

**The 9<sup>th</sup> Jordanian Chemical Conference**  
**9<sup>th</sup> JCC**

**Abstract Book**

Organized by

The Jordanian Chemical Society in Corporation with  
Chemistry Department at the Hashemite University

Tuesday, April 28<sup>th</sup>, 2009

### اللجنة التحضيرية

أ. د. سلطان أبو عرابي/ رئيس المؤتمر

د. كايد ابو صفية – مقررأ

أ. د. أحمد أبو شملة

د. موسى البرغوثي

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### اللجنة العلمية

د. كايد ابو صفية - مقررأ

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السيدة ليلى قدورة

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السيد عبد الكريم الجبارين

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السيد قاسم طلفاح

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السيد نبيه العرقسوسي

# The 9<sup>th</sup> Jordanian Chemical Conference

## 9<sup>th</sup> JCC

Lecture: L

Poster: P

### Conference Program

	Registration	التسجيل	8:30-9:00
	Opening Ceremony	الإفتتاح	9:00-9:45
	Break	استراحة	9:45-10:15
Session Chairs: Ahmad abu-Shamleh and Dr. Mikdad Al-Arif			
L1	<p><b>“Half-Sandwich group 6 Metal Complexes Containing Sulfur Ligands”</b></p> <p><u>Mohammad El-khateeb</u> (Chemistry Department, Jordan University of Science and Technology, Irbid, JORDAN) and Wolfgang Weigand (Institut für Anorganische und Analytische Chemie, Friedrich-Schiller-Universität Jena, August-Bebel Strasse 2, Jena, 07743 GERMANY).</p>		10:15-10:35
L2	<p><b>“Selective Chelation of Mercury in Aqueous Media”</b></p> <p><u>Amer Malkawi</u> (Chemistry Department, Yarmouk University, Irbid, Jordan).</p>		10:35-10:55
L3	<p><b>“Coupling Granular Activated Carbon with Common Metal Chelating Corrosion Inhibitors for Two Phase Transition Metal Immobilization”</b></p> <p><u>Muna A. Abu-Dalo</u> (Department of Water and Environmental Engineering, German Jordanian University, Amman, Jordan), <u>Svetlana Nevostrueva</u> (Department of Civil and Environmental Engineering, University of Colorado at Boulder, Campus Box 428, Boulder, CO 80309-0428, USA) and <u>Mark T. Hernandez</u> (Department of Civil and Environmental Engineering, University of Colorado at Boulder, Campus Box 428, Boulder, CO 80309-0428, USA).</p>		10:55-11:15
L4	<p><b>“Five-membered Heterocycles: Pyrazoline, Pyrazole, 1,2,3-Selenadiazole and 1,2,3-Thiadiazole Multi-arm Aromatic Compounds Syntheses, Reactions and Applications”</b></p> <p><u>Mousa L. Al-Smadi</u> (Department of Applied Chemical Sciences, Jordan University of Science and Technology, Irbid, Jordan).</p>		11:15-11:35
	Break	استراحة	11:35-2:00

Session Chairs: Dr. Mohamed Mubarak and Dr. Mohammad El-khateeb		
L5	<p><b>“Butyrylcholinesterase Inhibitory Activity of Testosterone and Some of its Metabolites”</b></p> <p><u>Amal Al-Aboudi</u>, Hana Odeh (Department of Chemistry, University of Jordan, Amman 11942, Jordan), Asaad Khalid (Medical Biochemistry Research Unit, Medicinal and Aromatic Plants Research Institute, National Center for Research, P.O. Box: 2404, Khartoum, Sudan ), Qamar Naz , M. Iqbal Choudhary, and Atta-Ur-Rahman (H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi-75270, Pakistan).</p>	12:00-12:20
L6	<p><b>"Synthesis and Mesomorphic Behaviour of Some Novel Compounds Containing 1,2,4-Triazole And 1,3,4-Thiadiazole Rings"</b></p> <p>Jumbed H. Tomma,( Department of Chemistry, College of Education, Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq), Ivan H. Rou'il (Department of Chemistry, College of Science, University of Al-Mustanseryia, Baghdad, Iraq), and <u>Ammar H. Al-Dujaili</u> (Department of Chemistry, College of Education, Ibn Al-Haitham, University of Baghdad, Baghdad, Iraq).</p>	12:20-12:40
L7	<p><b>“Fabrication And Preparation of Amino-Terminated Self-Assembled Monolayers by Chemical Reduction of Aromatic-Nitro Groups”</b></p> <p><u>Nathir A. F. Al-Rawashdeh</u>, W. Azzam, and Ch. Wöll.</p>	12:40-13:00
L8	<p><b>“Cucurbit[7]uril in Drug Delivery”</b></p> <p><u>Na'il Saleh</u> (Department of Chemistry, College of Science, Yarmouk University, Irbid, Jordan) and Werner M. Nau (School of Engineering &amp; Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen (Germany)).</p>	13:00-13:20
<b>Lunch and Poster Session</b>		13:20-15:00
Session Chairs: Dr. Hamzeh Abdel-Halim and Dr. Nathir A. F. Al-Rawashdeh		
L9	<p><b>“Molecular Dynamics Simulations of Protein (HLA-Cw6-β2m-KIR2DS2) Skin Disease Psoriasis”</b></p> <p><u>Mansour H. Almatarneh</u> (Al-Hussein Bin Talal University, Ma'an, Jordan) and Valarie Booth ( Department of Biochemistry, Memorial University, St.John's, NL, A1B 3X9, Canada).</p>	15:00-15:20

L10	<p><b>“Comparison of Calculated and Experimentally Determined Evaporation Path From an Emulsion”</b></p> <p><u>Abeer Al-bawab</u> (Chemistry Department, University of Jordan, Amman, Jordan).</p>	15:20-15:40
L11	<p><b>“A Comparative Study For the Determination of Doxycycline-hcl in Pharmaceutical Formulations by Flow Injection-Activated Chemiluminescence and Kinetic Spectrophotometric Methods”</b></p> <p><u>Suham Towfiq Ameen</u> ( Tikrit University, Iraq), Abdul majeed Korshed ( Karkuk University ,Iraq), and Ali Ebraheem Kalel (Tikrit University , Iraq).</p>	15:40-16:00
L12	<p><b>“Method Development for Analysis of Linear and Branched Alkyl Benzene Sulfonates and Comparison of Their Phase Behavior in Water and Oil Ternary Systems”</b></p> <p><u>Ayat Abed Al-Hafed Bozeya</u>, Abeer Al-Bawab and Manar Fayyad (Chemistry Department, University of Jordan, Amman, Jordan).</p>	16:00-16:20
Session Chairs: Jamal A. Sweileh and Dr. Yahya Tahboub		
L13	<p><b>“Simultaneous Determination of Fluoxetine, Norfluoxetine, Citalopram and Haloperidol in Plasma by LC-MS-ESI”</b></p> <p>Abdul-Wahab El-Rjoob (Department of Applied Chemistry, Jordan University of Science and Technology, Irbid, Jordan), Munther Tahtamouni (Prince Haya Center of Biotechnology, Jordan University of Science and Technology, 22110 Irbid, Jordan), and <u>Yahya Tahboub</u> ( Prince Haya Center of Biotechnology, Jordan University of Science and Technology, 22110 Irbid, Jordan).</p>	16:20-16:40
L14	<p><b>“Jordanian Zeolite: an Efficient Adsorbent for Water Purification”</b></p> <p><u>Rushdi I. Yousef</u> (Department of Chemistry, Faculty of Arts and Sciences, Petra University, Amman, Jordan) and Bassam El-Eswed (Zarka University College, Al-Balqa Applied University, Zarka, Jordan).</p>	16:40-17:00
L15	<p><b>“Flow injection – Sptrophotometric Determination of Selected Cephalosporines”</b></p> <p>S. A. Barakat (FHSS, Sohar University, Sohar P.O.Box 44 Postal code 311, Sohar, Sultanate of Oman).</p>	17:00-17:20

