First Tunisian Chemical Society Conference on Coordination Chemistry

JCC 2015

Organized by

Société Chimique de Tunisie
Tunisian Chemical Society

ROYAL SOCIETY OF **CHEMISTRY**
TUNISIA LOCAL SECTION

May 8-10, 2015

Sol Azur Beach Hotel, Hammamet, Tunisia

Lectures and Communications Abstracts
List of Participants

Tunisian Chemical Society - Short Program of the JCC 2015

Friday 8 May 2015	
14.00	**Welcoming participants, distribution of documents and check in**
15.00	**Plenary Lecture 1** **Pr. Hubert SCHMIDBAUR** *Technische Universität München, Germany*
15.45	**Oral Communications - First Session - OC 01 : OC 04**
16.45	**Coffee break + Poster Session 1 (P 1 - P 55) Alphabetical Order**
17.30	**Plenary Lecture 2** **Pr. Jean-François NIERENGARTEN** *Ecole Européenne de Chimie, Polymères et Matériaux, Strasbourg, France*
18.15	**Oral Communications - Second Session - OC 05 : OC 07**
19.00	**Welcome**
19.30	***Dinner***
Saturday 9 May 2015	
08.30	**Opening Ceremony**
09.00	**Plenary Lecture 3** **Pr. J Derek WOOLLINS** *University of St Andrews, St Andrews, United Kingdom*
09.45	**Oral Communications - Third Session - OC 08: OC 10**
10.30	***Coffee break***
11.00	**Plenary Lecture 4** **Pr. Dominique LUNEAU** *University of Claude Bernard, Lyon 1, France*
11.40	**Invited Lecture 1** **Dr. Med Abderrahmane SANHOURY** *University of Tunis El Manar, Faculty of Sciences of Tunis, Tunis, Tunisia*
12.15	**Oral Communications - Fourth Session - OC 11 : OC 13**
13.00	***Lunch***
14.30	**Plenary Lecture 5** **Pr. Klaus R KOCH** *Stellenbosch University, Stellenbosch, South Africa*
15.10	**Invited Lecture 2** **Dr. Noureddine RAOUAFI** *University of Tunis El Manar, Faculty of Sciences of Tunis, Tunis, Tunisia*
15.45	**Oral Communications - Fifth Session - OC 14 : OC 16**
16.30	**Coffee break + Poster Session 2 (P 56 - P 111) Alphabetical Order**
17.15	**Plenary Lecture 6** **Pr. Ouassini BENALI BAITICH** *University of Sciences and Technology Houari Boumediene, Algiers, Algeria*
18.00	**Oral Communications - Sixth Session - OC 17 : OC 20**
20.30	***Gala Dinner***
Sunday 10 May 2015	
08.30	**Plenary Lecture 7** **Pr. Arben MERKOÇI** *ICREA & Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain*
09.10	**Invited Lecture 3** **Dr. Salima BOUGHDIRI** *University of Tunis El Manar, Faculty of Sciences of Tunis, Tunis, Tunisia*
09.45	**Oral Communications - Seventh Session - OC 21 : OC 23**
10.30	***Coffee break***
11.00	**Plenary Lecture 8** **Pr. Azzedine BOUSSEKSOU** *Laboratoire de Chimie de Coordination, UPR, Toulouse, France*
11.45	**Oral Communications - Eighth Session - OC 24 : OC 26**
12.30	**Closing Remarks, Awards Distribution and JCC 2017 Announcing**
13.00	***Lunch and leaving the hotel***

FOREWORD

On behalf of the organizing committee, I am pleased to welcome you in Hammamet for this major event held under the auspices of the Tunisian Chemical Society (Societé Chimique de Tunisie, SCT) and the Royal Society of Chemistry.

This is the SCT Coordination Chemistry Conference First edition, which will see the participation of more than 10 African and European countries in addition to the Tunisian universities and with the participation of more than 170 participants from various countries. They will discuss themes involving the science of coordination chemistry, carefully distributed over 7 plenary lectures; 3 invited speakers, 26 oral communications and 110 posters presentations.

Many thanks for all participants and for all invited speakers who firmly accepted to contribute lectures at the event in order to make it a very successful meeting.

Happy First Conference on Coordination Chemistry to all.

Adel MEGRICHE

President of the
Tunisian Chemical Society

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Being on time is the main factor for conference's success

Friday 8 May 2015			
14.00	***Welcoming participants, distribution of documents and check in***		
15.00	**Plenary Lecture 1** **Pr. Hubert SCHMIDBAUR** *Technische Universität München, Germany* **The Silent Role of Metallophilic Bonding in the Chemistry of Gold, Silver and Mercury**		*Chairperson:* Mr Med Taieb Ben Dhia
Oral Communications - First Session - *Chairperson* : Mrs Ikram Chéhidi			
	Com.	*communicating*	
15.45	**OC-01**	**Susan Oruma Uchechukwu** *University of Nigeria - Nsukka, Enugu State, Nigeria*	
16.00	**OC-02**	**Ines Chniti** *FST - Tunis*	
16.15	**OC-03**	**Sana Dridi** *FSM - Monastir*	
16.30	**OC-04**	**Marwa Belkhiria** *FSM - Monastir*	
16.45	**C o f f e e b r e a k + Poster Session 1 (P 1 - P 55) Alphabetical Order**		
17.30	**Plenary Lecture 2** **Pr. Jean-François NIERENGARTEN** *EECPM, Strasbourg, France* **Macrocyclic Ligands for the Preparation of Luminescent Copper(I) Complexes**		*Chairperson:* Mr Adel Megriche
Oral Communications - Second Session - *Chairperson* : Mrs Taicir Ben Ayed			
	Com.	*communicating*	
18.15	**OC-05**	**Zayed Baccari** *FST - Tunis*	
18.30	**OC-06**	**Sarra Darghouthi** *University of Tunis El Manar - Tunis*	
18.45	**OC-07**	**Asanda Vincent Busa** *University of the Western Cape - Bellville, South Africa*	
19.00	***W e l c o m e***		
19.30	***D i n n e r***		

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Saturday 9 May 2015 (morning)			
08.30	**O p e n i n g C e r e m o n y**		
09.00	**Plenary Lecture 3** **Pr. J Derek WOOLLINS** *University of St Andrews, St Andrews, United Kingdom* **Coordination Chemistry with Group 16 Ligands**		*Chairperson:* Mr Med Abderrahmane Sanhoury
Oral Communications - Third Session - *Chairperson* : Mr Farhat Rezgui			
	Com.	*communicating*	
09.45	**OC-08**	**Leila Bahri** *FST - Tunis*	
10.00	**OC-09**	**Olfa Naouali** *FSB - Bizerte*	
10.15	**OC-10**	**Hamida Maouati** *FST - Tunis*	
10.30	***C o f f e e b r e a k***		
11.00	**Plenary Lecture 4** **Pr. Dominique LUNEAU** *University of Claude Bernard, Lyon 1, France* **Coordination Chemistry at the Quest of the Molecule-Based Magnets**		*Chairpersons:* Mrs Rym Abidi & Mr Med Rachid Khaddar
11.40	**Invited Lecture 1** **Dr. Med Abderrahmane SANHOURY** *University of Tunis El Manar, Faculty of Sciences of Tunis, Tunis, Tunisia* **Development of Phosphoramidates as New Ligands for Drug Design**		
Oral Communications - Fourth Session - *Chairperson* : Mr Faouzi Sediri			
	Com.	*communicating*	
12.15	**OC-11**	**Fatma Hmida** *FSM - Monastir*	
12.30	**OC-12**	**Firas Aboumessaad** *CNRSM - Borj Cédria*	
12.45	**OC-13**	**Olfa Ouled Ltaief** *ENIS - Sfax*	
13.00	***L u n c h***		

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Saturday 9 May 2015 (afternoon)			
14.30	**Plenary Lecture 5** **Pr. Klaus R KOCH** *Stellenbosch University, Stellenbosch, South Africa* **What's in the ^{195}Pt and ^{103}Rh NMR Chemical Shift of deceptively 'simple' complexes of such precious metals?**		*Chairpersons:* Mr Habib Batis & Mr Béchir Chaouachi
15.10	**Invited Lecture 2** **Dr. Noureddine RAOUAFI** *University of Tunis El Manar, Faculty of Sciences of Tunis, Tunis, Tunisia* **New Platforms Based on Ferrocene-Functionalized Gold Nanoparticles for Assessing Host-Guest Recognition in Biosensing Devices**		
Oral Communications - Fifth Session - *Chairperson*: Mr Lotfi Efrit			
	Com.	*communicating*	
15.45	**OC-14**	**Radhia Msaadi** *FSG - Gabès*	
16.00	**OC-15**	**Oumeyma Ben Ahmed** *FST - Tunis*	
16.15	**OC-16**	**Rania Omrani** *FST - Tunis*	
16.30	**C o f f e e b r e a k + Poster Session 2 (P 56 - P 111) Alphabetical Order**		
17.15	**Plenary Lecture 6** **Pr. Ouassini BENALI BAITICH** *University of Sciences and Technology Houari Boumediene, Algiers, Algeria* **Coordination Chemistry and Medicine**		*Chairperson:* Mrs Salima Boughdiri
Oral Communications - Sixth Session - *Chairperson* : Mr Med Rezaigui			
	Com.	*communicating*	
18.00	**OC-17**	**Brahim Ould Elemine** *FST - Nouakchott, Mauritania*	
18.15	**OC-18**	**Hallouma Bilel** *ISSTE - Borj Cedria*	
18.30	**OC-19**	**Samuel Tetteh** *University of Cape Coast, Ghana*	
18.45	**OC-20**	**Amira Amouri** *FSS - Sfax*	
20.30	***G a l a D i n n e r***		

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Sunday 10 May 2015			
08.30	**Plenary Lecture 7** **Pr. Arben MERKOÇI** *ICREA & Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain* **Nanomaterials and Plastic/Paper-Based Sensors for Diagnostics Applications**		*Chairpersons:* Mr Noureddine Raouafi & Mr Nizar Belakhal
09.10	**Invited Lecture 3** **Dr. Salima BOUGHDIRI** *University of Tunis El Manar, Faculty of Sciences of Tunis, Tunis, Tunisia* **The contribution of theoretical chemistry to the interpretation of metal-ligand coordination**		
Oral Communications - Seventh Session - *Chairperson:* Mr Halim Hammi			
	Com.	*communicating*	
09.45	**OC-21**	**Haifa Khemir** *FST - Tunis*	
10.00	**OC-22**	**Zied Gouid** *FST - Tunis*	
10.15	**OC-23**	**Salah Belaidi** *University of Biskra - Algeria*	
10.30	***Coffee break***		
11.00	**Plenary Lecture 8** **Pr. Azzedine BOUSSEKSOU** *Laboratoire de Chimie de Coordination, UPR, Toulouse, France* **Molecular Spin Crossover Phenomenon at the nanoscale**		*Chairperson:* Mrs Thouraya Barhoumi -Slimi
Oral Communications - Eighth Session - *Chairperson:* Mr Hatem Ben Romdhane			
	Com.	*communicating*	
11.45	**OC-24**	**Aida Benchaabane** *FST - Tunis*	
12.00	**OC-25**	**Melek HAJJI** *FSM - Monastir*	
12.15	**OC-26**	**Mama Désiré Bikele** *University of Douala - Cameroon*	
12.30	**Closing Remarks, Awards Distribution and JCC 2017 Announcing**		
13.00	***Lunch and leaving the hotel***		

Speakers' Abstracts

The Silent Role of Metallophilic Bonding in the Chemistry of Gold, Silver and Mercury

Hubert SCHMIDBAUR

Department Chemie, Technische Universität München, 85747 Garching, Germany

Aurophilic, argentophilic and mercurophilic interactions have recently been the subject of a large number of studies in the coordination chemistry of the metals concerned.[1] Surprisingly, the contributions are particularly obvious in homo- and hetero-metallic complexes of Au(I) and Ag(I) even though attractions M^+--M^+ are counterintuitive considering their d^{10} closed-shell electronic comfiguration and the Coulomb repulsion expected between cations. However, although the coordination chemistry of gold and silver shows the common parallels of congeners in the coinage metal group, there are also staggering differences, some of which are clearly related to different qualities in the intra- and intermolecular metal-metal interactions. This has become more and more evident as the number of precisely investigated pairs of examples has increased very rapidly. A comparison of the situation in the coordination chemistry of Au(I) and Hg(II) reveals a very different performance of the two cations with a strongly reduced metallophilic affinity for the latter. Examples selected from recently presented prototypes illustrate on the one hand the impressive impact that metallophilicity may have on specific compositions and structures, but show on the other hand the limited significance especially for Hg(II). Relativistic effects are known to be most relevant in this context.

[1] H. Schmidbaur, A. Schier, *Chem. Soc. Rev.* **2012**, *41*(1) 370-412; *Angew. Chem. Int. Ed*. **2015**, *53*, 746-784. *Organometallics* **2015.** DOI 10.1021/om501125c.

Macrocyclic Ligands for the Preparation of Luminescent Copper(I) Complexes

Jean-François NIERENGARTEN

Laboratoire de Chimie des Matériaux Moléculaires, Université de Strasbourg et CNRS (UMR 7509), Ecole Européenne de Chimie, Polymères et Matériaux, 25 rue Becquerel, 67087 Strasbourg (France). E-mail : nierengarten@unistra.fr

The increasing market demand for low cost flat-panel displays and efficient lighting sources is a strong driving force for intensive research on light-emitting devices. Fluorescent semi-conducting polymers have been widely used for such applications. However, the internal quantum efficiency of the resulting devices is limited to 25% by the non-emissive triplet excitons produced in OLEDs based on singlet emitters. To overcome this problem, devices employing triplet emitters have been developed in the past few years. Such OLEDs using phosphorescent heavy metal complexes can, in principle, reach a quantitative internal quantum efficiency as both singlet and triplet excitons participate to the emission owing to intersystem crossing of the singlet excited states to the triplet states. To date, the main part of the electrophosphorescent materials used for OLED applications are complexes of noble metal ions, in particular Ir(III) coordination compounds. There are however several drawbacks in the use of iridium complexes as emitters for OLEDs. One is the high price of iridium (it is the least abundant chemical elements in the earth's crust). The other is related to environmental concerns. Existing alternatives, such as Ru(II) and Os(II), have the same inherent limitations. In recent years, an attractive alternative has emerged in the form of Cu(I) coordination compounds. Importantly, copper is less toxic, less expensive, and environmentally friendly when compared to ruthenium or iridium. As part of this research, we became interested in electrophosphorescentheterolepticCu(I) complexes containing 1,10-phenanthroline (NN) and bis-phosphine (PP) ligands.[1] Whereas such complexes are stable in the solid state, equilibrium between the homoleptic and the heteroleptic complexes is often observed in solution. This major limitation for the preparation of $[Cu(NN)(PP)]^+$ derivatives results from the exceptionally high thermodynamic stability of the corresponding homoleptic $[Cu(NN)_2]^+$ and $[Cu(PP)_2]^+$ complexes. In order to prevent the formation of a stable homoleptic complex from the NN ligand, we have recently incorporated the 2,9-disubstituted-1,10-phenanthroline subunit in a macrocyclic structure. The preparation of the heterolepticCu(I) complexes from various PP ligands and macrocyclicphenanthroline derivatives provided stable Cu(I)-complexed pseudo-rotaxanes.[2] Comparison with analogous Cu(I) complexes prepared from acyclic phenanthroline derivatives clearly revealed a strong macrocyclic effect allowing the preparation of stable heteroleptic Cu(I) complexes whatever the PP ligand. Importantly, this is the case even when the formation of the corresponding acyclic derivative is not favorable. This recent result represents a major breakthrough for the synthesis of stable luminescent $[Cu(NN)(PP)]^+$ derivatives.

1) A. Kaeser, M. Mohankumar, J. Mohanraj, F. Monti, M. Holler, J.-J. Cid, O. Moudam, I. Nierengarten, L. Karmazin-Brelot, C. Duhayon, B. Delavaux-Nicot, N. Armaroli, J.-F. Nierengarten, *Inorg. Chem*. **2013**, *52*, 12140-12151.

2) M. Mohankumar, M. Holler, J.-F. Nierengarten, J.-P. Sauvage, *Chem. Eur. J*. **2012**, *18*, 12192-12195. M. Mohankumar, F. Monti, M. Holler, F. Niess, B. Delavaux-Nicot, N. Armaroli, J.-P. Sauvage, J.-F. Nierengarten, *Chem. Eur. J.***2014**, *20*, 12083-12090.

Coordination Chemistry with Group 16 Ligands

J Derek Woollins

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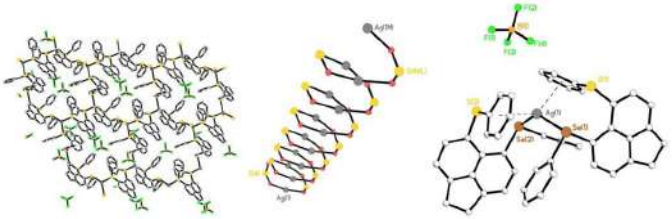
Coordination chemistry is an integral feature of inorganic and bioinorganic chemistry, with many applications in polymer design and materials science. In recent times, the metal-ligand interaction has emerged as an important tool for the manufacture of supramolecular metal complexes and is prominent in the design of organic solids and metal-organic frameworks (MOFs). Crystal engineering utilises the metal-ligand coordination bond to construct coordination networks, generally through the self-assembly of tuneable building blocks. Bridging organic ligands acting as rigid supports are linked in an ordered lattice, building extended and often multidimensional networks with central metal ions. Self-assembly, which dictates the structural motif of the final complex is controlled by experimental conditions. Factors such as the central metal ion oxidation state, the coordination geometry, the metal-to-ligand ratio, the nature and spacer length of the bridging ligand, the presence of solvents and the type of counter-anions, all play a significant role.
This lecture will examine the utility of inorganic sulfur and selnium ligands as well as peri substituted chalcogen-donor ligands $[NaphthE_2]^{2-}$ and Acenap[EPh][E`Ph] (Acenap = acenaphthene-5,6-diyl; E/E` = S, Se, Te) to form simple coordination complexes as well multimetallic systems and supramolecular arrays.



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- L. M. Diamond, F. R. Knight, R. A. M. Randall, A. L. Fuller, A. M. Z. Slawin and J. D. Woollins, *Inorg.Chim Acta*, 2014, **423**, 313-319
- Platinum *bis*-phosphine complexes of 1,8-naphthosultone . L. M. Diamond, F. R. Knight, D. B. Cordes, A. L. Fuller, A. M. Z. Slawin and J. D. Woollins, *Polyhedron*, 2014, **81**, 356-363

Coordination chemistry at the quest of the molecule-based magnets

Prof. Dominique LUNEAU

Laboratoire des Multimatériaux et Interfaces (UMR 5615)
Université Claude Bernard Lyon 1
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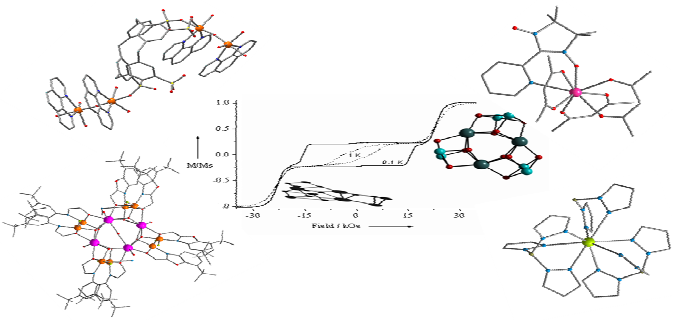
luneau@univ-lyon1.fr

During our lecture we will first introduce how coordination chemistry is intimately associated to the quest of the molecule-based magnets. Then we will illustrate our talk by some results of our own researches in the field, for which we follow different approaches to assemble *3d* and/or *4f* metal ions into magnetic complexes with various nuclearities using b-diketone [1], calixarene [2, 4], oxazole [3], scorpionate or nitronyl nitroxide free radicals [5] as ligands.



The synthesis, structures and magnetic behaviors of some of these compounds will be presented and discussed.

