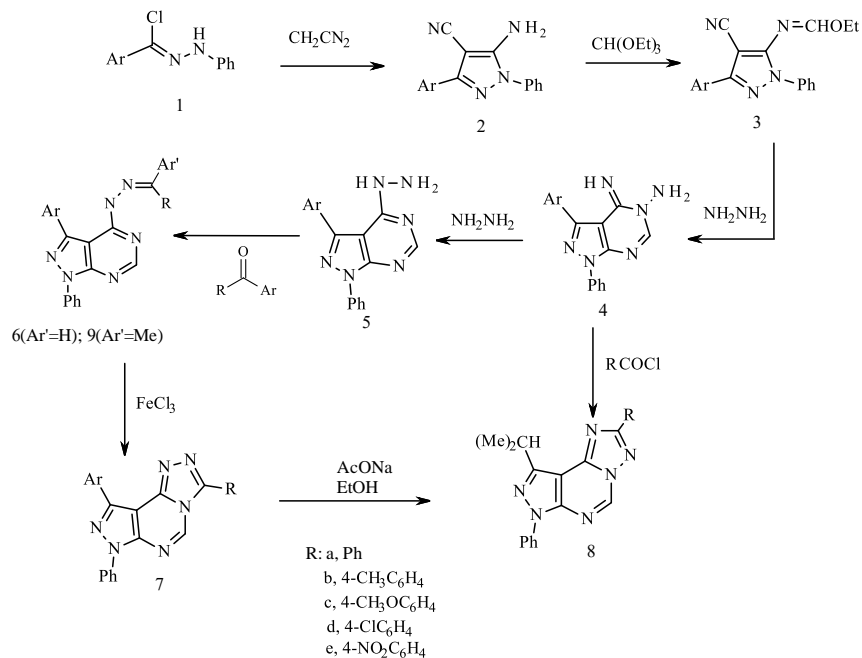
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ABSTRACT

Treatment of *N*-phenyl-substituted benzenecarbohydrazonoyl chlorides **1** with malononitrile in sodium ethoxide solution afforded 5-amino-4-cyanopyrazole derivative **2**, which converted to formidate derivative **3** upon refluxing with TEOF in acetic anhydride. The reaction of the latter product with hydrazine hydrate afforded imino-amine derivative **4**, which was converted to hydrazino derivative **5** by refluxing with hydrazine hydrate. Hydrazino as well as imino amino derivatives undergo condensation and cyclization reactions to give pyrazolo[3,4-*d*]pyrimidine and pyrazolo[4,3-*e*][1,2,4]triazolo[3,4-*c*]pyrimidine derivatives, respectively. Antimicrobial activities of some new synthesized compounds were studied.





Thiothymine In The Synthesis Of Triazolotriazine And Hydrazone Compounds. Evaluation Of Antimicrobial Activity Of Some Hydrazones

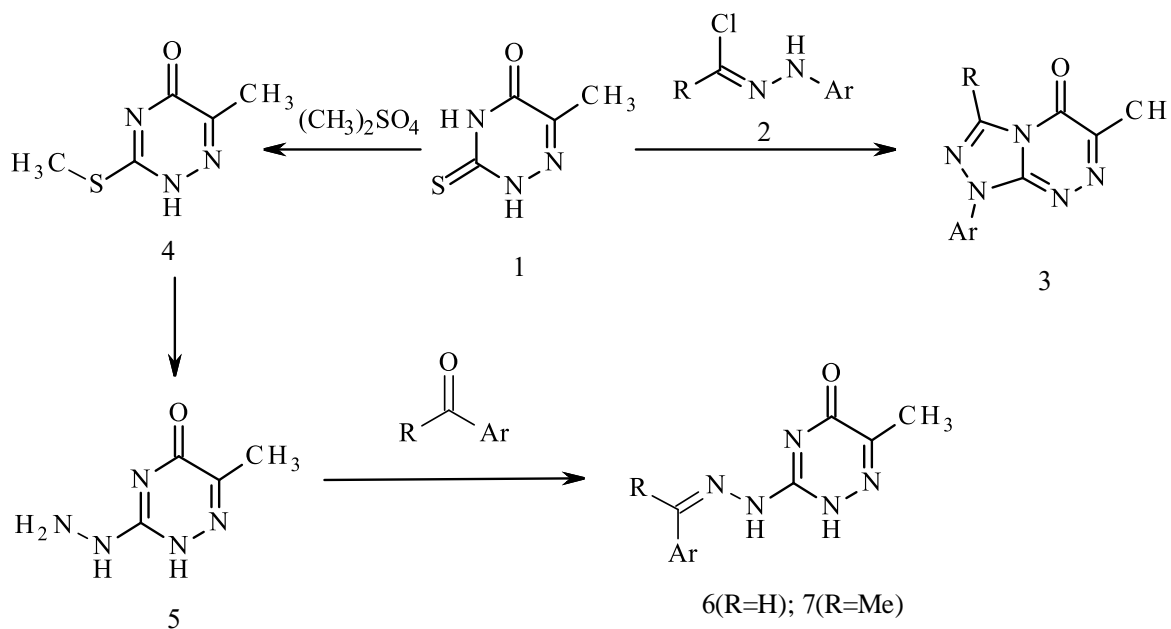
Hamdi M. Hassaneen^{a*}, Tayseer A. Abdallah^a, Fatma M. Saleh^aYasmin Sh. Mohamed^b, and Enas M. Awad^c

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ABSTRACT

Reaction of 6-methyl-3-thioxo-3,4-dihydro-1,2,4-triazin-5(2H)-one **1** with hydrazonoyl chloride **2** in refluxing chloroform in the presence of triethylamine yielded triazolotriazine derivatives **3**. Stirring of **1** with dimethylsulphate in sodium hydroxide solution, yielded 6-methyl-3-(methylthio)-1,2,4-triazin-5(4H)-one **4** which converted into hydrazine derivative **5** upon refluxing with hydrazine hydrate in ethanol. The hydrazino derivative **5** undergoes condensation reactions with aldehydes, pyruvic acid, ethyl pyruvate and ketones to give the corresponding hydrazone derivatives **6** and **7**, respectively. Antimicrobial activities of some new synthesized compounds were studied.





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