L16	<p><b>“Synthesis and Characterization of Polycarbonates by Melt-Phase Interchange Reactions of Alkylene and Arylene Diacetates with Alkylene and Arylene Diphenyl Dicarbonates: a New Synthetic Approach”</b></p> <p>Bassam A. Sweileh (Department of Chemistry, Faculty of Science, University of Jordan, Amman 11942, Jordan) , Yusuf M. Al-Hiari ( Department of Pharmaceutical Sciences, Faculty of Pharmacy, University of Jordan, Amman 11942, Jordan) and Mohammad H. Kailani (Department of Chemistry, Faculty of Science, University of Jordan, Amman 11942, Jordan).</p>	17:20-17:40
L17	<p><b>"Adduct Formation and Stability of Methyltrioxorhenium(VII) with a Series of Aliphatic and Aromatic Nitrogen-Donor Ligands"</b></p> <p>Ahmad M. Al-Ajlouni* and Mazin Y. Shatnawi ( Department of Applied Chemical Sciences, Jordan University of Science and Technology, Irbid 22110, Jordan)</p>	17:40-18:00
<b>Closing Ceremony</b>		<b>حفل الختام</b>
		18:00

## Half-Sandwich Group 6 Metal Complexes Containing Sulfur Ligands

Mohammad El-khateeb<sup>a</sup>, Wolfgang Weigand<sup>b</sup>

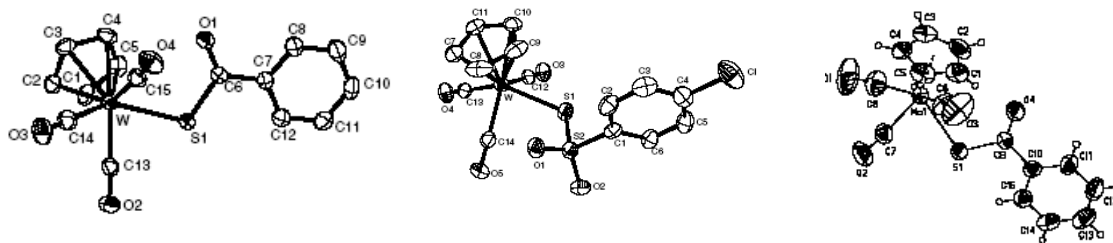
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<sup>b</sup> Institut für Anorganische und Analytische Chemie, Friedrich-Schiller-Universität Jena, August-Bebel Strasse 2, Jena, 07743 GERMANY

### ABSTRACT

The reactions of the metal hydrosulfido complexes  $[\text{CpM}(\text{CO})_3\text{SH}]$  ( $\text{M} = \text{Cr}, \text{Mo}, \text{W}$ ) of group 6 with electrophiles are under current investigation. The reaction of  $\text{CpM}(\text{CO})_3\text{SH}$  with acid chlorides gave the corresponding thiocarboxylates  $\text{CpM}(\text{CO})_3\text{SCOR}$  [1, 2]. The tungsten thiosulfonates were prepared by the interaction of the corresponding hydrosulfido complex with sulfonyl chlorides [1].

Our proposal to the Humboldt foundation, which was supported and this event is part of it will also include the preparations of thiosulfonate, thiocarbonate, dithiocarbonate,  $\text{SCS}_2\text{R}$  and *O*-alkyl thio-oxalates. Dimeric complexes can be obtained from the reaction of the hydrosulfido complexes with bi-functional electrophiles (diacid chlorides and compounds bearing the sulfonyl and acid chloride groups). The mono-metallic compounds ( $\text{CpM}(\text{CO})_3\text{SCOZCOCl}$  or  $\text{CpM}(\text{CO})_3\text{SCOZSO}_2\text{Cl}$ ;  $\text{Z} = \text{C}_6\text{H}_4$ ) are also possible to be obtained by a 1:1 molar ratio of  $\text{CpM}(\text{CO})_3\text{SH}$  to  $\text{ClCOZSO}_2\text{Cl}$ . Organic transformation reactions of the latter complexes will produce functionalized derivatives.



1. M. El-khateeb, H. Goerls, W. Weigand, *J. Organomet. Chem.* 691 (2006) 5816.
2. M. El-khateeb, T. Rueffer, H. Lang, *Polyhedron* 25 (2006) 3413.

## Selective Chelation of Mercury in Aqueous Media

Amer Malkawi  
*Chemistry Department, Yarmouk University*  
*Irbid Jordan*

### ABSTRACT

The need for environmental chelation and monitoring of mercury levels in water is driven by its known acute neurotoxicity. Implementation of chelation/surface chemistry to alter selectivity of chelates toward mercuric ion is a novel and effective mean for selective removal of Hg(II) from aquatic environments. Comparative studies involving chelation reactions of Hg(II), Cd(II) and Pb(II) with Dimercaptosuccinic acid (among other chelates) in solution and on silica surface and how the surface attachment has altered the metal binding characteristics of the chelate will be presented in this talk. How chelates are covalently tethered to silica material and selectively interacted with Hg(II) as evidenced by IR spectroscopy will be also demonstrated in the talk

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2. X. Wang, Z. Li, B. Wei, J. Yang, *Synthetic Communications*, **32(7)**, 1097 (2002).
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13. Hwang, J. Y. et al. *Journal of Combinatorial Chemistry* **7**, 816 (2005).

## Coupling Granular Activated Carbon with Common Metal Chelating Corrosion Inhibitors for Two Phase Transition Metal Immobilization

Muna A. Abu-Dalo<sup>a</sup>, Svetlana Nevostrueva<sup>b</sup> Mark T. Hernandez<sup>c</sup>

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### ABSTRACT

Benzotriazole derivatives form very strong bonds with transition metals, and are the most widely used type of industrial corrosion inhibitor. Because of their unique chemical architecture — an aromatic ring conjugated to a triazole ring — this class of compounds has a strong amphipathic behavior that enables them to bind metal ions, while at the same time, maintain a strong surface sorption character. The environmental chemistry of benzotriazoles, and their metal immobilization potential remains relatively unknown. Of particular environmental engineering interest are the most commercially significant and lowest cost benzotriazoles, which are simple methylated derivatives. Methylated benzotriazoles retain selective biodegradation responses and carry a significant degree of toxicity and environmental risk as judged by common ecosystem receptor models.

Laboratory microcosms and small scale columns experiments were used to evaluate the effectiveness of BTA for removing soluble transition metals from acidic water by sequentially adding benzotriazole and granular activated carbon (GAC) to acidic waters or adding premixed benzotriazole-metal solution to GAC. Tests were conducted at different acidic pH values and metal to ligand (triazole) ratio to determine the optimum treatment conditions.

The amphipathic behavior and metal-binding capacity of benzotriazoles were leveraged to remove selected transition metal ions from model industrial wastewaters and acid mine drainage. The amount of metal ions sequestered from solution was sensitive to pH changes as well as the metal to ligand ratio. These results suggested that some types of activated carbon can sequester benzotriazoles from acidic solutions and be useful in some industrial waste treatment and biological waste treatment scenarios. Either where toxicity to a biological process is an issue or where an effluent limit must be met.