References:

[1] C. Aronica, G. Pilet, G. Chastanet, W. Wernsdorfer, J.-F. Jacquot, D. Luneau *Angew. Chem. Int. Ed.* **2006**, *45*, 4659-4662

[2] S. Petit, G. Pilet, D. Luneau, L. F. Chibotaru, L. Ungur *Dalton Trans.*, ***2007***, *4582-4588.*

[3] O. Iasco, G. Novitchi, E. Jeanneau, W. Wernsdorfer, D. Luneau Inorg. Chem. **2011**, 50, 7373–7375

[4] N. Mattoussi, G. Pilet, G. Novitchi, F. Meganem, D. Luneau *Eur. J. Inorg. Chem.* **2013**, 2652–2656

[5] A. Lannes, M. Intissar, Y. Suffren, C. Reber, D. Luneau *Inorg. Chem.* ***2014****, 53, 9548−9560*

DEVELOPMENT OF NEW PHOSPHORAMIDATES AS LIGANDS FOR DRUG DESIGN

Med Abderrahmane SANHOURY

Laboratory of Structural Organic Chemistry: Synthesis and Physicochemical Studies, Coordination Chemistry Group, Department of Chemistry, Faculty of Sciences of Tunis, Campus Universitaire, 2092, El Manar I, Tunis, Tunisia
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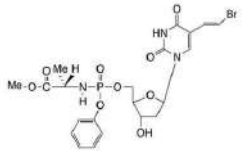
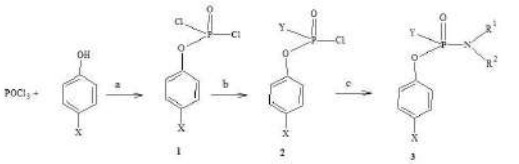
The development of phosphoramidate prodrug strategies have attracted much interest in anticancer and antiviral therapy and drugs containing these molecules are increasingly being explored in other therapeutic areas [1,2]. Recently, the phosphoramidate ProTides were shown to be potential prodrugs, especially as antiviral agents [3,4]. For instance, McGuigan *et al*. have tuned the lead anti-cancer agent thymectacin in the ester and amino acid regions and revealed a substantial enhancement in *in vitro* potency versus colon and prostate cancer cell lines [5]. In this presentation we will give an overview of the different approaches and phosphoramidate technologies through phosphorylation of various anti-HIV agents. Specifically in this context and as a continuation of our interest in organophosphorus chemistry [6,7], we will also dscribe our own synthesis of new aryloxy phosphoramidates **3** in which various amino acid ester groups were incorporated as preliminary mimics of phosphoramidate prodrugs. These products were fully characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR, IR and HRMS analyses. The ^{31}P and ^{1}H NMR data clearly reveal for some of these derivatives the presence of two phosphoramidate diastereoisomers, as expected, in roughly equi-molar proportions. In addition, the effect of the nature and sequence of the addition of different substituents in particular that of the amino acid on the reaction yield will be discussed and compared.



Thymectacin (anti-HIV agent)



X = H, CH_3 or NO_2; Y = OR or NR_2; R^1 = H, CH_3, or $CH_2CH(CH_3)_2$; R^2 = Me or Et.

Keywords: Organophosphorus compounds, aryl phosphoramidates, ProTides, amino acids, NMR spectroscopy.

References

[1] B. Hong, F.M. Raushel *Biochemistry*, **1999**, 38, 1159.
[2] J.A. Madden, P.B. Hoyer, P.J. Devine, A.F. Keating *Toxicol. Appl. Pharm.*, **2014**, 277, 1.
[3] C. McGuigan, O. M. Wedgwood, E. De Clercq, J. Balzarini *Bioorg. Med. Chem. Lett.* **1996**, 6, 2359.
[4] T. K. Venkatachalam, S. Qazi, F. M. Uckun *Bioorg. Med. Chem.* **2006**, 14, 5161.
[5] C. McGuigan, J.-C. Thiery, F. Daverio, W. G. Jiang, G. Davies, M. Mason *Bioorg. Med. Chem.* **2005**, 13, 3219.
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What's in the ^{195}Pt and ^{103}Rh NMR Chemical Shift of deceptively 'simple' complexes of such precious metals?

From unique *intrinsic isotope effects* as "spectroscopic-fingerprints" for unambiguous chemical speciation, to photo-induced geometric isomerism in solution.

Klaus R Koch

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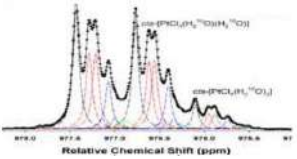
Our research over the last decade focused on applications of high-resolution multinuclear magnetic resonance spectroscopy to fundamental and applied aspects of the deceptively simple coordination chemistry of the platinum group metals, in the context of their separation and refining chemistry. ^{195}Pt and ^{103}Rh nuclear shielding, as reflected in the chemical shifts of Pt^{IV} and Rh^{III} complexes, is extremely sensitive to several factors *inter alia* temperature, solvent composition, and $^{35}/^{37}$Cl *intrinsic isotope effects* resulting from coordinated halide and partially 18O enriched *aqua* or hydroxido ligands. To date, the potential of isotope effects as a structural tool has not widely been studied.

This talk will highlight an overview of two aspects of our recent work. The remarkably well resolved *intrinsic* ^{35}Cl/^{37}Cl (and ^{16}O/^{18}O) *isotope effects* visible the ^{195}Pt and ^{103}Rh chemical shifts of complexes constitute unique "isotope-mass-resolved" ^{195}Pt and ^{103}Rh NMR fingerprints,[1-3] suitable for unambiguous chemical speciation of all the $[PtCl_{6-n}(H_2O)_n]^{(4-2+n)-}$ (n = 0-5) complexes in acid solutions, as well as their corresponding hydroxido-complexes $[PtCl_{6-m}(OH)m]^-$ (m = 0-5) in alkaline solutions. Moreover, some remarkable differences between these two series of related complexes is observed. These isotope effects are ascribed to the extreme sensitivity of the ^{195}Pt NMR shielding to tiny differences in the M–^{35}Cl/^{37}Cl and M–^{16}O/^{18}O bond displacements at the 10^{-5} Å level, as recently confirmed by DFT calculations4.



An expanded ^{195}Pt NMR signal of *cis*-$[Pt^{35/37}Cl_4(H_2{}^{16/18}O)_2]$ resolved by intrinsic isotope effects

Secondly, I will illustrate some aspects of our work concerning the rich coordination chemistry of the long-known simple N-acyl-N',N'-dialkylthioureas (HL-*S,O*) of Pt^{II}, Pd^{II} and Rh^{III} complexes. Recent studies concerning the photo-induced, reversible *cis/trans* isomerization of $[M(L^n\text{-}S,O)_2]$ type complexes (M=Pt or Pd) has been established as the key to preparing the *trans*isomers, long thought not preparable by conventional means. This phenomenon can *inter alia* be conveniently studied using *in situ* laser-irradiation of complexes directly monitored by ^{1}H and ^{195}Pt NMR spectroscopy. This technique yields some interesting surprises.

$$cis\text{-}[M(L^n\text{-}S,O)_2] \underset{\triangle}{\overset{h\nu}{\rightleftharpoons}} trans\text{-}[M(L^n\text{-}S,O)_2]$$

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New platforms based on ferrocene-functionalized gold nanoparticles for assessing host-guest recognition in biosensing devices

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Historically gold nanoparticles are the first to be prepared in a controlled synthesis in 1857. Their stability, usability and ease of functionalization especially with sulfur-containing compounds inspired extensive investigations to unveil their physicochemical properties and to develop applications. In this talk, I will review the works that we achieved in the functionalization of gold nanoparticles by different ferrocenyl derivatives to develop new biosensing platforms to follow host-guest recognition in a series of biosensors. The electrochemical output signal can be tuned depending on used monoclonal or polyclonal antibodies. Similarly, the ferrocene derivative tethered to gold nanoclusters allowed developing a sensitive platform for immuno- and enzymatic sensing. Detection of Ochratoxin A has also been made using an aptamer-modified gold nanoparticles functionalized by ferrocene. The electron-transfer rate constants of several ferrocenyl esters having different chain lengths have been determined and exploited to develop useful immunosensor for the ApoE detection, which is a biomarker of Alzheimer's disease. Ferrocene bipodal derivative was also used to build a new type of ferrocene potential-shifting biosensors.

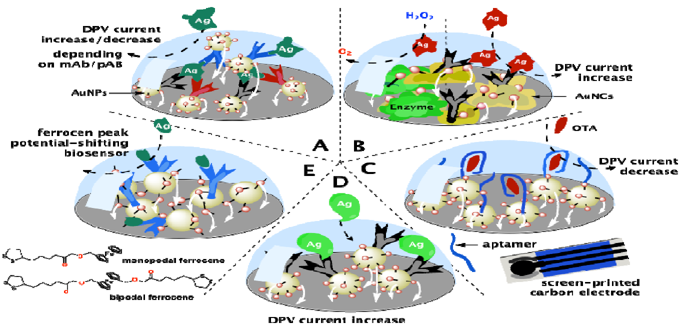

Figure. Different strategies adopted for the preparation of a series of gold nanoparticle-based biosensors ligand-based potential-shifting biosensor.

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COORDINATION CHEMISTRY AND MEDICINE

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The discovery of the antitumoral properties of the cisplatin in the 70s, and its use successfully in the treatment of certain cancers from the 80s has initiated a whole domain of research in Inorganic Chemistry. This new field born from the coordination chemistry and the biology, called Medicinal Inorganic Chemistry is dedicated to the study of the role of the metals in the biological processes as well as the study of the medical applications of their coordination compounds.

A review of the main coordination compounds having a marketing authorization and those under development is presented.

Therapeutic agents:

- Antimicrobial and antiviral: Complexes of silver(I) and mercury
- Anticancer : The square planar complexes of the platinum(II) family, the octahedral complexes of platinum(IV), complexes of other metallic elements in particular those of ruthenium.
- Antiarthritic: Complexes of gold(I) with thiolates.
- Antidiabetic agents: Complexes of vanadium(IV) and vanadium(V) with bidentate ligands.

Diagnostic agents:

- The radiopharmaceuticals: Complexes of technetium (^{99m}Tc), used as contrast agents for the medical imaging by scintigraphy.
- The agents of contrast for medical imaging by magnetic resonance (MRI): high spin complexes of gadolinium(III) and manganese(II).

Finally it is important to note the use of the chelation in the treatment of the poisoning by metals, and in Wilson and Alzheimer diseases.

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NANOMATERIALS AND PLASTIC/PAPER-BASED SENSORS FOR DIAGNOSTICS APPLICATIONS

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Development of novel diagnostic tools with interest for point of care applications represents one of the main research fields for the nanobiotechnology. Either brand new devices or improvement of existing ones are being developed thanks to the use of nanomaterials and nanotechnologies. Between the various devices biosensing systems based on electrical and electrochemical transducing schemes are overall in the focus of interest given the simplicity and cost efficiency of detection. Among the various biosensing system performance requirements the high sensitivity and selectivity of the response are crucial for applications in clinical diagnostics. The fulfilment of such requirements means the detection of low levels of clinical biomarkers in human fluids. Due to the fact that the biomarkers are present in very low concentrations the need for biosensing systems that can detect these analytes with high sensitivity and selectivity that include very low detection limits along with high reproducibility is an important challenge. To overcome the difficulties in accomplishing all these requirements the main efforts are driven toward signal amplification and noise reduction of biosensing systems by the incorporation of nanomaterials. Nanomaterials (NMs) such as carbon nanotubes, graphene, metallic nanoparticles, nanowires and quantum dots are showing to be excellent materials to be used as electrochemical transducers or labels in DNA (or genosensors) sensors beside enzymatic sensors, immunosensors, or cell sensors. The amplification of the detection of biorecognition events (ex. DNA hybridization reactions etc) are the most important objectives of the current bioanalytical chemistry. In this context integration of the catalytic properties of some biomolecules with those of nanomaterials is appearing to be a promising way to enhance the sensitivity of the bioassays. Examples related to various clinical biomarkers will be shown. The developed devices and strategies are intended to be of low cost while offering high analytical performance in screening scenarios beside other applications. Special emphasis will be given to lab-on-a-chip platforms with integrated electrochemical detection with interest for clinical applications. In addition simple paper-based platforms that operate in lateral flow formats with interest for various detections will be shown.

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THE CONTRIBUTION OF THEORETICAL CHEMISTRY TO THE INTERPRETATION OF METAL- LIGAND COORDINATION

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Nowadays, many researchers are focusing on the development of industrially practical transition metal complexes [1], because of their outstanding reactivity and their important roles in a wide range of chemical processes in catalysis and synthesis.

A huge number of complexes have been synthesized and characterized through spectroscopic techniques such as UV, IR, NMR, NγR . Generally, the assignment of signals in a spectrum provides a mixture of two or more isomers that are close in energy. This may be due to the different spin states easily accessible in some transition metal complexes. In that cases, the small gaps in energy between d-orbitals enable different combinations of occupation depending on the metal oxidation state, the nature of the ligands and their disposition in the metal coordination sphere. This is why, and despite the experimental researches, fundamental aspects of their chemistry remain not fully understood such as relative isomers stabilities, the nature of the ligand–metal interaction, spin state energetics of complexes of metallic centre with ligands …..

Thus, an understanding of these tasks is crucial for the advancement of this area of chemistry and will allow researchers to better control and manipulate the outcome of their reaction.

Quantum chemical methods today have become useful and practical tools in study of metal complexes, to explain the nature of the ligand–metal interaction in such complexes and have made qualitatively accurate predictions of their structures and their chemistry possible at a reasonable computational cost [2]., which will help synthetic chemists in their efforts toward fully characterizing such species. Some topical examples will be illustrated in my talk.

Keywords: Metal-ligand coordination, theoretical chemistry.

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Molecular Spin Crossover Phenomenon at the nanoscale

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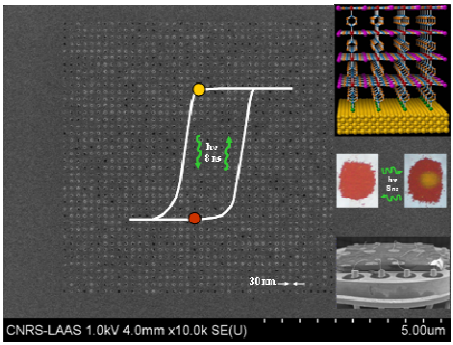
The spin crossover phenomenon in inorganic materials is one of the most spectacular examples of molecular bistability, which means that these molecules may exist in two different electronic states within a certain range of external perturbations. Most notably, the existence of a thermal hysteresis in certain complexes (in the solid state) confers a memory effect on these systems.[1-4] In our group we are particularly interested in the synthetic elaboration of nanometric thin films[5] and nano-sized patterns[6] that we obtain by electron beam lithography and in the application of an external perturbation in the hysteresis loop of spin crossover materials leading to an irreversible switching of their physical properties.[4] **recent hot results concerning the spatio-temporal spin propagation and visualisation of nucleation and growth of spin domains in spin crossover single crystals will be presented.**
Besides generating new fundamental knowledge on size-reduction effects and the dynamics of the spin crossover phenomenon, this research aims also at the development of **practical applications such as sensor, display, information storage and nanophotonic devices**.[1-12]
In this talk, I will discuss recent work in the field of molecule-based spin crossover materials with a special focus on these emerging issues, including chemical synthesis, physical properties, practical applications and theoretical aspects as well.



Combined Top - Down and Bottom - Up Apporoach for the nanoscale pattering of {Fe(Pyrazine)[Pt(CN)$_4$]}. Inserts: Schematic structure on Gold surface of {Fe(Pyrazine)[Pt(CN)$_4$]}; reversible nanosecond photo-switching in the hysteresis loop at room temperature and memory device prototype using the dielectric properties of spin crossover compounds.

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Oral Communications' List

(alphabetically authors' name)

Name	Ref
F. Aboumessaad, Y. Arfaoui, M.L. Efrit, E. Srasra, N. Besbes *CNRSM - Borj Cédria* Preparation and application of alumina, silica and acid activated clay: Synthesis and thoretical studies of 2-methyl-1,3-dioxolane	**OC12**
A. Amouri, M. T. Sougrati, N. Abdelmoula, H.Khemakhem *FSS - Sfax* Improved of multiferroic properties in (1-x)$BiFeO_3$-xBa[$Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}$]$O_3$ system	**OC20**
Z. Baccari, T. Barhoumi-Slimi, M.A.K. Sanhoury, M.T. Ben Dhia *FST - Tunis* Synthesis, characterization and coordination chemistry of new fluorinated α-aminophosphonates	**OC5**
L. Bahri, T. Barhoumi-Slimi, M.A.K. Sanhoury, M.T. Ben Dhia *FST - Tunis* New allylic phosphate tin(IV) complexes : Synthesis and multinuclear (^{1}H, ^{19}F, ^{31}P and ^{119}Sn) NMR Characterization	**OC8**
S. Belaidi *University of Biskra - Algeria* In silico study of a new series of coordination compounds derived from TTF-TCNQ	**OC23**
M. Belkhiria, A. Mechria, M. Msaddek *FSM - Monastir* Synthesis, characterization and crystal structure of new tetrachlorocobaltates(ii) of protonated beta-diimines	**OC4**
O. Ben Ahmed, M.T. Ben Dhia, T. Barhoumi-Slimi *FST - Tunis* Synthesis and characterization of cinnamaldehyde schiff base derivatives	**OC15**
A. Benchaabane, M.A. Sanhoury, M. Lejeune, F. Kouki, A. Zeinert, H. Bouchriha *FST - Tunis* Performance of bulk heterojunction photovoltaic cells based on P3OT matrix and cadmium selenide nanoparticles	**OC24**
M.D. Bikele, M. Nsangou, D. Lissouck, E. Younang *University of Douala - Cameroon* Coordination ability of 4-benzylidenamino-4, 5-dihydro- 1h-1,2,4-triazol-5-one derivatives: A density functional theory study of divalent metal cations	**OC26**

Name	Ref
H. Bilel, N. Hamdi, F. Zagrouba, C. Fischmeister, C. Bruneau *ISSTE - Borj Cedria* Catalysis and metathesis: valorization of natural products by organometallic catalysis	**OC18**
A.V. Busa, E. Nordlander, M. Onani *University of the Western Cape - Bellville, South Africa* Towards Discovery of New Organometallic Complexes: Synthesis, Characterization and Biological Activity	**OC7**
I. Chniti, M.A.K Sanhoury, D. Merlet, I. Chehidi *FST - Tunis* Synthesis, characterization and structural study of new *O-F*-alkyl thiocarbamate mercury(II) complexes	**OC2**
S. Dargouthi, S. Boughdiri, B. Tangour *University of Tunis El Manar - Tunisia* Stabilizing of the transitory species $(TIO_2)_2$ by encapsulation into carbon nanotubes	**OC6**
S. Dridi, Ali Mechria, Moncef Msaddek *FSM - Monastir* Novel cationic dinuclear methallyl palladium complexes containing N,N'-DONOR bridging ligands: Synthesis, characterization and crystal structure	**OC3**
Z. Gouid, R. Ben Said, M.A.K. Sanhoury, M.T. Ben Dhia, S. Boughdiri *FST - Tunis* Zinc(II) complexes with tributylphosphine chalcogenides: An experimental and theoretical study	**OC22**
M. Hajji, T. Guerfel *FSM - Monastir* Structural, thermal, vibrational and DFT studies of a new nonlinear optical chlorocadmate	**OC25**
F. Hmida, B. Ayed, A. Haddad *FSM - Monastir* Synthesis, structure and characterization of an inorganic-organic hybrid Dawson polyoxotungstate $(C_6H_8NO)_6[P_2W_{18}O_{62}].6H_2O$	**OC11**
H. Khemir, F. Moussa, B. Tangour *FST - Tunis* Drug vectorization by a carbon nanocone: In silico study	**OC21**
H. Maouati, M.A.K. Sanhoury, D. Merlet, I. Chehidi *FST - Tunis* Synthesis and characterization of bis(thiocarbamatophosphoramides)	**OC10**

Name	Ref
R. Msaadi, N. Hamdi, L. Baklouti *FSB - Bizerte* Cation binding properties of some coumarin derivatives	**OC9**
O. Naouali, M.A.K. Sanhoury, T. Ben Dhia, M. L. Efrit, A. Ben Akacha *FST - Tunis* Synthesis and characterization of tin tetrachloride complexes with phosphonothioamidates	**OC16**
R. Omrani, M.A.K. Sanhoury, T. Barhoumi-Slimi, M.R. Khaddar, M.T. Ben Dhia *FST - Nouakchott, Mauritany* Synthesis and NMR characterization of new tin complexes with aryl phosphoramidates bearing amino acid groups	**OC17**
B. Ould Elemine, S. Siffert, S. Fourmentin, M. Benzina *ENIS - Sfax* Performances of exchanged zeolite for the degradation of methyl orange dye via photo-Fenton process	**OC13**
O. Ouled Ltaief, D.K. Dodoo, R. Appiah-Opong, I. Tuffour *University of Cape Coast, Ghana* Palladium(II) chloride complexes with nucleobase ligands: Effective cytotoxic agents	**OC19**
S. Tetteh, E. Chinyere Nkpozi, P. Oziri Ukoha *University of Nigeria - Nsukka, Enugu State, Nigeria* Extractive determination of Zn(II) and Cd(II) in industrial samples using 1, 5-dimethyl-2-phenyl-4[(E)-2,3,4- trihydroxyphenyl)]diazenyl-1,2-dihydroxyl-3H-pyrazol-3-one, (H_3L)	**OC1**
S.O. Uchechukwu, Y. Arfaoui, M.L. Efrit, E. Srasra, N. Besbes *CNRSM - Borj Cédria* Preparation and application of alumina, silica and acid activated clay: Synthesis and thoretical studies of 2-methyl-1,3-dioxolane	**OC12**

Oral Communications' Abstracts

Program of Friday, May 8th 2015

EXTRACTIVE DETERMINATION OF Zn(II) AND Cd(II) IN INDUSTRIAL SAMPLES USING 1, 5- DIMETHYL-2-PHENYL-4[(E)-2,3,4- TRIHYDROXYPHENYL)]DIAZENYL-1,2-DIHYDROXYL-3H-PYRAZOL-3-ONE, (H_3L).

Uchechukwu Susan Oruma* Edith Chinyere Nkpozi, and Pius Oziri Ukoha

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H_3L was synthesized by coupling diazotized 4- aminoantipyrene with 1, 2, 3,-trihydroxybenzene. It coordinated as a tetradentate ligand to Zn(II) and Cd(II) to form $[Zn(H_2L)_2]$ and $[Cd(H_2L)_2]$ respectively. The ligand was characterized by ^1H and ^{13}C NMR, Infrared and UV spectroscopy whereas the complexes were characterized via UV and IR spectroscopy as well as conductivity and mole ratio determinations. Extractive determinations were based on the formation of darkbrown hydrophilic complexes of Zn(II) and Cd(II) by H_3L, which are readily extractible into chloroform. Effects of extraction variables like pH, salting –out agents, masking agents and concentration of H^+ was studied. Cd(II) was quantitatively extracted in 0.001M HCl up to 100% but masked by 0.001M of either SCN^- or tartrate up to 90% under five minutes. Extraction of Zn(II) with $H_3L/CHCl_3$ was also quantitative(96%) in 0.001M HCl within 70 min, but was masked by CN^- and SCN^- up to 79% and 67% respectively. Cd(II) was successfully separated from Zn(II) in a four cycle extraction in 0.001M HCl using $H_3L/CHCl_3$ in the presence of 1M CN^-. Recovery of Zn(II) and Cd(II) from rubber carpet following the procedure reached 90% and 85% respectively.

Keywords: 1, 5- Dimethyl-2-phenyl-4[(E)-2,3,4- trihydroxyphenyl)]diazenyl-1,2-dihydroxyl-3H-pyrazol-3-one, (H_3L), extractive determination of Zn(II) and Cd(II).

SYNTHESIS, CHARACTERIZATION AND STRUCTURAL STUDY OF NEW *O*-*F*-ALKYL THIOCARBAMATE MERCURY(II) COMPLEXES

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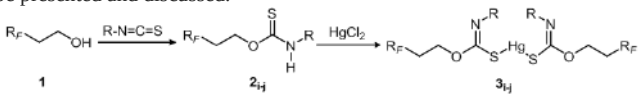
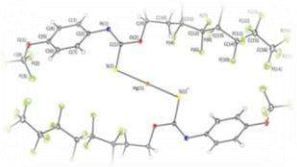
[b]*Equipe de RMN en Milieu Orienté, ICMMO – UMR 8182, Université Paris-Sud, Bâtiment 410, 91405 ORSAY Cedex.*

Thiocarbamates are known for their biological activity and are widely used as bactericides [1], pesticides [2], and herbicides [3]. Isothiocyanates proved to be excellent intermediates for the preparation of these derivatives of synthetic, biological, and pharmaceutical interest [4]. Furthermore, thiocarbamates were shown to have high affinity to heavy metal cations, forming stable metal complexes [5]. Such compounds can be used as sulfhydryl group antidotes and may have potential utility in medical or marine environmental detoxification [6]. In a previous work, we have described the synthesis of a series of *O*-**perfluoroalkyl**thiocarbamates by the reaction of aryl/alkylisothiocyanates **2(a-j)** with different *F*-alkyl alcohols [7]. In this study, these *O*-*F*-alkyl thiocarbamates were reacted with $HgCl_2$ to give new stable metal–organic compounds, bis[*O*-alkylthiocarbamato]mercury, **3(a-j)**, showing the strong affinity of thiocarbamates **2(a-j)** for mercury. All these new mercury complexes were characterized by multinuclear (^{1}H, ^{13}C, ^{19}F and ^{199}Hg) NMR, IR, HRMS and X-ray analyses. The effect of different substituents on the mercury-thiocarbamate interaction as well as the structure of the complex formed will be presented and discussed.



R= Ph, Pyridyl, NO_2-C_6H_4, Bn, Et
R_F= C_6F_{13}, C_8F_{17}



Keywords: Isothiocyanates, *O*-perfluoroalkylthiocarbamates, mercury(II) complex, ^{199}Hg NMR.

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NOVEL CATIONIC DINUCLEAR METHALLYL PALLADIUM COMPLEXES CONTAINING N,N'-DONOR BRIDGING LIGANDS: SYNTHESIS, CHARACTERIZATION AND CRYSTAL STRUCTURE

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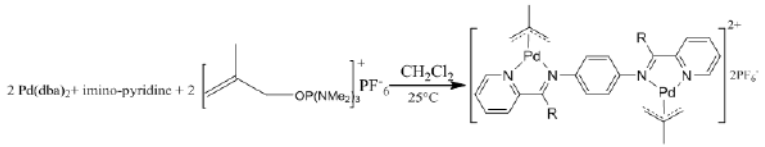
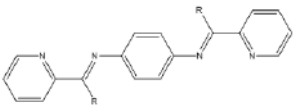
A series of dinucleating ligands, each with two bidentate imino-pyridine compartments, have been used to prepare the corresponding dinuclear complexes. Ligands p-phenylene-bis(picoline)-aldamine (L1), N,N′-Bis[1-(pyridin-2yl) ethylidene]benzene-1,4-diamine (L2) were obtained by classic condensation reactions. These ligands react with $Pd(dba)_2$ in the presence of methallyloxy tris(dimethylamino)phosphonium hexafluorophosphate $[C_4H_7OP(NMe_2)_3]^+PF_6^-$ to give the corresponding bimetallic cationic η^3-methallylpalladium complexes in high yields. The reaction was carried out in CH_2Cl_2 at room temperature. These new complexes have been characterized by IR spectroscopy and X-ray analysis.



Imino-pyridine:



L1: R = H
L2: R = Me

Key words: imino-pyridine, methallyloxytris(dimethylamino)phosphonium hexafluorophosphate

SYNTHESIS, CHARACTERIZATION AND CRYSTAL STRUCTURE OF NEW TETRACHLOROCOBALTATES(II) OF PROTONATED BETA-DIIMINES

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Tetrachlorocobaltates(II) of protonated beta-diimines with the formula $[(C_{21}H_{26}N_2)_2]$ $[CoCl_4]$ (1), $[(C_{17}H_{14}N_2)_2]$ $[CoCl_4]$ (2) and $[(C_{19}H_{20}N_2)_2]$ $[CoCl_4]$ (3) compounds were synthesized and characterized by IR and RMN spectroscopy. Crystal structure for compound (1) has been determined. It crystallize in space group C2/c with cell parameters of a = 12,345 Å, b = 28,804 Å and c = 12,38 Å; $\alpha = \gamma = 90°$,$\beta = 90,74°$.

The structure of (1) consists of a tetrachlocobaltate anion and two cations N-(-4-(2,6-dimethylphenylimino)pent-2-en-2-yl)-2,6-dimethylbenzenamine. These salts are soluble in polar solvents such as methanol.

Key words: Cobalt, β-diimine Ligands

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SYNTHESIS, CHARACTERIZATION AND COORDINATION CHEMISTRY OF NEW FLUORINATED α-AMINOPHOSPHONATES

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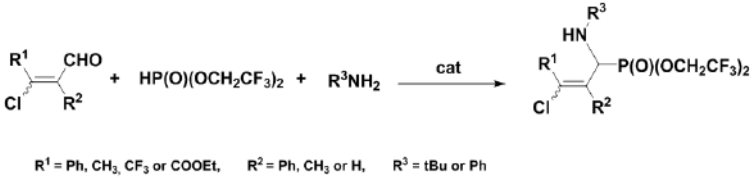
As natural amino acid analogs, α-aminophosphonates constitute an important class of compounds owing to their biological and physical properties as well as their utility as synthetic intermediates [1–3]. The synthesis of α-aminophosphonates has received increasing attentions over the last 20 years. The Kabachnik–Fields reaction [4] represents one of the most direct and efficient methods for the synthesis of α-aminophosphonate. In the present work, we describe the synthesis of new bis(trifluoroethyl) α-aminophosphonates from imines generated in situ using β-choloro-α,β-unsaturated aldehydes is reported. The starting β-chloro-α,β-unsaturated aldehydes and the aminophosphonates were prepared and fully characterized by multinuclear (^{1}H, ^{13}C, ^{19}F, ^{31}P and ^{119}Sn) NMR and IR spectroscopy. The new biologically interesting aminophosphonates were obtained through the three-component Kabachnik-Fields reaction of aldehydes, primary amines and bis(2,2,2,trifluoroethyl)phosphite using either $SnCl_4$ or TiO_2 as catalysts. The coordination chemistry of these **α**-aminophosphonates as new ligands towards tin tetrachloride will be also presented.



Keywords: β-chlorovinyl aldehydes, α-aminophosphonates Kabachnik Fields reaction NMR.

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STABILIZING OF THE TRANSITORY SPECIES $(TIO_2)_2$ BY ENCAPSULATION INTO CARBON NANOTUBES

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The aim of this paper is studying the encapsulation effect of carbon nanotubes (CNTs) on the stabilizing process of titanium dioxide molecule dimers $(TiO_2)_2$. First, a theoretical study was performed concerning the guest species that are various titanium dioxide dimers. Five structures were treated as following: i) Cis (C) or ii)Trans (T) relatively to a square shaped fragment Ti_2O_2, iii) a mixed Tetrahedral/Pyramidal (T/P) disposition while two titanium atoms are sharing three oxygen atoms, and finally not bonded dimers in iv) parallel (P) and v) orthogonal (O) positions respectively. Only the (T), (C) and (T/P) isomers may be considered as stable compounds. The structure of the T-dimer is more stable than the Cis one by only 6.5 kcal mol^{-1}. Typically, intra and extracyclic Ti-O bond lengths are 1.84Å and 1.61Å respectively. (T/P) dimer can be described as a metastable structure since its energy is higher than (T) one by 19 kcal mol^{-1}. NBO analysis highlights the participation of dative bonding between oxygen lone pair and vacant titanium 3d orbitals. (P) and (O) structures represent transitory species that transform into the more stable structure which is the T-dimer. The second and principal part of this work concerns the re-optimization of the studied structures placed inside the CNT (12,0). Only (T), (C) and (P) dimers are stabilized by encapsulation through the establishment of strong interactions with the CNT wall. The (T / P) and (O) isomers which are converted into (T) and (P) dimers respectively, are leaving the nanotube while they still interacting with its edge. These favorable results are indicating in one hand the possibly detection of (T) and (C) isomers, and in another hand that the process of polymerization of the TiO_2 molecule which is leading to nanostructured materials could be controlled by encapsulation within the CNTs

Keywords: Titanium dioxide, carbon nanotube, confinement, encapsulation, transitory species.

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Towards Discovery of New Organometallic Complexes: Synthesis, Characterization and Biological Activity

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In the 21st century with enormous advancement in modern medicine, malaria remains one of the greatest problems facing developing nations, especially in sub-Saharan Africa. The battle against malaria is intensified by the constant development of resistance to current treatments hence there is a large drive to develop novel antimalarial compounds [1, 2].

The focal point of the chemistry that has been studied in the present study can be viewed as a summation of three principal aspects, viz.: (i) Synthesis, (ii) Characterization and (iii) Biological Activity. Synthesis of designed chloroquine analogue ligands bearing a pyrazole scaffold resulted in ligands with an attractive secondary site for metal coordination in addition to the quinoline nitrogen. All ligands were synthesized from the primary amine N-(7-chloroquinolin-4-yl)ethane-1,2-diamine and different symmetric pyrazoles. The ligands were reacted with different palladium, platinum, iridium and rhodium starting materials to afford the targeted complexes. Thorough characterization of the complexes was done using various spectroscopic (UV-VIS, IR, NMR, ESI-mass) techniques in combination with elemental (C, H, N) analysis.

In general, the new pyrazole-containing derivatives show good, moderate to weak inhibitory effects relative to chloroquine and artesunate. In the chloroquine-sensitive strain (**NF54**), the results revealed that the compounds are the most active, with IC_{50} values less than 50 nM.

Keywords: Malaria, antimalarial, chloroquine.

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Program of Saturday, May 9th 2015

NEW ALLYLIC PHOSPHATE TIN(IV) COMPLEXES : SYNTHESIS AND MULTINUCLEAR (^{1}H, ^{19}F, ^{31}P and ^{119}Sn) NMR CHARACTERIZATION

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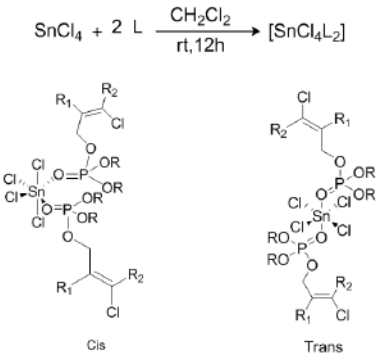
Octahedral tin(IV) complexes of the general formula SnX_4L_2 (X = halide and L is the phosphoryl ligand), continue to provide fundamental information about both the Lewis acid–base model and the reactivity of tin(IV) species [1,2]. The stereochemistry of $[SnX_4L_2]$ adducts depends considerably on the substituents directly bound to the phosphorus atom. In these compounds two isomers, with the ligand L in *cis* or *trans* mutual orientations, are possible [3,4]. In this work, we show that allylic phosphates (L) bearing different vinyl substituents readily form stable complexes with tin(IV) chloride to yield new allyl phosphate tin complexes as intensively yellow colored oils. The characterization of these complexes was carried out in solution using variable temperature multinuclear (^{1}H, ^{13}C, and ^{119}Sn) NMR spectroscopy. The comparison of the solution structures as well as the effects of the nature of allyl substituents on the donor ability of the P=O group in these new ligands will be presented and discussed.



(R = Et or Ph; R_1 = Ph or CO_2Et; R_2 = CH_3 or CF_3)

Keywords : Tin(IV) chloride; Lewis base; ^{119}Sn NMR; allylic phosphates.

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CATION BINDING PROPERTIES OF SOME COUMARIN DERIVATIVES

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Coumarins (2H-1-chromene-2-ones) are abundant in Nature and are common motifs found in drugs, dyes, spices, and agricultural chemicals. In particular, 3,4-unsubstituted coumarins are the most common naturally occurring coumarins, which show potential antimalarial,[1] antioxidant,[2] antimicrobial, anti-inflammatory, and antitumor activity.[3]

The complexation properties of some coumarin derivatives toward alkali metal, alkaline earth metal, some transition metal and some heavy metal cations have been investigated in acetonitrile by means of UV spectrophotometry absorption and conductivity. Thus, the stoichiometries of complexes formed and their stability constants were determined by digital processing of data.

Keywords: Coumarin derivatives; Stoichiometry; Complexation; Cation binding properties.

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SYNTHESIS AND CHARACTERIZATION OF BIS(THIOCARBAMATOPHOSPHORAMIDES)

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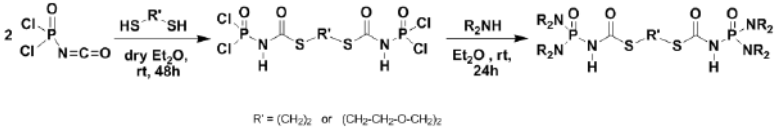
Thiocarbamates and carbamates find their applications in various fields such as agriculture as pesticides and herbicides [1, 2], industry as adhesives [3] and medicine as antitumor agents and drug intermediates [4, 5]. In a previous work, we described the synthesis of variously substituted bis(thiocarbamates) by the reaction of dithiols with alkyl or aryl isocyanates [6]. In the present work, we extend this reaction to isocyanatophosphonic dichloride which reacts with dithiols giving the corresponding bis(thiocarbamatophosphonic dichlorides). The latter undergo smooth aminolysis to afford the new bis(thiocarbamatophosphoramides) in good yields. These products were characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR and IR spectroscopic techniques. In addition, the coordination chemistry of these diphosphoramide-containing bithiocarbamtes as new bidentate ligands will be presented and discussed.



Keywords: Isocayanates, bis(thiocarbamates), isocyanatophosphonic dichloride, dithiols, NMR.

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SYNTHESIS, STRUCTURE AND CHARACTERIZATION OF AN INORGANIC-ORGANIC HYBRID DAWSON POLYOXOTUNGSTATE $(C_6H_8NO)_6[P_2W_{18}O_{62}].6H_2O$

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The polyoxometalates (POMs) form a significant class of inorganic metal–oxygen clusters with intriguing architectures and diverse physicochemical properties. These materials have attracted increasing attention worldwide because of their particular interesting nanosized structures. That's why a new inorganic-organic hybrid Wells-Dawson type polyoxotungstate, $(C_6H_8NO)_6[P_2W_{18}O_{62}]\cdot 3H_2O$ (1), has been synthesized under hydrothermal conditions and characterized by IR spectroscopy, UV spectroscopy, TG analysis, cyclic voltammetry and single crystal X-ray structural analysis.
The compound $(C_6H_8NO)_6[P_2W_{18}O_{62}]\cdot 6H_2O$ is a three-dimensional network composed of $[P_2W_{18}O_{62}]^{6-}$ polyanions, $(C_6H_8NO)^+$ cations, and water molecules (Fig. 1). 1 crystallizes as a monoclinic system, in C2/c space group; with a = 22.227(1) Å, b = 19.240(1) Å, c = 22.099(1) Å, β = 115.020(1) °, V = 8564.25Å^3, Z =4.

Keywords: Polyoxotungstate hybride Well-Dawson type, hydrothermal condition.

Fig. 1
A packing view of $(C_6H_8NO)_6[P_2W_{18}O_{62}]\cdot 6H_2O$ along the a axis.

PREPARATION AND APPLICATION OF ALUMINA, SILICA AND ACID ACTIVATED CLAY: SYNTHESIS AND THORETICAL STUDIES OF 2-METHYL-1,3-DIOXOLANE

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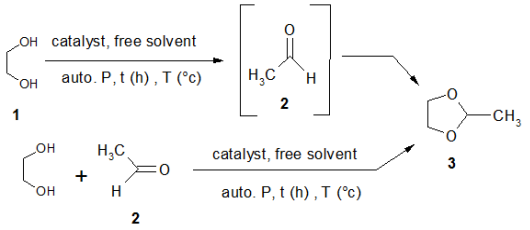
We have previously reported that the heterogenous supports based silica and alumina catalyzed the rearrangement of N-acyl-2,2-dimethylaziridines into mixture of oxazolines, methallylamides and amidoalcohols [1].
In order to improve our understanding the role of alumina and Tunisian heterogeneous catalysts as acid activated clay and silica and alumina [2] during organic reactions, we decided to synthesize the 2-methyl-1,3-dioxolane **3**, from pure ethylene glycol **1** or a mixture of ethylene glycol **1** and acetaldehyde **2** *via* tetracoodinated alumina and pentacoordinated silica intermediaries.



A kinetic study of this acetalization reaction and theoretical calculation were performed to determine and characterise the more stable geometries of these compounds **1-3** [3].

Keywords: alumina, silica, acid activated clay, theoretical calculation

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Performances of exchanged zeolite for the degradation of Methyl orange dye via photo-Fenton process

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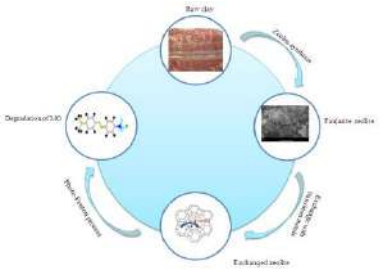
Many industries, such as the textile, paint and plastics industries currently use synthetic dyes in their production processes.The environmental impact of the wastewater resulting from those industries is dramatic. Those pigments are characterized with both high stability and toxicity.These aromatic amines which are characterized by the presence of N=N groups cannot easily be degraded and are apt to be carcinogenic and mutagenic to humans. One of the most used is methyl orange[1].Various technologies are utilized to remove dyes, such as biological, thermal, chemical treatments. However, these treatment technologies are less effective and still need to be improved. Advanced oxidation processes have become a popular method for wastewater treatment because they convert contaminants into stable, inorganic compounds, like carbon dioxide and water. Among them an especial interest has been focused to the Fenton's and photo-Fenton catalytic process. Among the possible catalysis materials, metal exchanged zeolites[2] are obvious candidates due to their high sorption capacities, good chemical and structural proprieties. .Cations (e.g., Na) located in the zeolite cages, channels and cavities can be exchanged by other metal cations. The size, number and position of the exchanged cations contribute significantly to the catalyst activity. In the present work, for the first time, a faujasite type zeolite (FAU zeo) was synthesized from low grade Tunisian clay. In the second time, various ions of transition metals: Cu, Co and Fe have been exchanged into the zeolite to be used as photo-Fenton catalysts for degradation methyl orange (MO) in water in presence of visible irradiation. Products have been characterized in terms of mineralogical composition by X-ray diffraction and in term of specific surface area. The results confirmed that the framework and crystallinity of zeolite were not destroyed during the preparation of catalysts.

The effects of various operating parameters like catalyst amount, H_2O_2 dose and methyl orange initial concentration on the degradation of dye were studied at atmospheric pressure. The results indicated that the Fe doped zeolite exhibited the higher degradation efficiency in comparison with catalysts prepared with other transition metals. Measurements of the mineralization of MO by TOC analysis reached 94% for the synthesized zeolite exchanged with Fe ions after 20 min of contact time and under UVC irradiation.