In addition, results from this work show the potential implications for improving the cost-effective remediation of industrial wastewater, metal plating electronics manufacture, acid mine drainage (AMD), radionuclide treatment, improve health, water quality, and serve as the basis for a novel precious metal recovery process.

**keywords:** Benzotriazoles, GAC, corrosion inhibitor, metal removal.

## Five-membered Heterocycles: Pyrazoline, Pyrazole, 1,2,3-Selenadiazole and 1,2,3-Thiadiazole Multi-arm Aromatic Compounds Syntheses, Reactions and Applications

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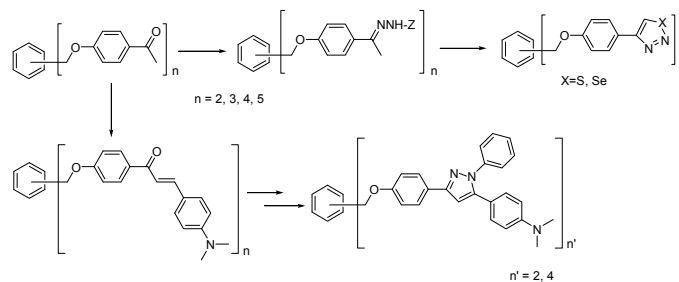
E-mail: mariam10@just.edu.jo

### ABSTRACT

Heterocyclic compounds are of interest due to their biological and synthetic applications. pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole and derivatives are well known and have attracted the attention being a versatile intermediates in organic synthesis. Many substituted pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole and derivatives were prepared and most of them showed high antibacterial activity. The antifungal activity of other substituted pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole was also determined. It has been found that the introduction of pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole ring to molecules of known biologically active compounds changes their activities and in some cases lead to an increase in their biological activity. Other heterocyclic compounds containing triazole, oxazole, benzoxazole, quinazoline, pyridazoline, pyridazine and thiazole rings were found to be biologically active substances. Derivatives of pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole are important in industry, medicine and agriculture<sup>[1]</sup>.

Heterocyclic systems with multi-arm pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole were recently prepared from the corresponding multi-arm ketones.

On the other hand, the chemical reactivity of the multi-arm pyrazoline, pyrazole, 1,2,3-selenadiazole and 1,2,3-thiadiazole derivatives was studied under thermal and photochemical conditions<sup>[2-6]</sup>.



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6. M. Al-Smadi and S. Mohammad, *J. Heterocyclic Chem.*, accepted (2008).

**Butyrylcholinesterase Inhibitory Activity of Testosterone  
and Some of Its Metabolites**

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Qamar Naz<sup>3</sup> M. Iqbal Choudhary<sup>3</sup>, and Atta-Ur-Rahman<sup>3</sup>

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<sup>3</sup>*H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological  
Sciences, University of Karachi, Karachi-75270, Pakistan*

**ABSTRACT**

Testosterone and ten of its metabolites were examined as inhibitors of butyrylcholinesterase. A significant enzyme inhibition activity ( $IC_{50} = 1.55 \mu M$ ) was observed for androst-4-en-3,7-dione. The kinetic parameters of butyrylcholinesterase inhibition were determined. Molecular docking was carried out in order to develop a better understanding of the inhibitor-enzyme interactions. The results showed that the inhibition was non-competitive, stabilized mainly by hydrogen bonds and hydrophobic interactions between the inhibitor and butyrylcholinesterase.

**Keywords:** Testosterone, androstenedione, butyrylcholinesterase, cholinergic hypothesis.

## Synthesis and Mesomorphic Behaviour of Some Novel Compounds Containing 1,2,4-Triazole and 1,3,4-Thiadiazole Rings

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<sup>a</sup>*Department of Chemistry, College of Education, Ibn Al-Haitham,  
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<sup>b</sup>*Department of Chemistry, College of Science, University of Al-Mustanseryia,  
Baghdad, Iraq*

### ABSTRACT

Two new mesogenic homologous series of liquid crystalline compounds containing 1,2,4-triazole and 1,3,4-thiadiazole in the molecule viz. 1,4-bis{3-[2-(4-alkoxybenzylideneamino)-1,3,4-thiadiazole-5-yl]phenyl} and 5-(4-methoxyphenyl)-3-[2-(4-alkoxybenzylideneamino)-1,3,4-thiadiazole-5-yl] were synthesized by many step procedures. Both series have been characterized by elemental analysis, FT-IR, mass spectrometry, <sup>1</sup>H-NMR, and <sup>13</sup>C-NMR. Phase transition temperature and the thermal parameters were obtained from differential scanning calorimetry (DSC). The texture observations were performed under hot-stage polarizing optical microscopy (POM). All compounds of the first series exhibited enantiotropic nematic mesophase. The compounds of the second series exhibited enantiotropic nematic mesophase, and that with propyloxy terminal substituent shows enantiotropic nematic phase on heating and monotropic smectic A (SmA) phase on cooling, while the homologue with ethoxy terminal substituent do not show any liquid crystalline properties. The mesomorphic behaviour has been analyzed in terms of structural property relationship.

## Fabrication and Preparation of Amino-Terminated Self-Assembled Monolayers by Chemical Reduction of Aromatic-Nitro Groups

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<sup>b</sup>*Department of Applied Chemical Sciences, Jordan University of Science & Technology, P.O.Box 3030, Irbid-22110, Jordan, E-mail: [nathir@just.edu.jo](mailto:nathir@just.edu.jo)*

<sup>c</sup>*Department of Chemistry, Tafila Technical University, Tafila-Jordan.*

### ABSTRACT

Nano-self-assembled monolayers (SAMs) formed from 4'-nitro-1,1'-biphenyl-4-thiol (NBT) on gold were studied at different immersion times using infrared reflection-absorption spectroscopy. The IR results revealed that the straightforward approach for fabrication SAMs, namely, immersing the gold film in organothiols, leads to the formation of highly oriented SAMs. Furthermore, we demonstrated that the immersion time of the gold substrate into the ethanolic solution of NBT has no effect on the orientation of NBT SAMs. To prepare highly oriented amino-terminated SAMs, the nitro-terminated SAMs were immersed into ZnCl<sub>2</sub>/HCl solution to reduce the nitro group to amino group. IR spectra recorded for this conversion revealed that the SAMs should be immersed in the acidic solution of ZnCl<sub>2</sub> for a short period of time (45 min). Immersion for a longer time results in the etching of the formed film by the acidic solution. IR data recorded for the amino-terminated SAMs reveal the formation of highly oriented organothiolate monolayers via the chemical reduction (ZnCl<sub>2</sub>/HCl) of the nitro group.

## Cucurbit[7]uril in Drug Delivery

Na`il Saleh<sup>a\*</sup> and Werner M. Nau<sup>b</sup>

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<sup>b</sup>*School of Engineering & Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen (Germany).*

### ABSTRACT

Important examples of potential drug vehicles at the nano-scale are safe and water-soluble compounds with a rigid pocket-like supramolecular structure, which can transport the drugs through non-covalent interactions of a host-guest type. We present the use of cucurbit[7]uril (CB7) for the activation of proton-pump inhibitors, such as omeprazole, which are used worldwide to cure gastric acid-related diseases. We demonstrate how the complexation of these drugs catalyzes with a 15-fold rate enhancement an intramolecular nucleophilic substitution reaction, which leads to the formation of a cyclic sulfenamide as the active form of the drug. This effect combines with a 500-fold increase in stability of the active form in its complex. The complex also retains its medicinally relevant reactivity with cysteine. By comparison with other benzimidazoles (BZs) drugs, we can rationalize the observed catalytic effect mechanistically through a supramolecular  $pK_a$  shift affected by the macrocycle. The obtained  $pK_a$  shifts by CB7 was also exploited to solubilize other BZs derivatives that are known as anticancer drugs, such as albendazole. Additionally, the potential use of CB7 to carry some ocular drugs with pH solubility profiles that resemble BZs drugs is also discussed. These results underscore the pharmaceutical potential of cucurbiturils as promising alternatives to cyclodextrins in drug delivery.

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## Molecular Dynamics Simulations of Protein (HLA-Cw6- $\beta$ 2m-KIR2DS2) Associated with Skin Disease Psoriasis

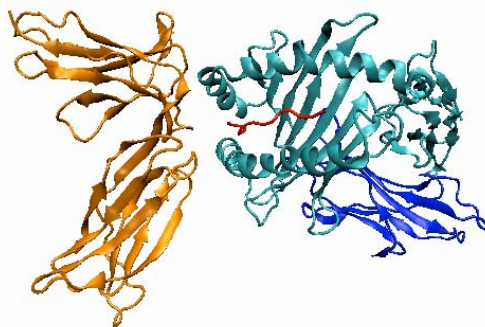
*Mansour H. Almatarneh* <[mansour@mun.ca](mailto:mansour@mun.ca)><sup>a</sup>; *Valarie Booth* <[vbooth@mun.ca](mailto:vbooth@mun.ca)><sup>b</sup>

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### ABSTRACT

Molecular dynamics (MD) simulations were performed to study the structure and dynamics of (HLA-Cw6- $\beta$ 2m-KIR2DS2) complex for better understanding of the skin disease psoriasis. Numerous studies have proved that Cw6 antigens is positively associated with psoriasis <sup>a</sup>. The overall aim of this study is to come up with a new peptide or a small protein therapeutic for psoriasis that is able to disrupt the interaction between HLA-Cw6 and its receptor. This project provides a detailed understanding of the HLA-Cw6- $\beta$ 2m-KIR2DS2 complex, which is not yet known by using MD simulations. Two complexes were constructed from HLA-Cw3- $\beta$ 2m-KIR2DL<sup>b</sup> and HLA-Cw4- $\beta$ 2m-KIR2DL1<sup>c</sup> by superposition and homology modeling using SWISS-MODEL. All MD simulations were performed using the Gromacs package. The OPLS-AA all-atom force field and Gromos96 was used with the SPC (single point charge) water model. The starting structure for all simulations was constructed by homology model from HLA-Cw3- $\beta$ 2m-KIR2DL2. The simulations were performed in triclinic and cubic periodic boundary conditions. The simulations time step was set to a 1.5 fs, and the MD simulation was performed up to  $1 \times 10^7$  time steps (15.0ns). The preliminary results, structures and the binding sites of the complex will be presented and discussed.



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<sup>b</sup> Boyington, J.C., Motyka, S. A., Schuck, P., Brooks, A.G. & Sun, P. D. (2000). *Nature* 405, 537-43.

<sup>c</sup> Fan, Q. R. & Wiley, D. C. (1999). *J. Exp. Med.* 190, 113-23.

## Comparison of Calculated and Experimentally Determined Evaporation Path From an Emulsion

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### ABSTRACT

The evaporation path from fragrance emulsions was experimentally determined and compared to estimations using phase diagrams of the emulsion system limiting the comparison to the case of insignificantly small relative humidities.

The experimentally determinations were made by evaporation from a rotating evaporator in order to eliminate the effect of kinetic factors and at a pressure of 0.2mmHg to ensure the relative humidity of the atmosphere to be without influence.

The agreement between the estimated and experimental values was excellent and the trend of the evaporation path as expected from the O/W ratios was reproduced in the experimental results.

The results are encouraging for estimations of evaporation paths from the phase diagrams to be a useful tool for fragrance emulsion formulation.

**A Comparative Study for The Determination of Doxycycline-hcl in Pharmaceutical Formulations by Flow Injection-Activated Chemiluminescence and Kinetic Spectrophotometric Methods.**

*Prof. Dr. Suham Towfiq Ameen, Tikrit University, Iraq*

*Dr. Abdul majeed Korshed, Karkuk University, Iraq*

*Dr. Ali Ebraheem Kalel, Tikrit University, Iraq*

**ABSTRACT**

This investigation involves development of a new flow injection-activated chemiluminescence (FIA-Cl) and a simple kinetic spectrophotometric methods for the determination of Doxycycline-HCl (Dox-HCl) in pharmaceutical preparations. The method of (FIA-Cl) was based on the activation of luminol-Cobalt-H<sub>2</sub>O<sub>2</sub> chemiluminescence by (10-80)  $\mu\text{g}\cdot\text{ml}^{-1}$  with detection limit of 7.2  $\mu\text{g}\cdot\text{ml}^{-1}$ , and correlation coefficient was 0.9994 (n=6) and the relative standard deviation RSD% was (0.12-1.02)%. Spectrophotometric method was based on the oxidation of the DOX-HCl with alkaline Potassium permanganate, the reaction is followed spectrometrically by measuring the rate of change of the absorbance at 600nm. A fixed time (at 24 min) method is adopted for determining the drug concentration. A linear calibration graph was in the range of (1-7)  $\mu\text{g}\cdot\text{ml}^{-1}$  with molar absorption coefficient was (4.2\*10<sup>5</sup>) L/mol.cm and correlation coefficient was 0.9999, detection limit of (0.221)  $\mu\text{g}\cdot\text{ml}^{-1}$  and a relative standard deviation was (0.73-1.61)%.

The two methods were applied successfully to determine the content of Dox-HCl in pharmaceutical preparations with a recovery of 98-99%.

## **Method Development for Analysis of Linear and Branched Alkyl Benzene Sulfonates and Comparison of Their Phase Behavior in Water and Oil Ternary Systems**

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### **ABSTRACT**

The first part of this work involved developing a high performance liquid chromatographic method for the separation and determination of linear and branched alkyl benzene sulfonate (LAS, BAS) in water samples. LAS and BAS were separated using Tthermo Hypersil Sax (250 x 4.6mm, 5 $\mu$ m) anion exchange column. Isocratic elution using (40/60 v/v) acetonitrile in water as a mobile phase containing 0.05 M sodium perchlorate was used, the flow rate was 1.5 ml/min and the UV detector was set at 280 nm. Detection limits obtained were 10 ppm for LAS and 25 ppm for BAS. It was found that this method can be used for the simultaneous determination of LAS and BAS surfactants in water samples.

The second part of the work involved systematic investigation of the phase behavior of a ternary system of LAS or BAS in oil (corn or olive) and water. The study showed that there are links between the surfactants chemical structure, aggregation properties, and the formation of micelles, the aggregation properties are dramatically affected by small structural variation of the hydrophobic group at constant carbon number. Micelles formation was found to correlate with the extent of chain branching by effecting oil-water tension, where the branched alkyl tail has significantly more ability to form micelles than the linear tail.