Graphical abstract

Keywords: photo-fenton, methyl orange, degradation, zeolite, clay.

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Post-synthesis surface-modified montmorillonite as adsorbent for heavy metal ion contaminant Pb (II)

Radhia Msaadi[1], Amor Ghorsalli[1], Samia Mahouche-Chergui[2], Sophie Nowak[3], Hanene Salmi[2], Benjamin Carbonnier[2], Salah Ammar[1,*], Mohamed M. Chehimi[3,*,#]

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Clay/mercaptosuccinic acid hybrids were prepared through radical thiol-ene coupling between methacrylate-silanized clay and mercaptosuccinic acid. First, the clay surface was modified by 3-trimethoxysilylpropylmethacrylate), then the so-silanized clay and mercaptosuccinic acid were clicked by the well-known thiol-ene click addition reaction which was triggered with UV light shining at 365nm. The clay-clicked mercaptosuccinic acid and silanised clay were characterized by X ray diffraction (XRD), diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) and X-Ray photoelectron spectrometry (XPS).As a demonstration of proof of concept, the acid-functionalized clay was found to adsorb much more PbII metal ions compared to the unreacted clay. From the above, it is clear that UV-triggered thiol-ene reaction is easy and efficient for designing reactive and functional materials.The Clay/mercaptosuccinic acid was then employed as an adsorbent for the removal of Pb(II) from the aqueous solution. Kinetic studies indicated that the adsorption of Pb(II) followed the pseudo- first-order equation. It was also found that the Langmuir model described the adsorption isotherm better than the Freundlich isotherm.

Keywords: Clay, click photochemistry, thiol-ene, silane, mercaptosuccinic acid, Heavy metal ions.

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SYNTHESIS AND CHARACTERIZATION OF CINNAMALDEHYDE SCHIFF BASE DERIVATIVES

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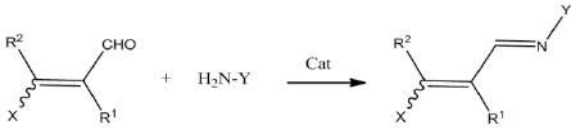
Schiff bases have been widely studied and areconsidered as an important class of organic compoundsin medical and pharmaceutical fields because of their broad spectrum of biological activities such asantibacterial and antifungal effects [1-4]. They have a large number of synthetic uses in organic chemistry and are used as precursors for the synthesis of various heterocyclic compounds and natural products [5, 6]. In this work, we describe the synthesis of a series of Schiff basesstarting mainly from cinnamaldehyde derivatives. In order to optimize conditions, reactions have been carried out without or in presence of catalysts. All the cinnamaldehyde Schiff base derivatives and corresponding tin(IV) chloride complexes were fully characterized by multinuclear (^{1}H,^{13}C and ^{119}Sn) NMR and IR spectroscopy. Preliminary results on the coordination chemistry of these Schiff bases as ligands towards tin(IV) chloride will be also presented.



X= H, Cl Y= iPr, NH_2

R^1= H, COOEt, CH_3

R^2= Ph, COOEt

Keywords: Schiff bases, catalysts, tin complexes.

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SYNTHESIS AND CHARACTERIZATION OF TIN TETRACHLORIDE COMPLEXES WITH PHOSPHONOTHIOAMIDATES

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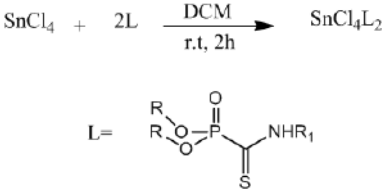
Phosphonothioamidates are known for their important biological and pharmaceutical activities such as antimicrobial, antihypertensive, antitumor, anti-inflammatory, anti-HIV and antidepressant properties [1-3]. It was generally shown that the coordination through the phosphoryl group or other heteroatoms in the molecule could be responsible of such biological activity [4]. In the present work, we describe the interaction of phosphonothioamidates [5] with tin(IV) tetrachloride and report on the resulting new tin complexes with these phosphonothioamidates. The compounds were characterized by multinuclear (^{1}H, ^{13}C, ^{31}P and ^{119}Sn) NMR, IR and UV-vis spectroscopic techniques. The effect of the alkyl group on the stability of the complex formed will also be presented.



Keywords: Phosphonothioamidates, Tin (IV) chloride, NMR spectroscopy.

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SYNTHESIS AND NMR CHARACTERIZATION OF NEW TIN COMPLEXES WITH ARYL PHOSPHORAMIDATES BEARING AMINO ACID GROUPS

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Organophosphorus compounds are known for their use as pesticides and chemical warfare agents [1,2]. For instance, phosphoramidates are attracting much attention as potential prodrugs due to their ability to inhibit acetylcholinestrase [1]. Their biological activity was shown to be more pronounced when amino acid groups are introduced into these compounds [3-5]. As a continuation of our interest in organophosphorus complexes with tin(IV), we report herein on the synthesis of new tin tetrachloride complexes with aryl phosphoramidates in which various amino acid ester groups were incorporated. These products were fully characterized by multinuclear (^{1}H, ^{13}C, ^{31}P and ^{119}Sn) NMR and IR spectroscopy. The ^{31}P and ^{119}Sn NMR show for these complexes the presence of two isomers, as expected, with the trans isomer being the dominant form. The results indicate that complex formation occurs only via the phosphoryl group and no interaction of the amino ester carbonyl group with the tin center was observed The effect of the nature of different substituents in particular that of the amino acid on the complex stability is also presented and discussed.

Keywords : Organophosphorus compounds, aryl phosphoramidates, amino acids, tin(IV) complex, NMR spectroscopy.

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Catalysis and metathesis: valorization of natural products by organometallic catalysis

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The utilization of renewable feedstocks arising from biomass has recently found a renewed interest for economic and ecological reasons. In this context, homogeneous catalytic transformations offer interesting perspectives towards green and sustainable chemistry. Olefin metathesis in the presence of commercially available ruthenium catalysts has given access to new functionalized terpenes using cross metathesis with electron deficient alkenes [1].

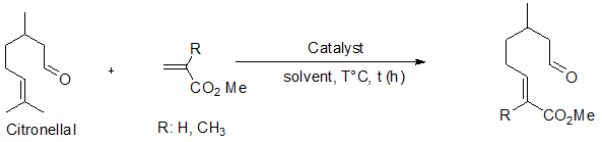

Figure 1: Functionalized terpenoid obtained from citronellal

A cascade reaction involving cross-metathesis of fatty ester, terpene and eugenol derivatives with allylic chlorides followed by an elimination reaction has led to a general method for the synthesis of terminal conjugated dienes [2].

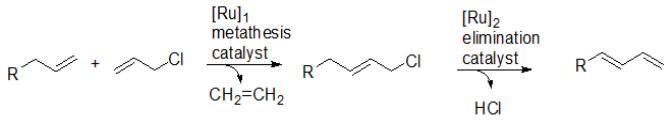

Figure 2: Two step ruthenium-catalyzed formation of conjugated dienes

The catalytic transformations of renewable resources have been carried out in green solvents such as dialkyl carbonates or without solvent under neat conditions, and thus fulfill several criteria of green chemistry.

Keywords: Terpenes, fatty esters, conjugated dienes, green chemistry.

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PALLADIUM(II) CHLORIDE COMPLEXES WITH NUCLEOBASE LIGANDS: EFFECTIVE CYTOTOXIC AGENTS

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Transition metal coordination complexes, such as cisplatin (cis-$[Pt(NH_3)_2Cl_2]$, are known to be cytotoxic on a number of cell lines and have been shown to have great potential for therapeutic interventions. The mode of action of these complexes is through the mediation of enzyme activities in signaling pathways essential for cellular functioning, and interfering with DNA through strand breaking or DNA-complex adduct formation [1]. Although cisplatin and its analogs such as carboplatin, nedaplatin, oxaliplatin etc have been successful clinically, the corresponding cispalladium (cis-$[Pd(NH_3)_2Cl_2]$) does not show anticancer activity [2]. Due to challenges with anticancer therapies such as drug resistance and toxicities to body organs the search for new drugs is imperative.

In this work, we have synthesized Palladium(II) chloride complexes bearing the nucleobases; Cytosine, Adenine and Guanine and in some cases ammonia. These complexes have been characterized by UV-vis spectrophotometric methods, magnetic susceptibility, molar conductivity, elemental analysis, FTIR and ^{1}H-NMR and ^{13}C-NMR. All the complexes have D_{4h} symmetry around the Pd(II) ion with the nucleobase ligands positioned *cis* to each other [3]. The complexes have shown significant *in vitro* cytotoxicity against HL-60, U937 and HepG2 cell lines. Complexes bearing Guanine ligands were the most cytotoxic. These complexes also showed significant antioxidant activity and inhibit Glutathione S-transferase inhibitory activity.

Key words: Palladium(II) complexes, nucleobases, apoptosis, cytotoxicity.

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IMPROVED OF MULTIFERROIC PROPERTIES IN $(1-x)BiFeO_3$-$xBa[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]0_3$ SYSTEM

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The polycrystalline samples of $(1-x)BiFeO_3$-$xBa[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]0_3$ (x = 0; 0.1; 0.2 and 0.3) were prepared by the conventional solid state reaction method. The phase purity and composition have been cheeked using powder X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDX) and X-ray photoelectron spectroscopy (XPS). The grain size and morphology of the ceramics have been confirmed by scanning electron microscopy (SEM). X-ray diffraction study showed that these compounds crystallized, at room temperature, in the Rhomboedral R3c distorted perovskite structure for x = 0 and in tetragonal P4mm one for compositions $0.1 \leq x \leq 0.3$. The effect of $Ba[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]0_3$ substitution on the structural, magnetic and ferroelectric properties shows improved magnetic and ferroelectric properties at room temperature. The highest magnetization was reported for composition x = 0.2 which is due enhanced canting angles, detected maxim concentration of Fe^{2+}, by XPS, which would possibly cause double exchange with Fe^{3+} ions and suppression of cycloid spin structure, as confirmed by ^{57}Fe Mossbauer spectroscopy. The electric polarization increases significantly for doped samples. A marked reduction in the leakage current compared to undoped $BiFeO_3$ was reported. Large electric field induced strains was observed for $Bi_{0.7}Ba_{0.3}Fe_{0.7}[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]_{0.3}0_3$, as an evidence of piezoelectric behavior. These results show that $Ba[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]0_3$ doped $BiFeO_3$ as a promising material for multifunctional devices.

Keywords: $BiFeO_3$; Perovskite; ceramics; Mossbauer; Multiferroic

Program of Sunday, May 10th 2015

DRUG VECTORIZATION BY A CARBON NANOCONE: IN SILICO STUDY

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This work concerns an *in silico* study of the potential of carbon nanohorns (CNH) in the field of drug vectorization. 6-Amino-penicillanic acid was used as active drug model. Preliminary computations of CNH showed that this compound may accumulate vectorization capabilities of both [60] fullerene (C_{60}) and carbon nanotubes. As compared to these two carbon nano-structures, the former exhibits greater polarization of the C-C bonds and a strong dipole moment of 10 Debye. Three grafting methods were studiedincluding1,3-dipolar addition on the apex, and a [1 + 2] grafting according to Bingel reaction on the walls or on the edge. The addition on the apex leads to the most stable compound and generates a large redistribution of single and double bonds on the entire cone. The three adducts are also characterized by a large change in the dipole moment from10 D to18 D, which could be attributed to by relative arrangement of the spacer-arm. One of the most remarkable results of this work is the identification of a great attraction of the σ skeleton of the spacer-arm with the π system of the cone.

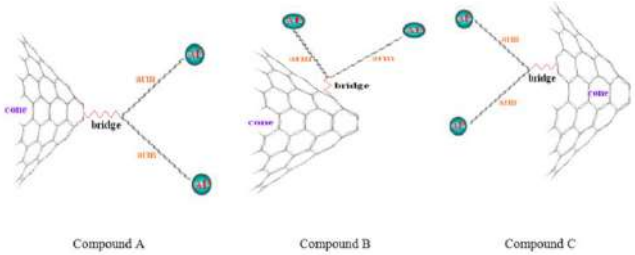

Figure 1: Artist representation of the three studied structures.

Key-words: Nanohorn, functionalization, drug vectorisation.

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ZINC(II) COMPLEXES WITH TRIBUTYLPHOSPHINE CHALCOGENIDES: AN EXPERIMENTAL AND THEORETICAL STUDY

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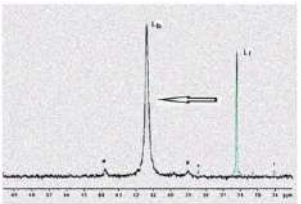
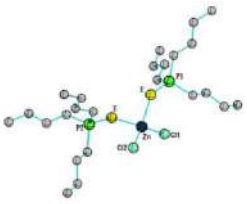
Phosphine chalcogenides are attracting increasing interest due to their complexing properties towards metal cations [1,2]. Recently, certain metal complexes of this class of compounds have shown to be suitable single-source precursors for the production of thin semiconducting films of metal chalcogenides, for example ME (M = Cd, Zn or Hg; E = O, S or Se) [3,4]. In this work, zinc(II) complexes of the type $ZnL_4(ClO_4)_2$ and ZnL_2Cl_2 (L =$Bu_3P(E)$ with E=O, S or Se)) have been synthesized and characterized by multinuclear (^1H, ^{13}C and ^{31}P) NMR, conductivity and IR techniques. The complex formation was confirmed by a coordination chemical shift of the ^{31}P NMR signals towards lower field compared to those of the free ligands The results show tha tthe ligand is coordinated to the zinc center through the chalcogenide atom of the group P=E. In addition, a DFT/B3LYP theoretical study through geometry optimization and NMR chemical shift calculations was carried out in order to support and complement the experimental data and to further investigate the nature of the chalcogenide-Zn interaction. The results show a good agreement between the experimental and theoretical data.



NMR spectrum of the complex in $CDCl_3$ of $Zn(Bu_3PSe)_4](ClO_4)_2$



DFT/B3LYP optimized structures of $[ZnCl_2(Bu_3PE)_2]$

NMR spectrum of the complex in $CDCl_3$ of $Zn(Bu_3PSe)_4](ClO_4)_2$
DFT/B3LYP optimized structures of $[ZnCl_2(Bu_3PE)_2]$

Keywords: Phosphine chalcogenide, zinc complexes, NMR, DFT/B3LYP.

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IN SILICO STUDY OF A NEW SERIES OF COORDINATION COMPOUNDS DERIVED FROM TTF-TCNQ

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Theoretical study of new series of charge transfer complexes derived from TTF-TCNQ, was performed by molecular modeling (molecular mechanics, molecular dynamics; Ab initio/HF and E.H.T). A good correlation between the theoretical and the experimental values were obtained; the complexes that have a specific conductivity between 0.1 and 150 S. cm^{-1} correspond to a charge transfer degree between 0.38 and 0.82 e/molecule and have a very restricted HOMO/LUMO gap from 0.108 to 0.128 eV.

Keywords: complexe, TTF, TCNQ, charge transfer, HF, EHT.

During the past few years, a considerable research effort has been focused upon the synthesis of more sophisticated tetrathiafulvalenes [1-3], as well as theoretical study [4-6].Over the past three decades, tetrathiafulvalene (TTF) and its derivatives have been extensively studied due to their unique electron-donating properties . In addition to the famous intermolecular charge transfer complexes related to organic metals and electrically conducting materials, TTF has been covalently linked to various electron-acceptor moieties.

In the present work, the structure of the donors and estimated degree of charge transfer between the donors of type tetrathiafulvalene (TTF) and the acceptors tetracyanoquinodimethane (TCNQ) are determined.

A good correlation between the theoretical and the experimental values were obtained; the complexes that have a specific conductivity between 0.1 and 150 S. cm^{-1} correspond to a charge transfer degree between 0.32 and 0.824 e/molecule and have a very restricted HOMO/LUMO gap from 0.108 to 0.128 eV.

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PERFORMANCE OF BULK HETEROJUNCTION PHOTOVOLTAIC CELLS BASED ON P3OT MATRIX AND CADMIUM SELENIDE NANOPARTICLES

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The use of phosphine chalcogenide metal complexes as single source precursors for the preparation cadmium chalcogenide nanoparticles is attracting special attention [1]. Specifically, hybrid nanocomposites consisting of inorganic nanoparticles and organic polymers represent a new class of materials that exhibit improved performance compared to their pure organic counterparts [2, 3]. In this work, photophysical properties of P3OT/CdSe composite films are investigated as a function of volume fraction f_v of CdSe nanoparticles (NPs) incorporated in these films. The results show that incorporation of CdSe NPs produces a quenching of the photoluminescence and improves the performance of solar cells based on the composites. The Stern-Volmer equation was used to determine the quenching rate constant of exciton, which was found to be $1.4.10^{-10}$ $cm^3.s^{-1}$. The different ITO/P3OT:CdSe/Al photovoltaic cell films prepared were characterized by Scanning Electron Microscopy (SEM) and J-V characteristics. The best result for the short-circuit current density (J_{sc}), open circuit voltages (V_{oc}), fill factor (FF) and efficiency (η) is obtained for the device with f_v = 0.135 that exhibits a considerable increase of the conversion efficiency, which is 17 times greater than the cell based on the pure polymer.

Keywords: Cadmium selenide NPs, P3OT polymer, photovoltaic cells.

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STRUCTURAL, THERMAL, VIBRATIONAL AND DFT STUDIES OF A NEW NONLINEAR OPTICAL CHLOROCADMATE

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Chemical preparation, X-ray single crystal diffraction, thermal analysis, electrochemical measurements, IR, Raman and UV spectroscopic investigations of a novel nonlinear optical organic-inorganic hybrid material $(C_5H_{16}N_2)_2Cd_3Cl_{10}$ are described. The catena-bis(3-dimethylammoniopropylammonium)decakis(μ_2-chloro)-tri-cadmium(II) crystallizes in the monoclinic system with the non-centrosymmetric space group P*c*. Its unit cell dimensions are a = 10.1393(4)Å, b = 13.9493(5)Å, c = 10.6629(4)Å and β = 112,627(8)° with V = 1392.04(9)Å^3 and Z = 2. The structure provides a new interesting example of infinite inorganic chains of $[Cd_3Cl_{10}]_n^{4n-}$ following the ***a*** crystallographic direction. The $[Cd_3Cl_{10}]^{4-}$ anions are interconnected by N–H···Cl hydrogen bonds. Acidic protons of the chloride group were transferred to the organic molecule, giving the doubly-protonated cations. The ability of ions to form a spontaneous three-dimensional structure through N–H···Cl hydrogen bond is fully utilized. These hydrogen bonds induce notable vibrational effects. The Hirshfeld surface and associated fingerprint plots of the compound have been presented to explore the nature of intermolecular interactions and their relative contributions in building the solid-state architecture. IR and Raman spectra are reported and discussed on the basis of group theoretical analysis and on quantum chemical density theory (DFT) calculation using B3LYP/6-311++G(d,p) approach. The molecular HOMO-LUMO compositions and their respective energy gaps were also drawn to explain the activity of our compound. The Mulliken charges and the first hyperpolarizability β_{tot} of the title compound were performed using DFT calculations. The optical study was also investigated by UV-vis. absorption spectrum. Thermal analysis reveals the anhydrous character of the compound. Cyclic voltammetry was studied to evaluate the spectral and structural changes accompanying electron transfer.

Keywords: Hybrid material. Crystal structure. NLO. Vibrational spectroscopy. DFT calculations. Thermal analysis (TG/DTA). Cyclic voltammetry.

COORDINATION ABILITY OF 4-BENZYLIDENAMINO-4, 5-DIHYDRO- 1H-1,2,4-TRIAZOL-5-ONE DERIVATIVES: A DENSITY FUNCTIONAL THEORY STUDY OF DIVALENT METAL CATIONS

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A detailed theoretical study of 4-benzylidenamino-4,5-dihydro-1*H*-1,2,4-triazol-5-one derivative (BDHTD) ligands coordinated to divalent doubly charged metal ions M^{2+} (M= Mg, Ca, Fe and Cu) has been investigated using the Becke-3-Lee-Yan-Parr (B3LYP) method [1]. Two distinct coordination modes (k^2-O,O and k^2-O,N) have been taken into account. The geometrical properties have been calculated in gas-phase and solution-phase: acetonitrile and N,N-dimethylformamide (DMF) with the basis set 6-31G(d,p). The B3LYP method was also used to calculate the stabilities and free energies of the 24 $[M\text{-}BDHTD]^{2+}$ complexes respectively in various media. These calculations lead to the conclusion that k^2-O,N structures are most stable in gas-phase. The influence of substitution on the stability in solution-phase has been also explored. The interaction energies of complexation process (coordination ability) in different media have been calculated at B3LYP/6-31G(d,p) and Coupled Cluster Single, Double and Triple (CCSD(T)) excitations level [2]. The Metal Ion Affinity (MIA) [3] of BDHTD with M^{2+} these media which is the enthalpy change during the complexation process has been also specified. The results show that the MIA highly varies with the coordination mode and substitution effect. From the calculated Gibbs energies of these processes, it is revealed that the complexation is only possible in gas and in acetonitrile. The ligand's affinity toward individual cation M^{2+} has been analysed. The comparison between the bond dissociation energies (BDEs) of X-H bond of the M^{2+}-BDHTD complexes and those its homolog of isolated ligands has revealed a significant reduce of the former ones. Such a reduce therefore confirmed the enhancement of the antioxidant activity by chelation with divalent metal cations as underlined in a previous theoretical analysis [4]. Our results show that the net charge on the metal atom is lower for k^2-(O,O) complexes. The k^2-(O,O) coordination mode then highly alters the redox potential of metal atom and render them more inactive. This confirms the fact that such a coordination mode leads to complexes with higher antioxidant activities [5].