**Simultaneous Determination of Fluoxetine, Norfluoxetine, Citalopram and Haloperidol  
in Plasma by LC-MS-ESI**

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**ABSTRACT**

A reliable method was developed for simultaneous determination of antidepressant drugs fluoxetine and its metabolite norfluoxetine and citalopram and antipsychotic drug haloperidole employing the antiepileptic lamotrigine as internal standard. The method is based on solid phase extraction followed by LC separation on a Agilent C<sub>18</sub> (4.6 mm x 150 mm, 5 µm) column at ambient temperature. Mobile phase was 5 mM ammonium acetate and on acetonitrile, and was pumped in a gradient of 30:70 V/V to 10:90 V/V and then back to 30:70 V/V over 15 min at a flow rate of 0.5 mL/min. Eluted compounds were ionized by electrospray ionization (ESI) ion source of the ion-trap mass spectrometer and were detected by selected ion monitoring (SIM) mode. Plasma endogenous compounds were eluted in the first five minutes and discarded by switching valve. Targeted drugs eluted in the period 5.5-11 min. Calibration curves were linear in the range 5 (10)- 400 ng/mL with correlation coefficients better than 0.999. LLOQs were 5 ng/mL for haloperidol and citalopram and 10 ng/mL for fluoxetine and norfluoxetine. Other statistical and validation results were within accepted range for clinical determinations.

## Jordanian Zeolite: an Efficient Adsorbent for Water Purification

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### ABSTRACT

Several studies were carried out by the first author on Jordanian zeolitic tuff which was chemically treated by different chemicals, viz., urea, thiourea, acetamide, DMSO, oxalic acid, salicylic acid, and surfactants. The capability of these zeolites to uptake some organic and inorganic pollutants from water was investigated. The outcome of these investigations revealed that Jordanian zeolite can be considered as an efficient adsorbent for water purification.

The aim of the present work is to get insight about one example on the use of zeolite in water purification, viz., interaction between phenols and Jordanian zeolite. The kinetics and thermodynamics of the adsorption of phenol, monochlorophenols (2- and 4-), and dichlorophenols (2,4- and 3,5-) on local zeolitic tuff was investigated. The rate of adsorption was found to increase with increasing the number of chloro-substituents on phenol (increase acidity and hydrophobicity of phenols). On the other hand, the adsorption capacity was found to decrease with increasing the number of chloro-substituents on phenol (increase size of phenol). The adsorption process was found to be exothermic with  $\Delta H$  values ranges from -20 to -80 kJ/mol, which are comparable with those reported for adsorption of water (-20 kJ/mol) and ethanol (-25 kJ/mol) onto natural zeolite.

**Flow injection – Spectrophotometric Determination of Selected Cephalosporines.**

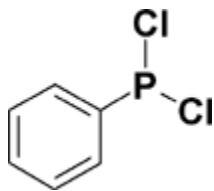
S. A. Barakat\*

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[salem\\_barakat@yahoo.com](mailto:salem_barakat@yahoo.com)

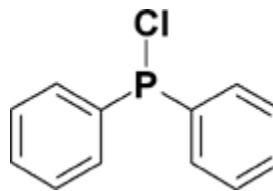
**ABSTRACT**

A rapid, sensitive and accurate flow injection method for the determination of Dichlorophenylphosphine and diphenylchlorophosphine has been developed. It is based on the oxidation reduction reaction between cephalosporines and iron(III), The excess iron(III) is determined spectrophotometrically using thiocyanate coloring agent. Aliquots of each cephalosporines are hydrolyzed using NaOH and filtered to be ready for injection in a simple manifold composed of 3-channels, injector, reaction coil and a spectrophotometer.

Variables such as concentration of reactants, reaction coil length, injection volume, flow rate. etc. are studied and optimized. Reproducibility, linearity, detection limit and statistical evaluation are shown. The methods results are in good agreement to other standard methods.



Dichlorophenylphosphine (dcpp),



Diphenylchlorophosphine(dpcp)

**Synthesis and Characterization of Polycarbonates by Melt-Phase Interchange Reactions of Alkylene and Arylene Diacetates with Alkylene and Arylene Diphenyl Dicarbonates: A New Synthetic Approach**

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**ABSTRACT**

A new method of synthesis of polycarbonates based on interchange reactions of alkylene and arylene diacetates with alkylene and arylene diphenyl dicarbonates is presented. The diphenyl dicarbonates are prepared from phenyl chloroformate and the corresponding dihydroxy compounds. The polycarbonates are synthesized by melt-phase polycondensation of the diacetates with diphenyl dicarbonates as monomers. The process involved a precondensation step under a stream of argon gas followed by melt polycondensation at high temperature and low pressure. The reaction was accompanied with the occurrence of partial randomization of the monomers in the polymer backbone, and in some cases by cyclization and subsequent elimination of cyclic aliphatic carbonates. The potential of this reaction was demonstrated by the successful synthesis of two series of polycarbonates involving several aromatic-aromatic, aromatic-aliphatic and aliphatic-aliphatic polymers. Using alkylene or arylene diacetates with alkylene or arylene diphenyl dicarbonate as monomers, it was possible to prepare polycarbonates having inherent viscosity values in the range 0.15–0.46 dL/g. The glass transition temperature values of the polycarbonates were in the range 13–108 °C. The present approach may permit the use of alkylene and arylene diacetates containing other organic functional groups leading to the synthesis of polycarbonates containing those groups.

## Adduct Formation and Stability of Methyltrioxorhenium(VII) with a Series of Aliphatic and Aromatic Nitrogen-Donor Ligands

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### ABSTRACT

The stability of a variety of aromatic and aliphatic N-donor ligand adducts of methyltrioxorhenium(VII) ( $\text{CH}_3\text{ReO}_3$ , MTO) was investigated using acetonitrile ( $\text{CH}_3\text{CN}$ ) as a solvent. The formation constants were determined by the utilization of obtained spectrophotometric data based on a 1:1 adduct formation. The adduct formation constants ( $K_f$ ) for MTO:L (L = nitrogen donor ligand) are very sensitive to the electronic nature of the ligand and increase with the ligand donating ability. Adducts of aliphatic N-donor ligands are less stable towards decomposition by basic solutions and produce polymeric rhenium material, methane and perrhenate. The kinetics of the adduct decomposition were investigated in solution at room temperature under pseudo-first-order conditions. Linear correlations between the adduct decomposition rate constants ( $k_d$ ) and ( $K_a$ ) values of the N-donor ligand have shown that the decomposition rate constants increasing with the N-donor ligand basicity. A comparative study between the values of  $K_f$  and  $k_d$  revealed that imidazole forms the most stable adduct with MTO among the N-donor ligands investigated in this study.

## Iron Complexes of Heterocyclic-Thiocarboxylate Complexes

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### ABSTRACT

The reaction of  $(\mu\text{-S}_x)[\text{CpFe}(\text{CO})_2]_2$  ( $x= 3, 4$ ) with acid chlorides give  $\text{CpFe}(\text{CO})_2\text{SCOR}$  [1]. The photolytic reaction between the iron thiocarboxylate complexes  $\text{CpFe}(\text{CO})_2\text{SCOR}$  and  $\text{EPh}_3$  ligands ( $E = \text{P, As, Sb}$ ) [2] which gave, exclusively, the monosubstituted complexes  $\text{CpFe}(\text{CO})(\text{EPh}_3)\text{SCOR}$  in high yield. The photolytic reaction of these thiocarboxylate complexes with bisphosphine ligands,  $\text{Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2$  was found to produce both the mono-substituted complexes  $\text{CpFe}(\text{CO})(\kappa^1\text{-P, Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2)\text{SCOR}$  or  $\text{CpFe}(\kappa^2\text{-P, P-Ph}_2\text{P}(\text{CH}_2)_n\text{PPh}_2)\text{SCOR}$  depending upon the bisphosphine chain length [3, 4]. Heterocyclic-thiocarboxylate complexes of iron  $\text{CpFe}(\text{CO})_2\text{SCO-het}$  ( $\text{het} = 2\text{-C}_4\text{H}_4\text{O, 2-C}_4\text{H}_4\text{S, 1-C}_4\text{H}_8\text{N}$ ) can be made similarly. The substitution reactions of these heterocyclic thiocarboxylates are under investigations. The structure of  $\text{CpFe}(\text{CO})_2\text{SCO-(2-C}_4\text{H}_4\text{S)}$  is reported.