Key words: Metal chelation, BDHTD, MIA , BDEs , ligand's affinity

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D. Tashobya, J. Wasswa *Uganda National Bureau of Standards - Kampala, Uganda* Assessing the impact of socio-economic activities in fort portal town on the water quality of River Mpanga	**PC93**
M. Tassadit, S. Mouanni, D. Amitouche, L. Mouheb, A. Boumchhour, M.R. Guerroudj, S. Benadji, L. Dermeche, C. Roch Marchal, C. Rabia *Mouloud Mammeri University - Tizi Ouzou, Algeria* An alternative path for clean synthesis of adipic acid catalyzed by an heteropolyacid drived complexe	**PC94**
M. Tassadit, D. Amitouche, S. Mouanni, L. Mouheb, A. Boumchhour, M.R. Guerroudj, S. Benadji, L. Dermeche, C. Roch Marchal, C. Rabia *Mouloud Mammeri University - Tizi Ouzou, Algeria* Transition metal-substituted polyoxometalates as catalysts in the oxidation of cyclohexanone to adipic acid with H_2O_2	**PC95**

Name	Ref
S.O. Uchechukwu, P. Oziri Ukoha, H. Obiajulu Echekwube *University of Nigeria - Nsukka, Enugu State, Nigeria* Synthesis, characterization and preliminary antimicrobial studies of three Schiff bases derived from indole-2, 3- dione and their Co(II) and Ni(II) complexes	**PC96**
S. Van Wyk, M. O. Onani, E. Nordlander *University of the Western Cape - South Africa* Novel bimetallic nickel and palladium complexes	**PC97**
I. Wekesa, Deogratius Jaganyi *University of KwaZulu-Natal - Pietermaritzburg, South Africa* Kinetic and Mechanistic Studies of 1,3-Bis(2-pyridylimino)isoindolate Pt(II) Derivatives. Experimental and new Computational Approach	**PC98**
M. Wubshet, I. Diaz *Aksum University - Axum, Ethiopia* Encapsulation of Co (II) complex with a Schiff base ligands derived from 1,10-phenantroline-5,6-dione and O-phenylene diamine in zeolite Y	**PC99**
A. Zaïdi, M. Merabet-Khelassi, L. Aribi-Zouioueche *Badji Mokhtar University - Annaba, Algeria* Enantioselective synthesis of some benzylic acetates precursors of drugs *via* enzymatic kinetic resolution	**PC100**
A. Zaïdi, M. Merabet-Khelassi, L. Aribi-Zouioueche, O. Riant *Badji Mokhtar University - Annaba, Algeria* *CAL-B* catalyzed tranesterification as key step to deracemization of benzylic alcohols through combined *CAL-B*/ Ruthenium catalysis	**PC101**
M. Zaied, H. Mekki, E. Ammar *FSS - Sfax* Valorisation des phosphogypses par leur integration dans les materiaux de construction	**PC102**
D. Zammel, I. Nagazi, A. Haddad *FSM - Monastir* Synthesis and caracterisation of a new Strandberg-type polyoxomolybdate $(NH_4)Rb_3[Se_2Mo_5O_{21}].H_2O$	**PC103**
D. Zammel, I. Nagazi. A. Haddad *FSM - Monastir* Synthesis and caracterisation of a new Waugh-type polyoxometalate $K_{1.5}(NH_4)_{4.5}[MnMo_9O_{32}].4.2H_2O$	**PC104**
E. Zouaoui, F. Krid, S. Kharraf, M.S. Medjram *University of 20 Aout 1955 - Skikda, Algeria* Corrosion inhibition of carbon steel A 283 C using the acetylsalicylic acid	**PC105**

Posters Communications' Abstracts

THEORETICAL STUDY OF ELECTRONIC STRUCTURE AND STABILITY OF MIXED $Al_mB_{n-m}H_n^{2-}$ AND $C_mB_{n-m}H_n^{m-2}$ (n = 6, 10, 12 AND m = 1, 2) CLUSTERS

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Density functional theory (DFT) method with B3LYP [1] functional and 6-311++G(d,p) basis set has been used to predict the geometries, relative stabilities, electronic structures and bonding analysis of Mixed $Al_mB_{n-m}H_n^{2-}$ and $C_mB_{n-m}H_n^{m-2}$ (n = 6, 10, 12 and m = 1, 2) clusters; being compared to the $B_nH_n^{2-}$ ones. Therefore, the DFT results suggest that the replacing of boron by aluminium or carbon is governed by Natural net charges following Gimarc's [2] and Williams's rules. The $Al_mB_{n-m}H_n^{2-}$ structures are relatively distorted compared to those of $B_nH_n^{2-}$ and $C_mB_{n-m}H_n^{m-2}$. In $Al_mB_{n-m}H_n^{2-}$ structures Al atoms prefer the adjacent sites, however for the $C_2B_{n-2}H_n$ cluster cages, the carbon atoms are positioned at diametrically opposed sites. The large HOMO–LUMO gaps show that the predicted clusters have chemical stabilities, principally, those of $Al_mB_{n-m}H_n^{2-}$ ones, which are not experimentally isolated. The optimized geometries obtained through boron substitution by Al and C lead to compactness and to contracted structures, respectively, where B–B bonds are the shortest in mono- and di-carbaboranes.

Key words: Density functional theory . Isomer stabilities . Bonding analysis. NBO analysis . Molecular structures.

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Improving seed treatment methods: A key factor to reduce the risk of chemical insecticides to the environment

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Bee, this small little insect that works so tirelessly and quietly around us certainly is one of the reasons, if not a main reason, for the possibility of human development on earth. Without them, the development of life on earth, as we know it now, would have been much different and the conditions for human development may not have existed. Bees and other pollinators have a great importance in maintaining the biodiversity in almost all environments. Pollinators support the reproduction of nearly 85% of the world's flowering plants. However these important species are endangered through the use of pesticides. In late April 2008, dust drift containing insecticide resulted in the largest bee poisoning in Germany for 30 years. The reason for these incidents was the contamination of flowering bee forage plants with dust particles abraded from maize seeds treated with the neonicotinoid insecticide Clothianidin recorded in the Upper Rhine. Thus highly specialist techniques should be used when treating seeds with Plant Protection Products to avoid such problem. The current study investigated the amount of drift generated from seeds of two varieties of cotton using two formulation of the neonicotinoid insecticide imadocloprid through measuring the fine dust particles from various treatments using the Heubach methods, whereas a Heubach Dustmeter was used. The aim was to improve the seed treatment methodology to reduce the drift generated from seeds by drilling and hence saving of bees and other pollinators as well as reducing the risk of people handling the treated seeds during the sowing activities and people located in the vicinity of the sowing site. The increase in percentages of drift generated through Heubach Meter through tested formulation of imadocloprid relative to the control treatment were found to be in the range of 336-378% and 221-287 for the Water dispersible powder formulation (WS) for Hamid and Barakat cotton varieties, respectively. For the Flowable Concentrate (FS) formulation the percentage increase in the drift over the control was ranging 82-95% and 15-445 for Hamid and Barakat varieties respectively. The Heubach vaules were higher in case of WS formulations. They were ranging between 13.5 – 24.5 for Hamid variety and 23.3-25.4 for Barakat variety. The values for the FS formulation ranged between 7-8.8 and 2.64-14.7 for Hamid and Barakat, respectively. The pesticide residues measured were found to be more for WS formulation compared to FS formulation for both tested varieties. The results of the study indicated in General that the Flowable concentrate formulation for seed treatment is better than the Water dispersible powder formulation in reducing the drift generated from pesticide treated seeds and can play important role in improving seed dressing technology to save various pollinators.

Keywords: Seed treatment, insecticides, neonicotinoid, cotton varieties, Heubach, pesticide residues.

THORETICAL STUDIE OF 2-R-1,3-DIOXOLANES FORMED FROM ALDEHYDES AND ETHYLENE GLYCOL VIA ALUMINA AND SILICA INTERMEDIARIES

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Previously, we have studied the thermolysis of 2,2-dimethylaziridines N-substituted by propanoyl, benzyloyl and benzoyl groups into vinylamides, allylamides and oxazolines [1].
In this work we have shown that 2-R-1,3-dioxolanes **3a-f** by acetalysation of aldehydes **2a-f** with ethylene glycol **1** in presence of Tunisian activated clay under green chemistry [2]. We have advanced two ionic mechanisms via tetracoodinated alumina and pentacoordinated silica intermediaries.
The interesting experimental results led us to conduct a comparative theoretical study of ethylene glycol **1**, alkyl and unsaturated aldehydes **2a-e** and dioxolane **3a-e** [3]. We can conclude that the more stable geometries, atomic charges and bond lengths of main atoms closely depended of the nature alkyl or aryl groups of thus compounds.

Figure 1: More stable geometries of ethylene glycol **1**, propanaldehyde **2c** and 2-ethyl-1,3-dioxolane **3c**

Keywords: aldehyde, dioxolane, acid activated clay, theoretical calculation

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Nitrilotriacetic acid functionalized *Adansonia digitata* bio-adsorbent: A suitable adsorbent for waste water treatment in Africa

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Nitrilotriacetic acid functionalized *Adansonia digitata* (NFAD) bio-adsorbent has been synthesized using a simple and novel method. NFAD was characterized by X-ray Diffraction analysis technique (XRD), Scanning Electron Microscopy (SEM), Brunauer-Emmett-Teller (BET) surface area analyzer, Fourier Transform Infrared spectrometer (FTIR), particle size dispersion, zeta potential, elemental analysis (CHNS/O analyzer), thermogravimetric analysis (TGA), differential thermal analysis (DTA), derivative thermogravimetric analysis (DTG) and energy dispersive spectroscopy (EDS). The ability of NFAD as bio-adsorbent was evaluated for the removal of Pb^{2+} and Cu^{2+} ions from aqueous solutions. Equilibrium, thermodynamics and kinetic studies were conducted by considering the effects of pH, initial metal ions concentration, contact time and temperature. The equilibrium adsorption capacity was found to be 51.883 mg/g for Pb and 7.213 mg/g for Cu which was monolayer, chemisorptive and controlled by both intra-particle diffusion and liquid film diffusion. The values of ΔG^o, ΔH^o and ΔS^o obtained showed a stable adsorbent-adsorbate configuration which is endothermic. The results of this study compared better than some reported bio-adsorbents in literature.

Keywords: *Adansonia digitata*; Adsorption; Bio-adsorbent; Heavy metal; Nitrilotriacetic acid

DEVELOPMENT OF A CONCRETE FIBERES ULTRA HIGH PERFORMANCE

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The fiber concrete ultra high performance, are materials with cementitious matrix, characteristic strength compressive greater than 150 MPa, and up to 250 MPa. These materials are added to metal fibers, in order to obtain a ductile behavior in traction and overcome if possible the use of passive reinforcements. They may also include polymeric fibers.
Progress in the field of adjuvants, design methods and the use of ultrafine led to dramatic changes of concrete.

Key words: ultrafine, mechanical strengths, concrete fiber reinforced ultra-high performance.

Anisotropic growth of cobalt nanoparticles using a simple approach

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One dimensional (1-D) nanomaterials (nanorods, nanowires, fibers,…) have received a great attention among researcher due to their interesting properties and numerous technological applications (electronics, optics, photonics, and plasmonics,…) [1, 2]. Up to now, several methods have been proposed to synthesis these nanomaterials. Most of them used organic surfactant which selectively adsorb on the surface of the particles assuring their anisotropic growth. Here we proposed a simple and versatile method to develop 1-D cobalt NPs based on the application of an external magnetic field during nucleation and growth of the particles. Cobalt acetate tetrahydrate and sodium hydroxide were used as precursors, hydrazine monohydrate as reducing agent and EG as solvent. Cobalt fibers with about 0.6 µm in diameter and few micrometers in length were obtained. Depending on the synthesis conditions, these sub-micrometric fibers were formed by uniform and very smooth discs (Fig. 1a) or by flower like sub-micrometric spheres (Fig. 1b) that coalesce in the direction of the applied magnetic field. In the latest case, the microspheres consist of well crystallized nanosheets (inset of Fig. 1b) with an average thickness of about 20 nm which may let them of potential candidate for catalysis [3].

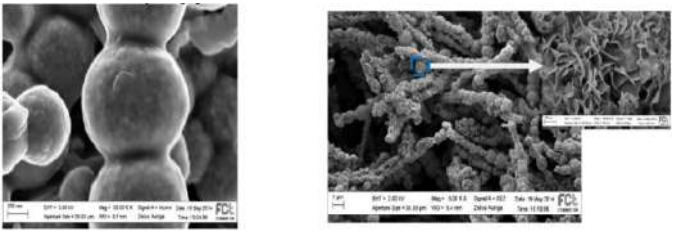

Figure 1: SEM images of cobalt sub-micrometric fibers obtained at low reducing ratio (a) and those obtained at high reducing ratio (inset Fig. 1b) microspheres with high magnification.

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A POLY (VINYL CHLORIDE) FUNCTIONALIZATION BY DIETHYLENETRIAMINE, 2,6-BIS (CHLOROMETHYL) PYRIDINE AND A CROWDED AROMATIC AMINE. INDUCTIVELY COUPLED PLASMA STUDY OF THE EXTRACTION OF La(III) AND Bi(III) BY MODIFIED PVC POLYMERS

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The aim of this study was to evaluate the efficiency of three new polymers obtained by functionalization of a commercial poly (vinyl chloride) (Mw = 48000) by grafting diethylenetriamine, 2,6-Bis (chloromethyl) pyridine and 1-chloro-2-phenylaminomethyl-6-phenylaminomethylene-cyclohex-1-ene groups to extract some metal cations from aqueous solutions. The structural properties of the polymers were systematically investigated by different analytical methods; namely elemental analysis (EA) and infrared spectroscopy (FT-IR). The percentage of extraction was determined by inductively coupled plasma-atomic emission spectrometry (ICP-AES). One of the obtained polymers gave an extraction ratio of La^{3+} = 99.57 % which highlight the importance of the substitution of chlorine atoms by amino groups.

Keywords: Poly (vinyl chloride); functionalization; metal cations; extraction; inductively coupled plasma-atomic emission spectrometry

CRYSTALLINE AND VIBRATIONAL PROPRETIES OF $Bi_{(1-x)}Ba_x[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]_xFe_{(1-x)}0_3$ NEW SOLID SOLUTION

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Materials that combine ferroic properties, such as ferromagnetism and ferroelectricity are highly desirable, yet rare. The number of candidate materials is limited and their effects are typically too small at room temperature to be useful in applications.

$Bi_{(1-x)}Ba_x[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]_xFe_{(1-x)}0_3$ new multiferroic solid solution have been prepared in the whole range of concentrations and studied at room-temperature by means of X-ray , Mossbauer spectroscopy and Raman scattering. X-ray measurements revealed rhombohedral-Tetragonal-cubic structure modifications depending on the contents of $Ba[Ti_{0.95}(Yb_{0.5}Nb_{0.5})_{0.05}]0_3$. Analyzing hyperfine Mossbauer parameters spectra confirms a modulated spiral structure. The distinct changes of the Raman spectra with increasing substitution were correlated with X-ray results. The modifications at high frequency of Raman spectra matches well with the hyperfine magnetic parameters. The broad phonon spectra indicated the disorder in the A and B sites. All these results indicate the existence of strong magnetoelectric coupling in our new solid solution.

Keywords: Ceramics, Magnetoelectric, Mossbauer, Raman.

Exploring the oxidation activities of a new series of hydroxo complexes against chemical and biological catalysis

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The oxidation catalytic activities against several biomasses and vinyl compounds were ensured by a new series of hydroxo complexes of transition metals and tested with H_2O_2 and OCl^- under mild conditions. Their products have been characterized by FTIR, NMR spectroscopies and GC-MS.

The series of hydroxo complexes of Fe (II), Ni(II), Cu(II) type $[M(L)(OH)_2]$ [L=diimin, 2,2'-bipyridin, 1,10-phenanthrolin, 3-methyl-1,2-cyclopentanedion] have been prepared by a simple and direct route, by the reaction of transition metal salts with sodium hydroxide and N- or O-donor ligands.

The new neutral catalyst have been characterized by FTIR, NMR spectro-scopies and X-ray diffraction data.

They present also an interesting antifungal activities, their cytotoxic activity is under study.

Keywords: hydroxo complexes, oxidation, biomasses, vinyl compounds.

PALLADIUM COMPLEXES WITH REACTIVE LIGANDS

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The free radicals of nitroxide are among the best groups characterizing the free radicals. They were mainly used as probes in the biological systems [1]. It is in the last decades when they became more used in magnetic materials. They allow the synthesis of molecular buildings with varied magnetic properties.
1,2,3-Triazoles and their by-products have wide applications including as pharmaceutical agents [2]. Their coordination with diverse metals, as the platinum, the iridium, and the tin, generate new complexes possessing a biological activity [3].
Here, we report synthesis and structure characterization of palladium complexes with triazole and stable nitronyl nitroxide radical ligands.
In the complex with nitronyl nitroxide radical, the palladium atom is bound to one chelating imino nitroxide radical through two N atoms, one from the pyridyl ring and the other from the imidazoline ring, the coordination of the metal is completed by two chlorine atoms in a cis configuration.
While In the complex with 1,2,3-mono-ferrocenyl triazole, the palladium atom is coordinated to two molecules of ferrocenyl triazole through the N1 atoms from triazole rings which are in trans configuration.

Key words: Palladium complexes, ferrocenyl triazole ligands, nitronyl nitroxide radical ligands.

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SYNTHESIS, CHARACTERIZATION AND CRYSTAL STRUCTURE OF A NOVEL Mo36-POLYOXOMOLYBDATES

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The chemistry of polyoxometalates have become a focus of contemporary chemical research, and witnessed remarkable achievements [1,2] due to the alluring topologies and potential applications in various fields such as catalysis, biology, medicine and materials science [3].

In this context, a new member of giant Mo36-polyoxomolybdate has been synthesized by reaction of potassium molybdate and potassium nitrate in aqueous solution acidified, characterized by IR spectroscopy and DSC-TG analysis. The title compound crystallizes in the monoclinic system, space group P21/n with a = 16.542 (50) A°, b = 18.517 (50) A°, c = 24.339 (50) A°, α= 90.00° , β= 90.58° , γ= 90.00° , V= 7351,29 $A°^3$ and Z = 2.

KEY WORDS : Giant polyoxomolybdate; synthesis and crystal structures.

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DIELS-ALDER REACTION AND CYCLOADDUCTS AROMATISATION

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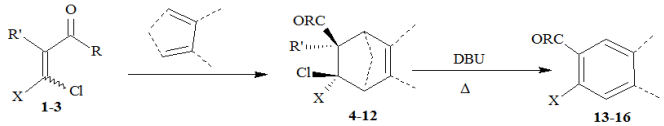
Polyfunctionalised benzene derivatives are abundant natural products and have a wide range of biological activity [1,2]. Furthermore, they are considered as versatile synthetic building blocks useful as precursors to the formation of a number of different compounds, such as dyestuffs [3], flavors and fragrances [4], nucleating agents and polymer additives [5].

The Diels-Alder cycloaddition reaction of β-chloro-α,β-unsaturated carbonyl compounds **1-3** with dienes as cyclopentadiene, Dimethylbutadiene and isoprene were carried out affording highly functionalized norbornenes **4-6** and cyclohexenes **6-12** in good yields. In some cases cycloadducts (CAs) undergo dehydrochlorination with subsequent aromatization in the presence of 1,8-diazabicyclo [5.4.0] undec-7-ene DBU leading to new substituted benzaldehydes **13-16**. Characterisation of all products was carried out by NMR, IR, MS and by elementary analysis. Structure assignments of isomers were made on the basis of NMR chemical shifts and coupling constants using 1D, 2D and heteroNOE NMR techniques.



R = CH_3, H
X = CF_3, COOEt
R' = H, COOEt

Keywords: β-Chloro-α,β-unsaturated carbonyls, Diels-Alder reaction, DBU, aromatisation, substituted benzaldehydes

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EFFECT OF ULTRASOUND IRRADIATION IN THE RESOLUTION OF (R, S)-2-PENTANOL CATALYZED BY LIPASE

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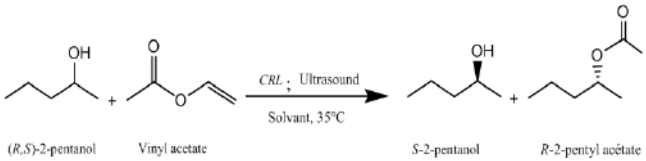
Methods for synthesis enantiomerically pure compounds have a great interest in pharmaceutical, agrochemical industry and other industries of fine chemistry [1]. The use of biocatalysts has proven to be an extremely useful method; lipases constitute the most important class of biocatalysts because they can catalyze variety of reactions such as: esterification, hydrolysis, aminolysis and trans-esterification, under milder and simpler process conditions, and with high activity and régio-selectivity [2-5]
However, one of its major drawbacks is its low reaction rate [6], which may seriously limit its industrial application. Ultrasound can enhance the reaction rate and its equipment is relatively inexpensive, making it economically attractive for large-scale application [7].
This work is devoted to study the effect of solvent on the tansesterfication of (*R, S*) 2-pentanol by the vinyl acetate as an acyl donor in the presence of *Candida rugosa lipase (CRL)* assisted by ultrasound.