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## Reactions of Ruthenium Hydrosulfido Complexes with Electrophiles

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### ABSTRACT

Cyclopentadienyl ruthenium hydrosulfido complexes  $\text{CpRu(L)(L')SH}$  ( $\text{Cp} = \eta^5\text{-C}_5\text{H}_5$ ;  $\text{L} = \text{L}' = \text{PPh}_3$ ;  $1/2 \text{ dppe}$ ;  $1/2 \text{ dpdm}$ ;  $\text{L} = \text{CO}$ ,  $\text{L}' = \text{PPh}_3$ ), were found to be active towards electrophiles. Reaction with acid chlorides [1] gave the thiocarboxylate complexes  $\text{CpRu(L)(L')SCOR}$ , with chloroformates [2] gave the thiocarbonate complexes  $\text{CpRu(L)(L')SCO}_2\text{R}$ , with O-alkyl oxalates [3] gave  $\text{CpRu(L)(L')SCOCO}_2\text{R}$  and with sulfonyl chlorides gave  $\text{CpRu(L)(L')SSO}_2\text{R}$  [4].

Cyclopentadienyl ruthenium thiocarboxylate dinuclear complexes of the general formula  $(\mu\text{-Z})[\text{CpRu(L)(L')SCO}]_2$  were prepared directly by reacting the cyclopentadienyl ruthenium hydrosulfido complexes  $\text{CpRu(L)(L')SH}$  with diacid chlorides (1,4- $\text{ClCOC}_6\text{H}_4\text{COCl}$ , 1,3- $\text{ClCOC}_6\text{H}_4\text{COCl}$  and  $\text{ClCO(CH}_2)_4\text{COCl}$ ) in THF at room temperature [5].

Complexes containing heterocyclic thiocarboxylates of the general formula  $\text{CpRu(L)(L')SCO-het}$  ( $\text{het} = 2\text{-C}_4\text{H}_4\text{O}$ ,  $2\text{-C}_4\text{H}_4\text{S}$ ,  $1\text{-C}_4\text{H}_8\text{N}$ ) can be obtained in a similar way.

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**Ruthenium(III), Rhodium(III) and Iridium(III) Complexes Bearing  
Bidentate Imine Ligands: Synthesis, Characterization, and Catalytic  
Application in Oxidation of Some Amino Acids**

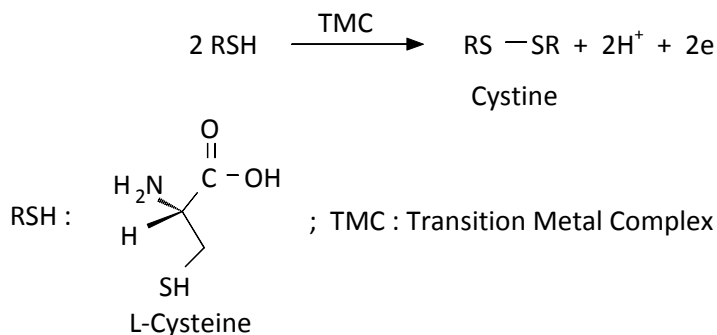
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**ABSTRACT**

Oxidation of amino acids by transition metal complexes is of great importance structurally, catalytically, and biologically. The oxidation reaction involves electron transfer reaction of the metal complex, which is an important process in coordination chemistry. The reaction has been studied by different methods, including: stopped-flow spectrophotometry, chemical analysis of products, and the use of radioactive and stable isotope tracers. [1]

In the present work, the synthesis of a new series of ruthenium(III), rhodium(III) and iridium(III) complexes of the general formula  $[M(L-L)_2Cl_2]Cl$  and  $[M(L-L)_3]Cl_3$  (L-L: N,N'-bis(1-naphthyl)-2,3-butandiimine (**BNB**), 1,10-phenanthroline (**Phen**), 2,2'-bipyridine (**bipy**)) is described. The isolated complexes were characterized by their physical properties, elemental analysis, magnetic susceptibility, infrared-, and UV/Vis- spectroscopy. The influence of metal center, geometry of the complex, auxiliary substituents, and the backbone of the ligand toward the rate of oxidation of L-cysteine (Scheme below) will be studied spectrophotometrically.

**Keywords:** Ruthenium(III), Rhodium(III), Iridium(III), diimine ligands, catalysis, oxidation, Amino acid.



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## Assessment of Multivariate Calibration and Liquid Chromatography for Quantification of Two Drugs Systems of Variable Spectral Overlap: A Comparative Study

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### ABSTRACT

The resolution power of multivariate calibration and liquid chromatography were evaluated for determination of paracetamol–caffeine (56.3% spectral overlap) and amoxicillin-clavulanic acid (93.6% spectral overlap) in their drugs formulations. Independently, the binary drugs mixtures were quantified in pure mixtures and after extraction from tablets by PLS-1 and liquid chromatography. With four latent variables, PLS-1 was able to quantify paracetamol and caffeine in the formulations with reasonable recoveries and precisions: 105.2(5.3%) for paracetamol and 94.6(4.9%) for caffeine. The analytical performance for the chromatographic method was almost similar to PLS-1, recoveries were ranged from 99.2 to 101.2 and R.S.D. values were ranged from 1.8–3.1%. For amoxicillin–clavulanic acid system, eight (for amoxicillin) and nine (for clavulanic acid) latent variables were needed to optimize PLS-1 calibration and quantify the drugs in their formulations. The performance of PLS-1 for amoxicillin-clavulanic acid resolution was relatively lower compared to paracetamol–caffeine system, the obtained values were 86.4(13.3%) and 91.6(11.6%) for amoxicillin and clavulanic acid; respectively. Using liquid chromatography, amoxicillin-clavulanic acid was accurately quantified with convincing recoveries (97.5–98.6%) and precisions (3.6–4.3%). Liquid chromatography outperformed PLS-1 for analyzing amoxicillin-clavulanic acid system and this was attributed to the high spectral overlap between drugs and presence of non-modeled excipients co-existed with the drugs.

*Keywords:* Paracetamol–Caffeine; Amoxicillin–Clavulanic Acid; Liquid Chromatography; ultivariate Calibration; Spectral Overlap; Excipients.

**Effect of Dimensions and Oxidation of Carbon Nanotubes on Preconcentration of Phenols**

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**ABSTRACT**

In this work, a solid phase extraction procedure of phenols (phenol, 2-chlorophenol, 3-chlorophenol, 4-chlorophenol, 2-nitrophenol, 4-nitrophenol and 2, 4-dinitrophenol) from aqueous medium using multiwalled carbon nanotubes (MWCNTs) was optimized. Various factors were studied, including: dimensions and oxidation of carbon nanotubes, mass of adsorbent, volume and type of eluting solvent, volume and pH of solution. The optimum procedure was applied on real water samples. The analytical performance of the method was studied and satisfactory results were achieved. Various phenols gave various behaviors. It was found that MWCNTs of various dimensions have different preconcentration abilities towards various phenols.

## Simple Microwave and Ultrasound Assisted Digestion Procedure of Phosphate Rock

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### ABSTRACT

In this work, a simple-fast digestion procedure of phosphate rock was optimized. The procedure is based mainly on the use of microwave and ultrasound. Various factors were optimized, including: type and concentration of leaching solvent, microwave power, the use of ultrasound, and number of repeating the digestion cycles. It was found that the use of ultrasound has significantly facilitated the digestion procedure, accompanied with the use of microwaves. The digested phosphate rock was analyzed for mercury determination using unspiked and spiked phosphate rock samples. The analytical performance of the method was studied and satisfactory results were achieved.

**Effect of Derivatization of Phenols on Their Selective Solid Phase Extraction (SPE) from Water using Molecularly Imprinted Polymers (MIP)**

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**ABSTRACT**

In this work a polymer imprinted with 2-chlorophenol was prepared. This molecularly imprinted polymer (MIP) was used for selective solid phase extraction (SPE) of 2-chlorophenol from aqueous medium in the presence of other phenolic compounds. A SPE method was then optimized for preconcentration of phenols from real water samples. The effect of derivatization of 2-chlorophenol on the SPE selectivity of the polymer was also investigated by preparing MIPs imprinted with 4-amino-antipyrine derivatized 2-chlorophenol. Another SPE was optimized for preconcentration of phenols from real water samples. The two SPE methods were compared to see the effect of derivatization of 2-chlorophenol on the MIP selectivity.



## Dynamics of Viologen-Cucurbituril Complexes in Aqueous Solution

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### ABSTRACT

In the present work molecular dynamics (MD) simulations have been used to study the dynamics of the inclusion complexes of methyl viologen with cucurbit[*n*]uril, CB<sub>*n*</sub>, (where *n* = 6, 7 and 8) in aqueous solution. The obtained MD trajectories were analyzed and post processed using Molecular mechanics-Poisson Boltzmann surface area (MM-PBSA) method to shine some light on the guest-host intermolecular forces that play a significant role in formation of the CB inclusion complexes. Methyl viologen exhibits partial inclusion into CB6 cavity while deep inclusion was observed for the larger macrocyclic hosts with the two cationic groups interacting with the carbonyl portals. The extracted snapshots reveal increase in the macrocycle distortion of CB6 and CB7 upon inclusion of the guest molecule. MM-PBSA calculations indicate that CB7 forms the most stable complex with methyl viologen. The guest-host electrostatic interactions are the dominant contribution to the complex stability. Furthermore, van der Waals interactions add significantly to the complex binding free energy. Potential of mean force (PMF) for the guest-host distance was obtained by umbrella sampling. No energy barriers were obtained for the guest movement inside the host cavity except in the case of CB6.

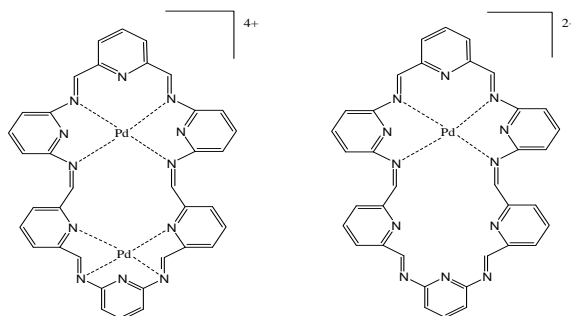
## Synthesis and Characterization of New [3+3] Macrocyclic Complexes

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\* *Mutah University, Al-Karak.*

### ABSTRACT

The [3+3] condensation reaction of 2,6-diformylpyridine with (2,6-diaminopyridine in acetonitrile in the presence of palladium salts ( $\text{Pd}^{+2}$ ,  $\text{Pd}^{+4}$ ) as templating agent to give new Schiff bases macrocyclic complexes. The formula obtained for the complexes are:  $\text{Pd}_2\text{C}_{36}\text{H}_{24}\text{N}_{12}(\text{BF}_4)_4 \cdot 8\text{H}_2\text{O}$ ,  $\text{PtC}_{36}\text{H}_{24}\text{N}_{12}\text{Br}_2$ ,

The isolated compounds were characterized based on their melting points, elemental analyses, conductivity measurements, nuclear magnetic resonance, FTIR and electronic absorption spectra.



**Chemical Composition of Essential Oils from Aerial Parts of *Sisymbrium irio*. From Jordan.**

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**ABSTRACT**

The volatile compounds obtained from *Sisymbrium irio* growing in Jordan has been analyzed by GC-MS. The major constituents are dioctyladipate (25.44 %), N-(*n*-proyl) acetamide (14.77 %), isopropyl isothiocyanate (11.55 %), isobutyl isothiocyanate (6.75 %), 3,7,11,15-tetramethyl-2-hexadecen-1-ol (6.52 %), cis-8,11,14-eicosatrienoic acid (6.30 %), heptacosane (3.89 %), palmitic acid (3.45 %), n-butyl isothiocyanate (2.85 %) and dimethoxyacetophenone (2.54 %).

**Keys words:** *Sisymbrium irio*, Cruciferae, isopropyl isothiocyanate, dioctyladipate

## Resolution of Glycopyrrolate Drug

Ala eddin Al-sarabi, Samer Ratrout, Wasim Abdellah , Ahmad Abu Mahthiyah.

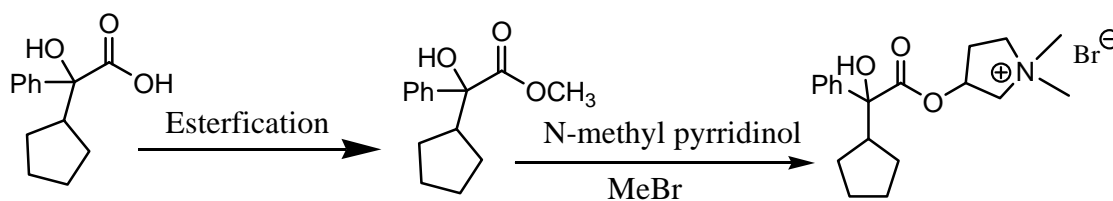
### ABSTRACT

Glycopyrrolate is a anticholinergic drug marketed under the brand name RBINUL and is one of the two diastereomeric forms 3-[(cyclopentylhydroxyphenylacetyl)]-1,1-dimethylpyrrolidinium bromide.

The four optical isomers exist as diastereometric pairs and just one pair of these two diastereoisomers is accepted according to global specification of the drug. USP show that the isomer with higher melting point is the desired drug.

This active compound has been established for long time but because it doesn't meet the requirements of the modern therapeutic rules according to difficulties in separating these pair of diastereoisomers and accordingly decreasing the limit of the un-desired isomer to the limit of unknown impurities.

The preparation of the crud drug occur by convert the manelic acid to methyl mandelate in methanol solvent using H<sub>2</sub>SO<sub>4</sub> as catalyst followed by transesterfication between the prepared ester and N-methyl pyrrolidinol in heptane using Dean-stark condition. Finally formation of dimethyl pyrrolidinium salt has been prepared using methyl bromide in ethyl methyl ketone as shown below.



## Synthesis and Characterization of New N-Oxide Schiff's Base of P-Flourobzaldehyde, as New Class of Potential Hypoxia PET Markers.