Two approaches were used in this study. In the first, ultrasounds are used during all the reaction; the other approach was to pre-irradiate the enzyme before its use. Compared with conventional shaking, ultrasound made the synthetic activity and the enantioselectivity increase 2.1-fold and 1.3-fold, respectively.

Key words: Ultrasound; Lipase; (*R,S*) 1-pentanol; enantioselectivity

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Mineralogical and physico-chemical characterization of Algerian palygorskite

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Palygorskite (also known as attapulgite) is a 2:1 phyllosilicate with a fibrous morphology. It is known to contain a continuous two dimensional tetrahedral sheet; commonly occupied by Si and Al; but differs from other layered silicates in lacking continuous octahedral sheets, coordinated at regular intervals, like ribbons, as in talc.

The Algerian palygorskite is a new mineral which was recently discovered in the east of Algeria. Many characterizations have been deeply investigated for an adequate study of the Algerian mineral. The X ray diffraction, the X ray fluorescence and the electronic transmittance microscopy proved that there are two varieties of Algerian palygorskite with their characteristic peaks at 10.5 Å (1 1 0), 6.49 Å (2 0 0) and 5.42 Å (1 3 0). The first variety is a carbonated mineral with calcite peaks at 3.03 Å (1 0 4), 2.28 Å (5 3 0) and 1.90 Å and the second is rich in dolomite. The FT-IR spectroscopy revealed the presence of the three water molecules of the fibrous clay; zeolitic, coordinated and structural water.

Metal organic frameworks as new antibiotics nanocarriers: Synthesis and cytotoxicity studies

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Metal organic frameworks (MOFs) are hybrid materials; resulted from the assembly, exclusively by strong bonds, of inorganic clusters and easily tunable organic linkers. They have several potential advantages over conventional nanomedicine such as their structural and chemical diversity, their high loading capacity, and their intrinsic biodegradability. Thanks to its high loading capacity, these inorganic materials have been investigated for applications in loading and releasing of several drug molecules. Actually, many interesting drugs cannot be successfully encapsulated in the current nanovectors (such as liposomes, polymers…). Thus, it was recently reported that nanoparticles of porous iron Metal Organic Frameworks (nanoMOFs) are used as a new alternative for the vectorization of challenging drugs.1 Nevertheless; the use of these solids as drug nanocarriers is conditioned to their physicochemical properties, their drug loading capacity, their stability in biological medium and their toxicity.
In this work we study the physicochemical properties of nanoMOFs synthesized by microwave chemistry heating reaction of iron as the transition biocompatible metal and trimesic acid as the organic linker. Then nanoparticles stability was studied in water and PBS. Moreover these nanoparticles were tested for antibiotics (Flumequine) loading capacity. Finally the cytotoxicity was assessed on normal human microvascular endothelial cells (HMEC) and human epithelial colorectal adenocarcinoma cells (Caco2). Preliminary results showed that nanoparticles size is in the range of 50 to 200 nm with pore sizes between 0.4 and ~ 6 nm, which is perfect for storage and/or delivery applications. Flumequine loading capacity was improved within 6 hours to achieve 32 % with a progressive release up to 72 hours. Cytotoxicity was not exceeding 25% of cells viability inhibition. This study has shown that the synthesis of nanoMOFs requires no specific and complex synthetic methods, paving the way for its use for Flumequine delivery notably in the veterinary medicine.

Key words: MOFs, nanocarrier, flumequin, cytotoxicity

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STUDY BY ^{1}H NMR OF THE INTERFACE: Poly (ethylene oxide) (PEO) grafted on silica

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Text of the abstract Nanocomposites of polymers and layered silicates and polymer grafting onto inorganic molecules like pyrogenic silica are among the current research activities in industry and academia. The modification of the characteristics of the nanocomposite polymer/solid interface depends essentially on the behavior of particular chains, such as conformation, mobility, …etc. Moreover the grafting of a macromolecule on a solid surface must introduce a significant effect on its motion.

The polymer/solid interface of Poly (ethylene oxide) (PEO) grafted on silica is studied by ^{1}H Nuclear Magnetic Resonance. Such technique permits some approaches to a monomer unit scale of the macromolecular grafted onto a silica.

The magic angle spinning technique is used. It allowed to confirm on one hand the existence of a residual dipolar interaction which reveals the high monomer units concentration at the surface and to follow on the other a physical parameter such "second moment", which gives in turn an indication of the local concentration of monomer units in the vicinity of the surface. This behavior has been studied as a function of molecular weight of the chains and grafting ratio parameters.

Key words: polymer /solid interface, Nuclear Magnetic Resonance, poly(ethylene oxide), silica, grafting ratio, residual dipolar interaction.

BROWNIAN DYNAMICS OF WATER CONFINED IN AOT REVERSE MICELLES: A FIELD-CYCLING NMR RELAXOMETRY AND NMR DIFFUSOMETRY STUDIES

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Reversed micelles can be used to solubilize biopolymers and genetic materials allowing to analyze their properties in confined geometry. Nuclear Magnetic Resonance Dispersion (NMRD) provides a powerful and a non-invasive experimental technique to probe the long term dynamics of these confined systems. However, the first step is to analyze and understand the slow dynamics of water inside these micro-reactors without any guest molecule. This is the aim of this presentation.

Experimental results have been obtained for proton ^1H, deuteron ^2H NMRD and NMR diffusometry of water (H_2O or D_2O) confined in reverse micelles of bis (2-ethylhexyl) sodium sulfosuccinate (AOT) dispersed in isooctane C_8H_{18}. The water content is expressed as the molar ratio W_0 = [water]/[AOT]. The radius of the spherical reversed micelles, R_w, increases almost linearly with W_0. In our case, W_0 is in the range $10 \leq W_0 \leq 50$ ($19 \leq R_w \leq 80$ Å).

The frequency dependence for spin-lattice relaxation rate $R_1(\omega)$ exhibits two regimes: a plateau at low frequency followed by an algebraic decay running as $\frac{1}{\omega^{\alpha}}$ where $0{,}5 < \alpha < 1{,}5$. The cut-off frequency between these two regimes, ω_c, evolves as $1/R_w^2$. ω_c can be directly related to an upper time cut-off of water diffusion inside these spherical geometries.

These typical relaxation features have been interpreted according to two processes :

(i) the molecular reorientation of water molecules coupled with translation diffusion inside a spherical confinement
(ii) the exchanges and collisions between reverse micelles.

Our experimental observations are discussed and compared to Brownian molecular dynamics of water molecules reported in literature.

Key words: AOT Reverse micelles, Field-cycling relaxometry, NMR diffusometry, Spin-lattice relaxation rate, Dynamics in confinement.

DFT STUDY OF ISOMERS OF THE RUTHENIUM DIHYDRIDE COMPLEX $RuH_2(CO)_2(AsMe_2Ph)_2$

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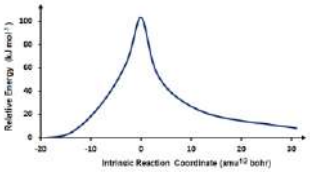
Ruthenium complexes have attracted considerable attention due to their ability to catalyze reactions [1,2]. The catalytic activity depends largely on the configuration of these complexes [3]. In the present work we report a density functional theory (DFT) study of cct-As, ccc and cct-CO isomers of the ruthenium dihydride complex $RuH_2(CO)_2(AsMe_2Ph)_2$. Complex geometries, relative energies of different isomers and NMR chemical shields have been calculated with both B3LYP and M06-2X functionals. The results show that the B3LYP calculated Boltzmann populations of cct-As, ccc and cct-CO isomers are 65.5%, 34.2% and 0.3%, respectively. These are in better agreement with the experimental data than those obtained at M06-2X level. However, the calculations of NMR parameters were found to be better described with M06-2X than with B3LYP. In addition, a transition state between the two most stable isomers was determined through DFT/B3LYP calculations along the IRC path.



Keywords: DFT/B3LYP, DFT/M06-2X, ruthenium dihydride complex, arsine, transition metal, NMR.

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SYNTHESIS AND CHARACTERIZATION OF TIN DIOXIDE NANOPARTICLES OBTAINED BY HYDROLYSIS IN POLYOL MEDIUM

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The synthesis of tin oxide in polyol medium results from a hydrolysis reaction governed by the hydrolysis ratio defined as h = n (water)/ n (metal) including the amount of water present in the precursor salt. When the preparations were carried out with a hydrolysis ratio inherent in the amount of water present in the metal acetates hydrates used as precursors. At this stage, we have studied the influence of the amount of water on the growth mechanism of hydrolysis ratio h = 17 and h = 20. It is determined by X-ray diffraction (XRD), Transmission Electron microscopy (TEM), Scanning Electron Microscopy (SEM), Fourier Transform Infra-Red spectroscopy (FTIR) and Nitrogen Sorption Porosimetry. FTIR indicate that tin oxide species were obtained with a complete removal of polyol residues and water after thermal treatment of 700 °C [1]. XRD patterns reveal that nanocrystallites of cassiterite, i.e. rutile-like tetragonal structure, SnO_2 were formed after annealing, the average crystallite size increasing with the hydrolysis ratio [2]. Moreover, TEM, SEM and N_2 sorption porosimetry show that the sample of the hydrolysis ratio h = 17 is composed of an aggregated network of almost spherical nanoparticles, their morphology was changed with the increase in hydrolysis rate at h = 20, the mesoporosity observed being related to the interparticle space [3].

Key words: Synthesis – Characterization – Nanoparticles - Hydrolysis ratio – Polyol - Tin oxide.

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STRUCTURAL, TEXTURAL AND OPTICAL PROPERTIES OF V-DOPED SNO_2 NANOPARTICLES SYNTHESIZED BY THE POLYOL METHOD

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Nanocrystalline mesoporous SnO_2 nanoparticles were synthesized by the polyol method followed by concentration of doped by vanadium varying from 0 to 6 % .The composition, texture and structure of the samples pure and vanadium doped tin oxide (SnO_2) were determined by X-ray diffraction (XRD), Fourier Transform Infra-Red spectroscopy (FTIR),UV-vis diffuse reflectance spectroscopy (DRS) and Nitrogen Sorption Porosimetry (BET). X-ray diffraction patterns show for all samples a typical rutile-type tetragonal structure of SnO_2. The FTIR spectroscopy reveals the presence of tin oxide and vanadium oxide with increase concentration of doping. According to UV–visible absorption measurements this decrease of particle size is accompanied by a decrease of the band gap value from 3.32 eV for SnO_2 down to 2.61 eV for 6 % V doping. Finally, N_2 sorption porosimetry show that the specific surface increase from 9.76 to 21.55 $m^2.g^{-1}$ with concentration increase of doping respectively from 0 to 6 %, the mesoporosity observed being related to the interparticle space.

Key words: Synthesis – Doping – Nanoparticles - Vanadium – Polyol - Tin oxide.

DFT and TDDFT studies of the planar form of the clusters $(ZnX)_6$ X=O, S, SE, TE

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The nanocristals of ZnX (X: O, S, Se, Te) are widely used in various industries such as rubber vulcanization, pharmaceutical productions and optoelectronic techniques. The development of new nanostructures of ZnX represents a great opportunity to create new materials for important applications such as the manufacture of solar cells, which are one of the promising renewable energy technologies for this century, since they have the ability to solve environmental problems worldwide.

In this work, we are interested in the theoretical study of a series of nanoclusters (ZnO) 6 by substituting all atoms of Oxygen by chalcogens of its group: sulfur (S), selenium (Se) and tellurium (Te). The studied clusters are represented in a planar form (crystalline form A).

Calculating the geometrical parameters of the ground state of the cluster (ZnO)6, (ZnS)6, (ZnSe) 6 and (ZnTe)6 was carried out using the density functional theory (DFT) with functional B3LYP and the basis LANL2DZ. The optimization of the first excited state is performed at the Hartree-Fock method, Single Configuration Interaction (HF / CIS). The transmission-absorption spectra are given by the method Time-Dependent Density Functional Theory (TDDFT). Our work has led us to significant results, especially for excited states which have a good process for application to materials in solar cells and optical applications that will be useful in the future theoretical and experimental scale. The figure below represents the geometry of one of the systems cited above.

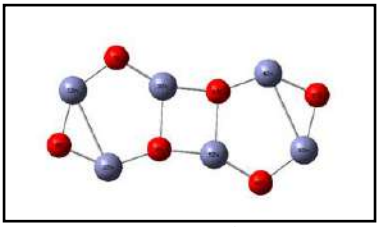

Figure 1: Planar geometry of the cluster $(ZnO)_6$

Keywords: $(ZnX)_6$, O, S, Se, Te, DFT, TDDFT

Transformations of eugenol and its derivatives *via* olefin cross metathesis

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Catalytic reactions that make possible straightforward transformations of natural compounds into high value-added products have potential from the perspective of utilizing renewable feedstock for fine chemistry [1]. Phenolic derivatives found in lignin represent important families of natural molecules with important potential for the access to polyfuctional products.
Olefin metathesis applied to eugenol derivatives controlling at the same time the position of their terminal double bond has provided access to new allylic derivatives of phenol by using acrylates, acrylonitrile and acrylamides as cross metathesis partners [2].

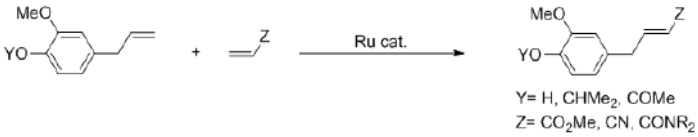

Figure 1: Polyfunctional phenol obtained from eugenol and its *O*-protected derivatives

The addition of 1,4-benzoquinone suppresses the undergo isomerization reactions before and after metathesis via carbon-carbon double bond migration and provides an efficient access to the formation of conjugated styrene derivatives [3].

Keywords: Eugenol, ruthenium, isomerization, 1,4-benzoquinone, cross metathesis.

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DOSAGE D'UN ANTIHYPERTENSEUR PAR COMPLEXATION DANS UNE FORMULATION PHARMACEUTIQUE PAR SPECTROPHOTOMETRIE UV/VIS : LE TRANDOLAPRIL

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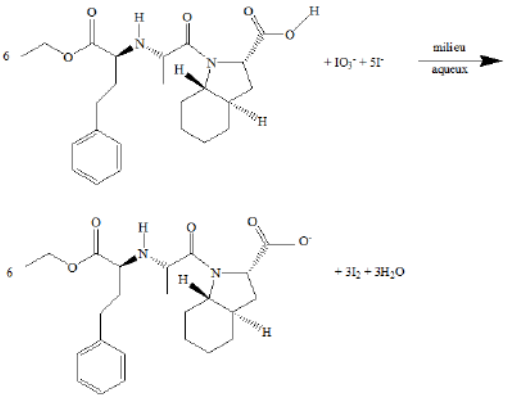
Le tandolapril ou Acide (2S, 3aR, 7aS)-1-[(2S)-2-{[(2S)-1-éthoxy-1-oxo-4-phénylbutan-2-ylamino} propanoyl]-octahydro-1H-indole-2-carboxylique) appartient à la famille des inhibiteurs de l'enzyme de conversion (IEC), agissant sur le système rénine-angiotensine-aldostérone [1]. Ce système, joue un rôle majeur dans la régulation de la pression artérielle. Diverses méthodes ont été développées pour le dosage du trandolapril dans la matière première et dans les formulations pharmaceutiques par spectrophotométrie UV-visible. On propose dans ce travail d'optimiser une méthode du dosage du trandolapril basée sur une réaction de complexation en présence d'un mélange KI/KIO_3. Suivi d'une validation analytique de la méthode optimisée. La deuxième partie sera consacrée à l'étude cinétique de la réaction de complexation pour la détermination de l'ordre de la réaction [2].



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PROPERTIES OF FUNCTIONAL MONTMORILLONITE-DENDRIMER BY Cu(0) / Pd(0) METALLIC NANOPARTICLES AS CO_2 / H_2 ADSORBENTS AND SENSORS

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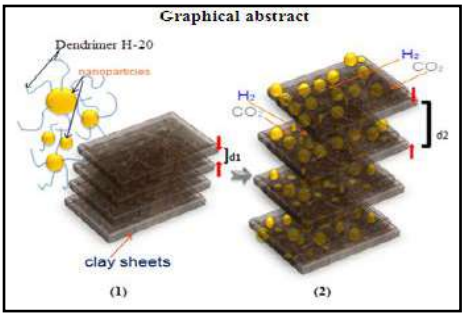
In order to better understand gas (H_2, CO_2) and water interaction with modified Montmorillonite (NaMt) by incorporation of metallic nanoparticles Cu(0), Pd(0) and dendrimer. We present a phenomenon to explain CO_2 and H_2 sorption in the presence of water in NaMt. Adsorption experiments have been performed on functional NaMt at 400° C and atmospheric pressures. Even so with presence of M-NNPs it found for both gases the distance between the minerals clay layers were dependencies on CO_2 and H_2 adsorption. However, the adsorption was also held between layers inters, which have distances larger than nanoparticles size (0.38 nm) and gives rise to the structure destruction such as NaMt lamellae. Based on the differences in H_2 and CO_2 adsorption capacity they infer that oxygen-containing functional groups represent the primary adsorption sites. The competitive interaction turns out to be a volumetric displacement independent of the gas type. As results, thermal analyzes programmed desorption (TPD) indicate an increased affinity for the carbon dioxide (CO_2) relative to the starting mineral. This was explained in terms of highest number of available adsorption sites and the enlargement entered interlayer spaces, which involves the CO_2 adsorption at least two kinds of adsorption sites.



Keywords: Nanoparticles, CO_2 and H_2 adsorption, clay layers, competitive interactions.

HEAVY METALS ACCUMULATION IN WILD PLANTS FROM ABANDONED MINE SITES IN NORTH TUNISIA

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Metal exploitation plays a very important role in the economical, technological and industrial development of the human society. Georesources' exploitation is one of the main foundations of Tunisia economical development. In the last few years, many mines have been abandoned leaving behind millions of tones of mine rocks and mine waste materials with high content of toxic trace elements. These sites represent a major concern because of their potential environmental contamination and risk to human health. Potential metal release and mobility from mine waste materials pose a threat to the local populations. The geochemical dynamics is controlled by the seasonal rain along with high evaporation rates. These factors produce minor acid mine drainage and metal leaching and pollute the groundwater and hence the water of irrigation for agricultural area. In this present study, we propose to restore the mining contaminated sites in North Tunisia by focusing on biological processes. During this study we identified the native species plants that are sampled from the tailings from two abandoned mines (mine of Jbel Erssas and mine of Fej Lehdoum) situated in North Tunisia. The rate of heavy metals especially Pb and Zn in soil and plant samples collected from both sites was investigated. The obtained results showed that effectively, the concentrations of the two heavy metals in the rhisophere were much higher than the eco-toxic required standard values. Among the plant species studied, two plants indicated a higher capacity in metal accumulation *Bacopa monnieri* and *Vetiver grass*. The highest content of Zn have been recorded in *Bacopa monnieri* the metal has been mainly distributed in the aboveground tissues and only small amounts transferred to the root tissues. The maximum Pb content was observed in *Vetiver grass* with the metal being mainly accumulated in the root tissues. These two species may be considered as hyperaccumulators plants and so they should be used as phytoremediation tools in abandoned mine areas rehabilitation programs.

Keywords: Heavy metals, phytoremediation, hyperaccumulator plant.

Synthesis and Reactivity of π-conjugated 2-AzabutadieneComplexes of Palladium and Platinum: Luminescence Properties and Crystal Structures.

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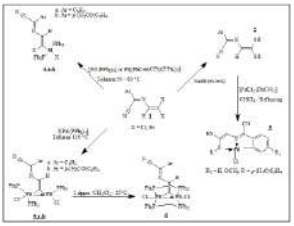
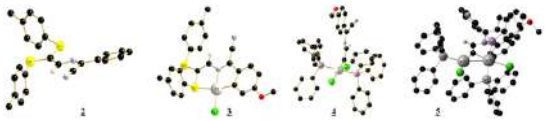
Due to the eminent role of palladium in organometallic synthesis and homogenous catalysis, several methods for formation of palladium-carbon bonds have been developed.[1,2] In continuation on our research on organometallic π-conjugated systems,[3,4] we have developed a straightforward preparative route for the synthesis of cyano-functionalized 2-azabutadiene ligands of type (**1**) and exploited the reactivity of the vinyl-halide bonds for oxidative addition reactions across low-valent metal centers to synthesize σ-alkenyl complexes *trans*-[MX{C(X)=C(H)-N=C(CN)Ar}(PPh_3)$_2$] (**4**) (M = Pd, Pt) possessing a π-conjugated organic array or dinuclear μ-vinylidene complexes of type (**5**). The functionalization of (**1**) by two thioether groups gives rise to polydentate ligands systems (**2**), thus allowing the preparation of cyclometallated Pd and Pt *N,C,S*-pincer complexes.[5]



The synthetic work is completed by a study of the luminescence properties of the azadienic ligands and their derived complexes. The molecular structures of (**2**), (**3**), (**4**) and (**5**) have been determined by X-ray diffraction studies.