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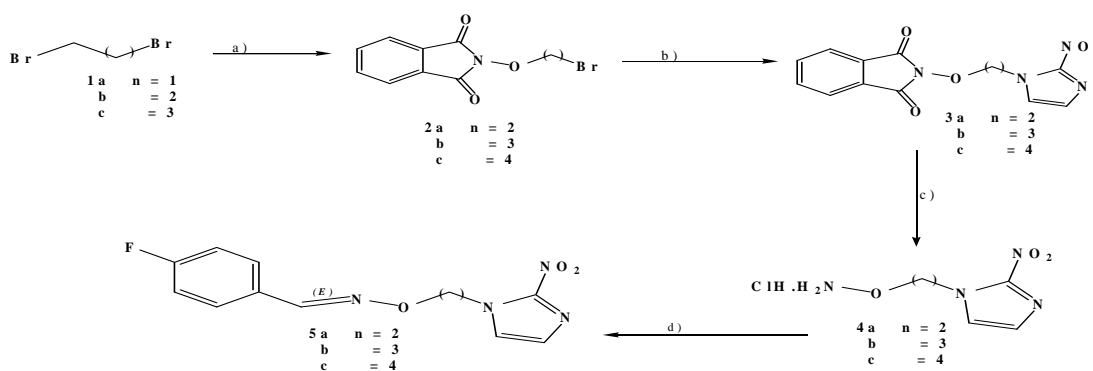
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### ABSTRACT

Hypoxia is a pathological condition in which the body as a whole or region of the body -tissue - is deprived of adequate oxygen supply, Hypoxia in which there is complete deprivation of oxygen supply is referred to as anoxia. The bioreductive metabolism of 2-nitroimidazoles provides a way of labeling hypoxic cells in vivo and a variety of isotopic labels have been proposed for the non-invasive detection of bound metabolites of these markers, the best of isotope is <sup>18</sup>F due to it is half life 110 min, which allow sufficient time to complex synthesis and biological studying, has lowest positron energy, and give sharpest imaging. In our research, we attempt to synthesis of N-Oxide Schiff's base of P-flourobzaldehyde with change long chain alkyl group attached to 2-nitroimidazolyl moiety, as a novel hypoxia PET marker. were synthesized in a four step sequence by reacting of N-hydroxy phthalimide with change long chain dibromo compound to give (2a-c), followed by Coupling with 2-nitroimidazole to give (3a-c) , followed by Hydrolysis by glacial acetic acid / hydrobromic acid or by reflux it in absolute ethanol with 98% NH<sub>2</sub>NH<sub>2</sub>.H<sub>2</sub>O to produce amine or salt of amine (4a-c), finally reacting the amine-salt- with P-flourobzaldehyde in presence of 1M of sodium hydroxide to give (5a-c).



a) N-Hydroxy phthalimide, DMF, Et<sub>3</sub>N, 17 h

b) 2-Nitroimidazole, K<sub>2</sub>CO<sub>3</sub>, DMF, 100 °C, 4 h

c) AcOH/HBr 1:1.5 (v/v), 30 min, or by NH<sub>2</sub>NH<sub>2</sub>.H<sub>2</sub>O, EtOH, reflux 4 h

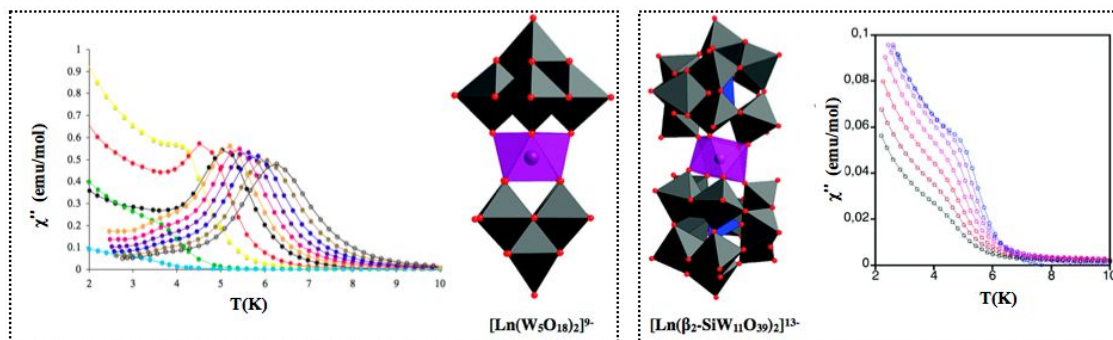
d) P-flourobzaldehyde, absolut EtOH, 1M NaOH, 24 h

## Molecular Magnetism of Polyoxometalates , A Tale of Single-Molecule Magnet

Murad AlDamen

### ABSTRACT

Due to their nanometric size, quantum effects on their magnetic properties, and extremely long magnetic relaxation times, single molecule magnets (SMMs)<sup>1</sup> have been considered as promising candidates for the development of high-density magnetic memories, molecular spintronic applications, and quantum computing devices. Recently, we showed - for the first time - that polyoxometalates (POMs) encapsulating lanthanides with local coordination geometries  $D_{4d}$  can also exhibit SMM behavior. This was demonstrated firstly in the sodium salt of the polyanion  $\text{Na}_9[\text{Er}(\text{W}_5\text{O}_{18})_2]^{9-}$ .<sup>2</sup> Also, we reported a detailed magnetostructural characterization for the whole families  $[\text{Ln}(\text{W}_5\text{O}_{18})_2]^{9-}$ ,  $\text{Ln}^{\text{III}}=(\text{Tb}, \text{Dy}, \text{Ho}, \text{and Er})$  and  $[\text{Ln}(\beta\text{-SiW}_{11}\text{O}_{39})_2]^{13-}$ ,  $\text{Ln}^{\text{III}}=(\text{Tb}, \text{Dy}, \text{Ho}, \text{and Er}, \text{Tm}, \text{and Yb})$ .<sup>3</sup>



<sup>1</sup> (a) Aromi, G.; Brechin, E.K., **Struct. Bonding** 2006, 122, 1–67 (b) Gatteschi, D.; Sessoli, R. **Angew. Chem., Int. Ed.**, 2003, 42, 268–297.

<sup>2</sup> AlDamen, M.A. et al., **J. Am. Chem. Soc.**, 2008, 130, 8874–8875.

<sup>3</sup> AlDamen, M.A. et al., **Inorg. Chem.**, 2009, 48(8), 3467–3479.

## A Thermodynamic Study between Viologens and Macrocycle Molecules

D-Marji, S-Mizyed and M-Shehab

### ABSTRACT

Intermolecular interactions between some viologens and macrocyclic molecules ( I – III ) will be investigated in ethanol solution. The formation constants of the CT complexes between viologens such as methyl viologen and benzyl viologen... with macromolecules ( I – III ) will be determined at different temperatures using UV-Vis spectroscopy.

Enthalpy and Entropy changes of complexes were determined using Vant Hoff equations.

Complexes were found to have 2:1 stoichiometry as obtained by Job plots and mole ratio methods.

Formation constant values for these complexes found that the complex between ( II ) and benzyl viologen has the largest  $k_{2:1}$  value.

Generally the complexation with benzyl viologen as acceptor gives  $k_{2:1}$  value larger than with methyl viologen for the same crown ether.

The  $k_{2:1}$  value for our complexes is order from the largest to the smallest, ( II ) with BV, ( III ) with MV, ( II ) with MV, ( I ) with BV, ( III )with BV and ( I ) with MV.

The thermodynamics parameter  $\Delta H^\circ$ ,  $\Delta S^\circ$  and  $\Delta G^\circ$  were calculated for these complexes.  $\Delta H^\circ$  values were all positive which means that complexes formation is enthalpy disfavored.  $\Delta S^\circ$  values were also positive which means that the complex formation is entropy favored.

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