Key words : Azabutadienes / σ-alkenyl complexes / Palladium / Platinum / Cyclometallation

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Aryldithiothers *p*-MeXC$_6$H$_4$SCH$_2$SC$_6$H$_4$XMe-*p* (X = O, S) as Assembling Ligands for the Construction of Coordination Polymers.

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In the context of our work on the organic and organometallic chemistry of sulfur-rich organic ligands, we have designed a rich panel of π-conjugated ligands such as 2-azabutadienes Ar_2C=N-C(H)=C(SR)$_2$, Ar(CN)C=N-C(H)=C(SR)$_2$ and vinylferrocenes Z-[(RS)(H)C=C(SR)-Fc] bearing thioether groups and investigated their coordination chemistry.[1,2] We have also used simple dithioether ligands to self-assemble coordination polymers (CPs) and Metal-Organic Frameworks (MOFs) of varying dimensionality incorporating soft Cu(I) and Hg(II) ions.[3,4,5] We have demonstrate that the reaction of aromatic and aliphatic dithioethers with variable flexibility of type RS-$(CH_2)_n$-SR (n = 1-8) with CuX and HgX_2 gives rise to CPs and MOFs, whose fascinating structural richness is not predictable. For example, with CuX salts we obtained CPs, in which dinuclear Cu(μ_2-X)$_2$Cu rhomboids, tetranuclear Cu_4I_4 cubane units, hexanuclear Cu_6I_6 clusters or octanuclear Cu_8I_8 clusters are present as secondary building units (SBUs). These SBUs act as connecting nodes, which are spanned by the dithioether ligands. We have extended our investigations on the synthesis and coordination chemistry of the short-bite dithioether ligands *p*-MeXC$_6$H$_4$SCH$_2$SC$_6$H$_4$XMe-*p* (X = O, S) bearing -OMe or -SMe groups at the *p*-position of the aryl cycle as additional potential donor sites. We present the use of these thioether ligands for the construction of crystallographically characterized CPs, which are in some cases strongly luminescent.

Figure 1. Example of a 1D coordination polymer obtained by reaction of CuBr with p-MeSC$_6$H$_4$SCH$_2$SC$_6$H$_4$SMe-p

Key words : Coordination polymers / Copper / Mercury / Thioether ligands / Luminescence.

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DICHLOROBIS(DIMETHYLSULFOXIDE-O)COPPER(II) : REDETERMINATION OF THE CRYSTAL STRUCTURE AND DFT CALCULATIONS

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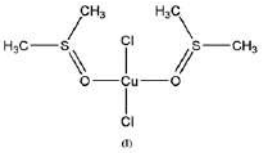

(I)

The crystal structure of the title compound, $[CuCl_2(DMSO)_2]$ (I), previously determined by Willett and Chang [1], has been reinvestigated. Our structure determination is of a significantly higher precision in terms of bond lengths, angles, and R factors [e.g. Cu1-O1= 1.9737(24) Å, O1-Cu1-O1^{i} =173.08(13)° (symmetry code: (i) x, ½-y, z) and $R(F^2)$ = 0.046 compared to 1.955(4) Å, 173.0(3)° and R(F) = 0.075]. In contrast to the previous investigation, all H atoms were clearly found and refined. In the title complex, the Cu^{II} atom is five coordinated in a distorted square pyramidal geometry. Thus, as it reported previously, it can be shown that the crystal structure consists of $[CuCl_2(DMSO)_2]$ molecules which, by virtue of long Cu-Cl interactions, are tied together to form infinite chains parallel to [100] direction. Density functional theory (DFT) optimized structure at B3LYP/6-311++G(2d,2p) level is compared with the experimentally determined structure. HOMO–LUMO energy gap and other related molecular properties are also calculated. Comprehensive theoretical and experimental structural studies on the complex have been carried out by FT-IR and UV-visible spectroscopy.

Key words: crystal structure, DFT calculation, FT-IR, UV-visible spectroscopy.

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VAN DER WAALS CLUSTERS DETECTION THROUGH THE ACTIVATION OF VISCOUS FLOW DERIVED PROPERTIES IN ISOBUTYRIC ACID + WATER BINARY MIXTURES NEAR AND FAR AWAY FROM CRITICAL TEMPERATURE

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Physical and chemical properties of solvent mixtures are important for understanding their thermodynamic behavior. One of the most important considerations is that these properties may provide information about molecular interactions. Excess molar volumes, viscosity deviations and excess molar Gibbs energy of activation of viscous flow in isobutyric acid + water binary mixtures from 302.15 K to 313.15 K. were calculated from experimental density and viscosity data presented in previous work. Here these experimental values were used to test the applicability of the correlative reduced Redlich-Kister equation and the Herráez and Belda equations as well as their corresponding relative properties. Their correlation ability at different temperatures, and the use of appropriate numbers of parameters, is discussed for the case of limited experimental data. The relative functions are important to reduce the effect of temperature and, consequently, to reveal the effects of different factors and types of interactions. Values of limiting excess partial molar thermodynamic properties at infinite dilution were deduced from different methods. In this system it was found that structural order is not much destroyed by the activation process, and consequently bonds are not so much broken between the associated molecules to form smaller clusters (IBA:8 W).

Key words: Binary liquid mixture, viscosity, Reduced Redlich-Kister equation, Molecular interaction, complex, cluster.

Complexation of metals ions using functionalized polystyrene with organophosphate group via amine linkage

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The commercial polystyrene (PS) was grafted with organophosphate groups via amine linkage. PS with amino group was initially prepared by nitration and reduction reactions. Then, the aminated PS was reacted with the tris-(2-chloroethyl) phosphate (TCEP) to conduit a chelating polymer named PS-NH-TCEP. The obtained products were characterized by infrared spectroscopy, elemental analysis and TGA, DTA analysis. These materials were tested for their ability to extract some metallic cations such as Zn(II), Cu(II) and Fe(III) in aqueous solutions.

Keywords: functionalization of polystyrene, Cross-linking polystyrene, Complexation.

CYCLOHEXANOL AND CYCLOHEXANONE OXIDATION TO ADIPIC ACID CATALYSED BY DAWSON-TYPE POLYOXOMETALATES

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Liquid-phase oxidation in heterogeneous system with clean oxidant such as H_2O_2 can lead to an environmentally friendly alternative. Adipic acid industrial production, from cyclohexane via cyclohexanone and cyclohexanol, uses nitric acid (50-60%) as oxidant and Cu/V as catalyst [1-3]. Unfortunately, this method also leads to the nitrogen oxides (NO_2, N_2O, NO) formation. Among them, N_2O contribute to the atmosphere pollution [4]. In this context, adipic acid synthesis from cyclohexanone and cyclohexanol oxidation was studied using Dawson type polyxometalate (POM) as catalyst and hydrogen peroxide as oxidant, according to a green protocol. Adipic acid, main precursor for nylon 6,6, is one of the most widely used chemicals in the world.

The aim of this work was to prepare a series of Dawson-type POMs, as potassium salts, of formula $K_{10}P_2W_{12}Mo_5MO_{62}$ with M=Mn or Co (noted $P_2W_{12}Mo_5M$) in order to examine the effect of the chemical composition on their catalytic performance for adipic acid (AA) synthesis. This last is obtained from heterogeneous liquid phase oxidation of mixture of cyclohexanone and cyclohexanol at 90°C, in the presence H_2O_2 (30%), free solvent. H_2O_2 is easy to handle, its reduction only leads to water and in addition its use requires an acid environment that could come from the POM.

The obtained catalytic results showed that amount of catalyst and composition of polyanion influence the adipic acid yields. With an amount of POM of 0.125g and 15mmol of substrate, $P_2W_{12}Mo_5Mn$ exhibits considerable catalytic performance with ca. 53% of AA yield. An increase of catalyst mass from 0.06 to 0.25g lead to an increase of adipic acid yield from 49 to 77% in presence of $P_2W_{12}Mo_5Mn$.

The use of both Dawson type polyxometalate as catalyst and hydrogen peroxide as oxidant in solvent free media can be an efficient strategy for adipic acid production. These results pave a promising eco-friendly way of reaction for adipic acid synthesis, compared to industrial process that uses nitric acid as oxidant, source of pollutant gas as nitrous oxide obtained as a by-product.

Keywords: Polyoxometalate, Adipic acid, Hydrogen peroxide, cyclohexanol oxidation, heterogeneous catalysis

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A NEW DIMERIC COPPER(II) COMPLEX CONTAINING OXALATE(2-) AND OXAMIDE DIOXIME LIGANDS

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Compound $[Cu(H_2oxado)(C_2O_4)(H_2O)]_2$ (**1**) was obtained as green prismatic crystals from aqueous solution, by the reaction of $K_2[Cu(C_2O_4)_2(H_2O)_2]$ or $(NH_4)_2[Cu(C_2O_4)_2(H_2O)_2]$, with oxamide dioxime. It was characterized by single crystal X-ray diffraction, thermal and elemental analyses, infrared and UV-Vis spectra. (**1**) crystallizes in a triclinic $P\bar{1}$ unit cell and is composed of two neutral $[Cu(C_2O_4)(H_2oxado)(H_2O)]$ entities connected by a Cu-O bond between an oxalate oxygen atom and an adjacent copper(II) ion, thereby producing a centrosymmetric dimer, with the Cu(II) center exhibiting a strongly distorted octahedral coordination (Fig. 1). Neighboring dimers are hydrogen bonded through O-H···O interactions leading overall to a layer structure.

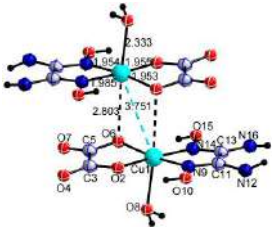

Fig. 1: ORTEP representation of $[Cu(C_2O_4)(H_2oxado)(H_2O)]_2$ (**1**).

It should be noted that a closely related platinum(II) complex $[Pt(C_2O_4)(C_6H_{14}N_2)(H_2O)_2]$ was recently obtained [1] with 1,2-diaminohexane in lieu of oxamide dioxime and exhibiting antitumor properties. Obviously, the isolation of (**1**) opens the door into a fascinating family of materials with potentially interesting properties.

Keywords: Oxamide dioxime, Oxalate, Copper(II) complex, Crystal structure.

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SYNTHESIS, AND CRYSTAL STRUCTURE OF A NEW CHROMIUM COMPLEX $(C_8H_7N_2)[Cr(C_2O_4)_2(H_2O)_2].2H_2O$

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Metal-organic frameworks have received extensive attention in recent years owing to their great specific properties, such as luminescent, magnetic and even industrial and as part of our ongoing studies of new bis(oxalato)chromate(III) species, we have focused our work on the synthesis and structural study of a new compound of formula $(C_8H_7N_2)[Cr(C_2O_4)_2(H_2O)_2].2H_2O$, 1,5-Naphthyridine Trans diaquadioxalatochromate(III) dihydrate. This compound crystallizes in the orthorhombic $Pna2_1$ space group with **a** = 22.645(4)Å, **b** = 11.665(1)Å, **c** = 12.395(1)Å and V= 3274.2(7)Å^3.

The resolution of the structure leads after several cycles of refinement followed by some Fourier-Differences to reliability factors R(F) = 3.75%, wR(F^2) = 10.17% and S= 1.061.

The structure of $(C_8H_7N_2)[Cr(C_2O_4)_2(H_2O)_2].2H_2O$ consists of $[Cr(ox)_2(H_2O)_2]^{2-}$ anion, one $(C_8H_6N_2)^+$ cation and two uncoordinated water molecule.

The structure of the title compound is consisted by layers of complex anion formed by $[Cr(C_2O_4)_2(H_2O)_2]^-$ intercalated by free water molecules and organic cations $(C_8H_6N_2)^+$ (Fig. 1).

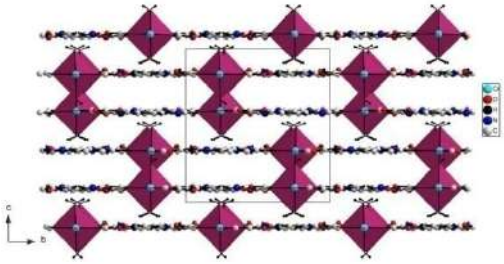

Figure 1: Projection of the $(C_8H_7N_2)[Cr(C_2O_4)_2(H_2O)_2].2H_2O$ structure along the *a* axis

The cohesion of the structure is ensured by O_H..O and N_H..O strong hydrogen bonds [1, 2] and Van Der Walls interactions leading to a three-dimensional framework.

Key words: chromium(III) complexes, Crystal structure, X-ray powder diffraction.

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SYTHNTESIS, CHARACTERIZATION AND CRYSTAL STRUCTURE OF CATIONIC BIS(PYRIDINYLIMINE)Ni(IV)

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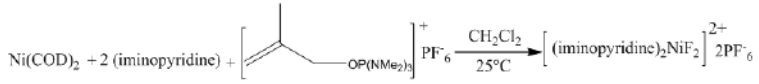
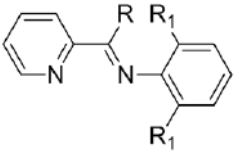
Ligands 2,6-diisopropyl-N-(1-(pyridine-2-ylmethylene)aniline (L1), 2,6-diisopro pyl-N-(1-(pyridin-2-yl)ethylidene)aniline (L2) and 2,6-dimethyl-N-(1-(pyridin-2-yl)ethylidene)aniline (L3) were obtained by condensation reactions.

The reactions of $Ni(COD)_2$ with the corresponding ligands L1–L3 in the presence of methallyloxytris(dimethylamino)phosphonium hexafluorophosphate $[C_4H_7OP(NMe_2)_3]^+PF_6^-$ afford in good yields the new cationic bis(pyridinylimine)Nickel(IV) fluoride complexes C1-C3. These new complexes C1–C3 have been characterized by IR spectroscopy. Solid state of complex C2 have been determined.



Iminopyridine:



L1: R = H, R_2 = iPr
L2: R = Me, R_2 = iPr
L3: R = Me, R_2 = Me

Key words: iminopyridine, methallyloxytris(dimethylamino)phosphonium hexafluorophosphate.

SYNTHESIS, CHARACTERIZATION AND ANTI-TUBERCULOSIS ACTIVITY OF COPPER(II) AND COBALT(II) COMPLEXES CONTAINING 4-AMINOPYRIDINE SCHIFF BASE

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The increasing reports of resistance of *Mycobacterium tuberculosis* (*M.TB*) to the classical anti-tuberculosis drugs pose a challenge to effective control of *M.TB* [1-2]. This drug resistance has led to renewed interest in the search for new classes of compounds active against *M.TB*. Novel bidentate Schiff bases namely (2-hydroxybenzylidene)pyridine-4-amine (**L1**), *N*-(5-nitro-2-hydroxybenzylidene)pyridine-4-amine(**L2**) and *N*-(5-bromo-2-hydroxybenzylidene)pyridine-4-amine (**L3**) have been synthesized. Copper(II) and cobalt(II) complexes of these ligands have been prepared. The compounds were characterized using by elemental analysis, infrared (IR), ^{1}H and ^{13}C nuclear magnetic resonance (NMR), electronic absorption, atomic absorption spectroscopy, and molar conductance measurements. The elemental analysis indicate that the stoichiometry of the complexes is CuL and CoL_2 (**L** = Schiff base ligand). The molar conductance measurements correspond to a non-electrolytic nature for all the complexes which can be formulated as [$\mathbf{M(L)_nX.H_2O}$] (where M = Cu(II), n = 1 and Co(II), n = 2; X = Cl^-). On the basis of IR and electronic spectral studies, a square planar geometry has been assigned to the Cu(II) complexes, whereas an octahedral geometry have been found for the Co(II) complexes. The synthesized compounds were evaluated for their *in-vitro* anti-tuberculosis activity against *Mycobacterium tuberculosis* $H_{37}Rv$ and a clinical isolate using the proportion method. The anti-tuberculosis activity of most of the Schiff bases increased in the presence of metal ion. The metal complexes have higher activity than the free ligands and can be considered as a good starting point to develop new lead compounds for the management of tuberculosis.

Keywords: Schiff base, 4-aminopyridine, Copper(II) and cobalt(II) complexes, anti-tuberculosis

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SYNTHESIS, CHARACTERIZATION AND STUCTURAL STUDY OF MERCURY AND CADMIUM COMPLEXES WITH TRIPIPERIDINOPHOSPHINE CHALCOGENIDES

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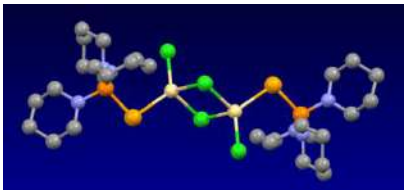
Organophosphine chalcogenides of the formula R_3PE (E = O, S, Se or Te) are attracting considerable interest due to their selective complexation properties towards 'hard/soft' metal cations [1-3]. Interestingly, certain metal complexes of this class of compounds have shown to be suitable single-source precursors for the production of nanocrystals of metal chalcogenides, for example ME (M = Cd, Zn or Hg; E = S or Se) [4,5]. In a previous work [6], we have synthesized a series of cadmium complexes with different phosphine tellurides. In this work, we report on the synthesis of the corresponding complexes with ligands of the type $Pip_3P(E)$ (Pip = piperidinyl ; E= O, S or Se). These complexes were fully characterised by multinuclear (^1H, ^{13}C and ^{31}P) NMR, IR spectroscopies, X-ray analysis and conductimetry. The sulfide and selenide ligands $Pip_3P(E)$ (E= S or Se) were shown to give stable complexes with mercury(II) and cadmium(II) whereas the oxide ligand $Pip_3P(O)$ forms more stable complexes with aluminum(III). Our results show also that the selenide ligand yields more stable complexes than does the sulfide analog. This indicates the clear effect of the nature of the chalcogen atom in these derivatives on their donor character. The X-ray structures reveal that whilst the cadmium chloride complex with Pip_3PS is monomeric, the other cadmium and mercury complexes are dimers with bridging chlorine atoms producing a structure of the type $M_2Cl_4L_2$.



Keywords : Phosphine chalcogenide, piperidinyl, mercury(II) and cadmium complexes, multinuclear NMR.

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SYNTHESIS, CHARACTERIZATION AND SOLUTION BEHAVIOR OF NEW TIN TETRACHLORIDE COMPLEXES WITH ALLYLIC PHOSPHONATES OF BAYLIS HILLMAN ADDUCTS-TYPE

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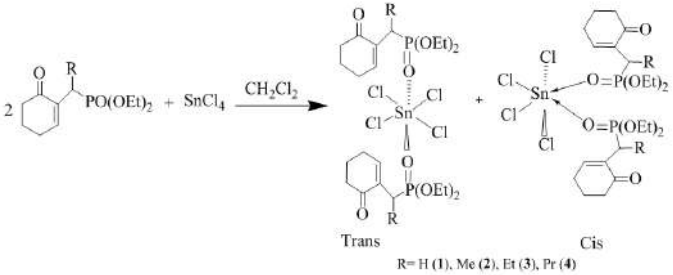
New octahedral complexes of the type $SnCl_4L_2$ (L = allylic phosphonate [1]) (**1**-**4**) were synthesized and characterized by multinuclear (^1H, ^{13}C, ^{31}P and ^{119}Sn) NMR spectroscopy. The NMR data show that these complexes exist in solution as a mixture of *cis* and *trans* isomers with the predominance of the latter form. Interestingly, the solution structure was confirmed by ^{119}Sn NMR spectra which show two triplets corresponding to the two isomers. The triplet feature is due to the coupling of the tin atom with two phosphorus nuclei, indicating that the metal is surrounded by two phosphonate ligands. Furthermore, the solution behavior of these complexes was studied by variable NMR temperature through metal-ligand exchange. The activation energies associated to this exchange were determined to be in the range 13.5-14.5 kcal/mol using the coalescence temperature method. On the basis of these results, the metal-ligand interaction was estimated and compared with closely related tin-phosphoryl complexes [2-4].



Keywords: Phosphonate, complexes, phosphonate ligands, coalescence temperature, tin phosphoryl complexes, Baylis Hillman adducts.

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CLIMATE-FRIENDLY SYNTHESIS OF RIFAMPICIN-LOADED STARCH-STABILIZED SILVER NANOPARTICLES FOR THE TREATMENT OF TUBERCULOSIS

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Background: With almost 30% of the world population suffering from tuberculosis (TB) including its resurgence in the developed world, better management of this global threat is highly desired. Estimates reveal that about 9 million cases occur globally, with Asia and Africa accounting for 85 %. Rifampicin (RIF), an effective antituberculosis drug used in many countries is poorly absorbed from the stomach; hence, low bioavailability remains its major challenge. Application of nanotechnology to solve this problem is gaining increasing interest in this regard. However, most of the researches on carrier systems use very expensive synthetic polymers, making the dosage forms out of the reach of many in developing countries.

Methods: We isolated and purified starch from a cheap and renewable source; *Manihot esculenta*. The purified starch was modified to obtain hydroxypropylated starch. NMR, FTIR and Raman spectroscopies were used to confirm the synthesis, while DSC-TGA, SEM, XRD, viscosity profile, water absorption and solubility indices were used to characterize the new polymer. We also report herein the binding of RIF to starch protected silver nanoparticles and its application in enhanced delivery of RIF for the treatment of TB. The RIF nanoparticles (RIF-NPs) were evaluated for mean particle size, polydispersity index, and zeta potential and further characterized by FTIR and SEM. *In vitro* release of RIF-NPs as well as the effect of nanoencapsulation of RIF-NPs on the antibacterial activity of RIF-NPs against gram-positive and gram-negative bacteria was also evaluated on BACTEC-MGIT960.

Results: Our results show that RIF-NPs were generally spherical with monodispersed size distribution. The nanoparticles were evaluated for mean particle size (273nm), polydispersity index (0.320) and zeta potential (18.16 mV) and further confirmed by UV, FTIR and SEM. *In vitro* release of encapsulated nanoparticles showed significant rapid release profile in acidic pH of the stomach. RIF-NPs exhibited minimum inhibitory concentration (MIC) value of 0.003 ug/mL, while RIF-free drug had MIC value of 0.07 ug/mL.

Conclusion: This study shows that, RIF-NPs prepared from a cheap, non-toxic, renewable and generally compatible natural polymer could considerably improve the RIF antibacterial efficacy, while still being more economical.

Keywords: Tuberculosis, Silver-Starch-nanocomposite, Climate-friendly

BERYLLIUM(II) COMPLEXES WITH $(R_2N)_nP(O)F_{3-n}$ (R = Me or Et; n = 0-3): A DFT STUDY

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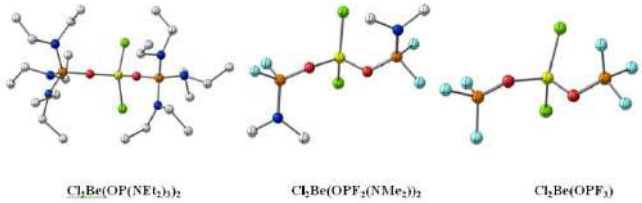
Beryllium is finding increasing use in modern industry because of its unique physical properties [1-3]. Despite this, the chemistry of beryllium is relatively unexplored compared to that of its neighbouring elements [4]. This is due to its high toxicity [5], which acts as a deterrent to the experimentalist if not to the rhetorician. In this present work, we report on the theoretical study of beryllium complexes with fluorophosphoryl ligands of the type $(R_2N)_nP(O)F_{3-n}$ by means of DFT geometry optimisation (B3LYP/6-31G(d) and NMR chemical shift calculations (B3LYP/6-31G(d)). A good correlation was found between calculated and experimental data. The results show that on going from complex $(R_2N)_3PO$ to F_3PO, the Be-OP bond underwent a considerable lengthening from 1.643Å to 1.740Å, while that of the Be-O-P bond angle was found to decrease from 163.0° to 124.1° for $(Et_2N)_3PO$ and F_3PO, respectively. The trends are in good agreement with the calculated metal–ligand binding energies of these complexes. Interestingly, the structural changes are accompanied by increased chemical shifts towards higher frequencies as the R_2N groups in the ligand are substituted by fluorine atoms. The theoretical results showed that the use of the 6-31G(d) basis set could efficiently predict the NMR chemical shifts in the phosphoryl beryllium complexes.



Keywords: Beryllium complexes; phosphoryl ligands; ^{31}P NMR; ^{9}Be NMR; DFT/B3LYP.

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LE LIGAND NEUTRE 1,3-DIÉTHYL-2,4-DIMÉTHYLAMINE-2,4-DITHIO-CYCLODIPHOSPHAZANE $[EtNP(S)NMe_2]_2$: ÉTUDES COMPARATIVES DES RÉSULTATS DE DIFFRACTION DES RAYONS X ET DE CALCUL DFT

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Le matériau $[EtNP(S)NMe_2]_2$ (I) est membre d'une famille de ligands pouvant être utilisés dans l'extraction de plusieurs métaux. Dans le but de mieux comprendre les propriétés complexantes de (I) ainsi que d'autres ligands homologues (ligand mono- ou bidendate, sites actifs,…), des études théoriques moyennant les méthodes semi-empiriques PM6 et DFT en utilisant la fonctionnelle B3LYP avec la base 6-31G(d) sont réalisées. Les résultats issus de ces méthodes sont comparés en premier lieu aux données structurales de (I) (Fig. 1), montrant un bon accord entre les paramètres géométriques théoriques et expérimentaux. En second lieu, ces résultats, en particulier les charges atomiques calculées au niveau B3LYP, montrent que (I) est un ligand potentiellement complexant par les atomes de soufre [1] avec des charges calculées de -0,37e (e : charge élémentaire), valeurs comparables à celles obtenues pour le ligand bis(N,N,N',N'-tétraméthylthiophosphoramidoyl)-méthylamine $P_2S_2N_5C_9H_{27}$ [2].

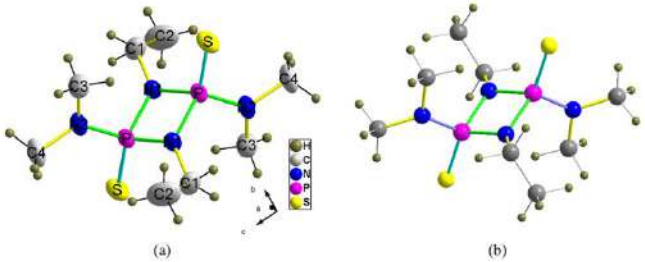

Figure 1 : Représentation en perspective de la molécule de $[EtNP(S)NMe_2]_2$ à partir des données de DRX (a) et de calcul DFT (b).

Keywords: Cyclodiphosphazane ligands; DRX ; ^{31}P NMR; ^{1}H NMR; PM6 ; DFT/B3LYP.

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EFFICIENT SYNTHESIS OF BISOXAPHOSPHOLE 2-OXIDE FROM BISALLENYLPHOSPHONATES

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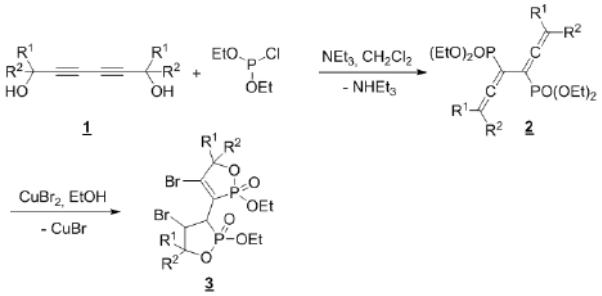
For many years, organophosphorus chemistry has been developed because of a great interest in diphosphorylated compounds owing to their many useful properties ranging from pharmacological activities to their heavy-metal-complexing ability[1,2]. For instance, bisphosphonates proved to be effective inhibitors of bone resorption, and have been used extensively for the treatment of metabolic bone diseases such as osteoporosis, Paget's disease, and bone-related cancers. On the other hand, bisphosphonates have interesting industrial applications as water-softeners, anti-scaling, anti-corrosive and complexing agents, mainly in the textile, fertilizer and oil industries.

With this in mind, we report in the present work, the synthesis of novel phosphorus bis-allene derivatives from the reaction of diyne diols **1** with diethyl chlorophosphite. The cyclisation of the obtained bis-allenylphosphonates **2**, performed in the presence of copper (II) bromide, gave bis-oxaphospholenes **3** in satisfactory yields (Scheme 1).



Scheme 1

Keywords: Bis-oxaphospholenes, bis-allenylphosphonates, diyne diols, cyclization.

References:

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DETERMINATION OF METAL UPTAKE OF COPOLYMER RESIN DERIVED FROM 8-HYDRXYQUINOLINE, PYROGALLOL AND FORMALDEHYDE IN THE PRESENCE OF VARIOUS ELECTROLYTE

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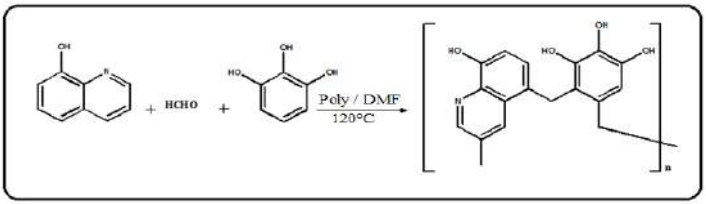
Separation, removal, and the enrichment of metals in trace amounts in aqueous solutions, have an important role in wastewater, industrial or geological sample analysis. The following experimental procedure was applied in order to study the effect of the nature of various electrolytes and concentrations on the amount of metal ion taken up by copolymer resin sample. The copolymer sample derived from 8-Hydrxyquinoline, pyrogallol and formaldehyde (8-HPF) [1] (25mg) was suspended in an electrolyte (NaCl, $NaNO_3$,Na_2SO_4, $NaClO_4$) solution (25ml) of known concentration.

The influence of chloride, nitrate, chlorate and sulphate at various concentrations [2] on the equilibrium of metal – resin interaction had been examined. Fig. 2 to Fig 7 show that the amount of metal ions taken up by a given amount of copolymer depends on the nature and concentrations of the electrolyte present in the solution. 8-HPF is a selective chelating ion exchange copolymer for certain metals. In addition, the copolymer showed a higher selectivity for metal ion Cu^{2+} than for Zn^{2+} and Pb^{2+}.

Key words: Metal ion, Copolymer resin, Chelating ion exchange, Electrolyte



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REMOVAL OF METHYL RED FROM AQUEOUS SOLUTIONS BY ADSORPTION ONTO BENTONITE-TYPE ALGERIAN CLAY

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A large variety of synthetic organic dyes is discharged into the effluents during their production and fabrics manufacturing process. At the same time, dye molecules are very visible in wastewaters due to their strong colour at very low concentrations and in consequence, the colour is one of the most obvious indicators of water pollution **[1]**. The environmental damage of coloured effluents is associated with their toxicity. Adsorption processes using suitable adsorbent have shown high removal efficiency and many economical, ecological and technological advantages **[2]**. Based on their adsorption performance, bentonite-type Algerian clay from Maghnia (N.W. Algeria) has been first acid-activated (HCl) and characterized by powder X-ray diffraction, FT-IR spectroscopy, and electron microscopy (SEM), and specific surface area. The acid-activated clay (AAC) was employed as adsorbent for the removal of methyl red from aqueous solutions using adsorption method. The influence of several parameters (kinetics, contact time, sorbent amount, adsorbate concentration, and pH) on the adsorption capacity was evaluated and discussed. The results indicated that the adsorption was favourable at lower pH **[3]**. Freundlich model provided the best fit to the experimental data with high correlation coefficient (R^2= 0,997) **[4]**. The monolayer adsorption capacity of Maghnia bentonite found to be 3,6 $mg.g^{-1}$. The adsorption kinetic data was modelled using the pseudo-first and pseudo-second orders. It was seen that pseudo-second order equation describes the adsorption kinetics. The results indicated that this bentonite-type clay is potential to be used as an economical adsorbent for the removal of Methyl Red dye.

Keywords: Removal; Bentonite Clay; Methyl Red; Activation; Adsorption

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SYNTHESIS OF NEW FUNCTIONALIZED PHOSPHONATED TRIAZOLES AS LIGANDS FOR METAL COMPLEXES

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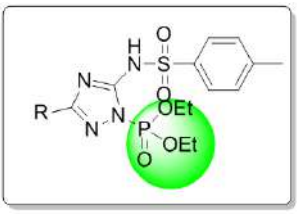
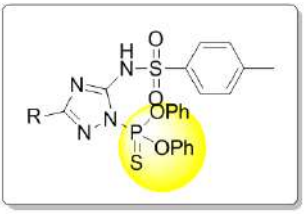
Heterocyclic compounds occur widely in nature and quite a few of these are essential to life processes. The literature on heterocyclic compounds is replete with examples of a large number of synthetic methods of naturally occurring systems which are pharmacologicall[1] active.
Indeed, phosphonated triazoles are used for various applications such as synthetic intermediates in organic chemistry and drug design[2] hybrid materials[3]. In most cases, these systems take advantage of the metal coordination properties of the phosphonate group.
In this context to extend the range of heterocyclic synthesized in our laboratory, we disclosed a new family of phosphonated triazoles ligands. They were prepared by reaction of N-sulfonylisocyanates iminoesters and phosphonated hydrazine.
The structures of all the newly prepared triazoles were confirmed by ^{1}H, ^{13}C NMR spectral data, and elemental analysis.





Key words: Heterocyclic compounds, phosphonated triazolylsulfonamides, Ligands.

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CRYSTAL STRUCTURE, VIBRATIONAL STUDIES, OPTICAL PROPERTIES AND TG-DTA ANALYSIS OF A NEW CHLORO-CADMATE TEMPLATED BY 1-METHYLIMIDAZOLIUM

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Chemical preparation, X-ray single crystal diffraction, thermal analysis, electrochemical measurements, IR, Raman and UV spectroscopic investigations of a novel organic-inorganic hybrid material $(C_4H_7N_2)CdCl_3(H_2O)$ are described. The 1-Methylimidazolium aquapentachlorocadmate(II) crystallizes in the monoclinic system with $P2_1/n$ space group. Its unit cell dimensions are a = 11.4543(6)Å, b = 7.4757(4)Å, c = 11.7675(6)Å and β = 98.997(7)° with V = 995.24(9)Å^3 and Z = 4. The structure provides a new interesting example of infinite inorganic layers of $[CdCl_3(H_2O)]_n^{n-}$ following the **[101]** crystallographic direction. The $[CdCl_5(H_2O)]^-$ anions are interconnected by O–H···Cl hydrogen bonds. Acidic protons of the chloride group were transferred to the organic molecule, giving the singly-protonated cation. The ability of ions to form a spontaneous three-dimensional structure through O–H···Cl and N–H···Cl hydrogen bond is fully utilized. These hydrogen bonds induce notable vibrational effects. IR and Raman spectra are reported and discussed on the basis of group theoretical analysis and on quantum chemical density theory (DFT) calculation using B3LYP/6-311++G(d,p) approach. The molecular HOMO-LUMO compositions and their respective energy gaps were also drawn to explain the activity of our compound. The role of the intermolecular interaction in this crystal is analyzed. The optical study was also investigated by UV–vis absorption spectrum. Thermal analysis reveals the hydrous character of the compound. Cyclic voltammetry was studied to evaluate the spectral and structural changes accompanying electron transfer.

Keywords: Chlorocadmate (II). X-ray diffraction. Thermal analysis (TG/DTA). Infrared, Raman and UV-Vis spectroscopy. DFT calculations. Cyclic voltammetry.

EXPERIMENTAL AND THEORETICAL STUDY OF INTERACTIONS BETWEEN TRIVALENT LANTHANIDES AND ANIONIC CALIX[n]ARENES

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The study of f-elements is of considerable relevance because of their impact in different fields of basic and applied science, including industry, medicine, biology and nanotechnology. The 4f elements are of particular importance because of their unusual photophysical and magnetic properties, which can be enhanced by organic and inorganic ligands or by an adequate matrix. Investigations of the complexation properties of lanthanide compounds have become noteworthy and have exponentially increased. Therefore, a considerable number of different types of linear and macrocyclic ligands have been specifically designed and synthesised for the synthesis of lanthanide complexes.

Over the past, calixarenes have found many applications for industry; chemistry, cosmetology and environmental technology[1]. Due to their great affinity for cations, the liquid-liquid extraction of alkali, alkaline earth, transition metals and lanthanides by calixarene has been extensively studied for decontaminating industrial effluents water and nuclear wastes[2] by complexing pollutants[3].

We report in this work the complexing properties of deprotonated calix[n]arenes towards some trivalent lanthanides (Ln^{3+}), then we have made an attempt to explain the interaction between trivalent lanthanides and anionic calix[n]arenes using density functional theory (DFT). Quantum chemical parameters such as E_{HOMO} (highest occupied molecular orbital energy), E_{LUMO} (lowest unoccupied molecular orbital energy), the energy gap(ΔE), hardness(η), Softness(S), dipole moment(μ), electron affinity(EA), ionization potential(IE), the absolute electronegativity (χ) , the fraction of electron transferred (ΔN), electrophilicity index(ω) and the back-donation ($\Delta E_{\text{Back-donation}}$) have been calculated.

Key words: calix[4]arene, complex, lanthanides, Theoretical calculations.

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QSAR Analysis Of Drug Design ligands: Pyrazole Derivatives

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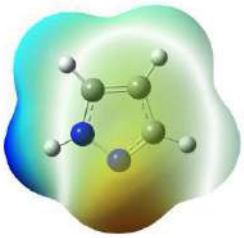
Quantitative structure-activity relationship (QSAR) has been playing a major role in the field of agriculture chemistry, pharmacology, and toxicology since last few years. It can increase the probability of success and reduce time and cost involvement in drug discovery process.

Molecular geometry, electronic structure, effect of the substitution and structure physicalchemical property relationship for pyrazole derivatives, have been studied by molecular mechanics, PM3, Ab initio, DFT and QSAR method. In the present work, the calculated values, namely net charges, MESP contours/surfaces has also been drawn to explain the electronic activity of pyrazole, bond lengths, Non-linear optical properties, electron-affinities, drug-likeness, LipE and QSAR properties, are reported and discussed in terms of the biological activity of pyrazole derivatives.



Key words: pyrazole, FMOs, NLO, MEP, ROV, QSAR properties, lipE

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SYNTHESIS AND CHARACTERIZATION OF A NEW DIPHOSPHOPENTAMOLYBDATE $[C_7H_7N_2]_2[H_2P_2Mo_5O_{23}]_{0.5}\cdot 3.5H_2O$

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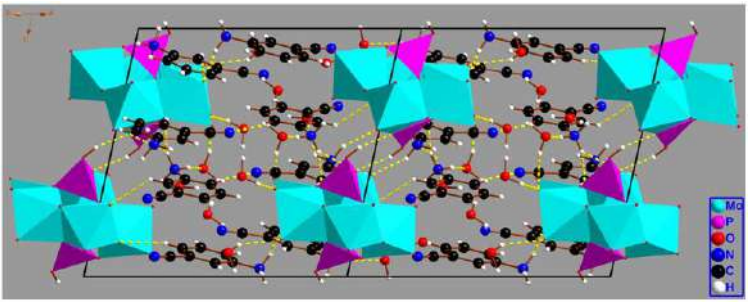
A new diphosphopentamolybdate (VI) $[C_7H_7N_2]_2[H_2P_2Mo_5O_{23}]_{0.5}\cdot 3.5H_2O$ (1) has been synthesized and structurally characterized by single crystal X-ray diffraction, scanning electron microscopy (SEM), IR, thermal stability analysis, Cyclic Voltammetry analyzes and UV–Vis. The compound 1 crystallizes in the monoclinic, space group *C* 2/*c*, *a* = 23.267(3) Å, *b* = 16.759(2) Å, *c* = 13.756(3) Å, β = 110.57(1)°, *Z*= 8. The crystal structure of 1 also contains the isolated polyanion units $[H_2P_2Mo_5O_{23}]^{4-}$ around the protonated 3-Aminbenzonitrile ions and lattice water. The hydrogen bond hold the components together into a three-dimensional network and make the crystal structure of the compound more stable.

Keywords: Diphosphopentamolybdate; Synthesis; Crystal structure; characterizations.



View along the [110] direction of compound (1)

SYNTHESIS AND CHARACTERIZATION OF A NEW β -OCTAMOLYBDATE: $[(C_7H_7N_2)_3(NH_4)]_2[MO_8O_{26}]_2 \cdot 4H_2O$

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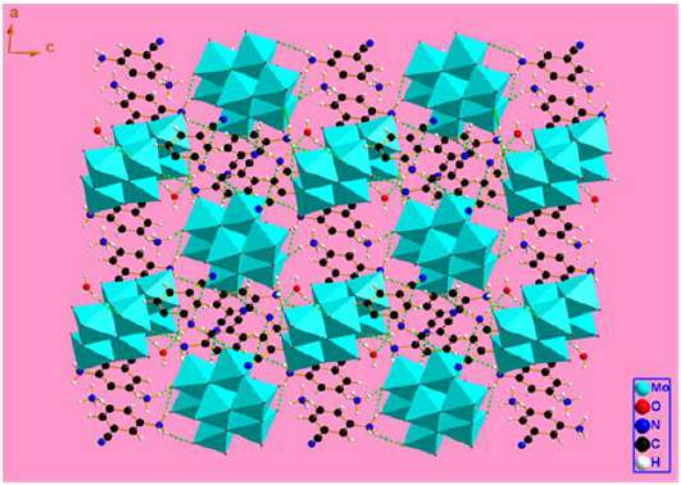
The reaction of $(NH_4)_6Mo_7O_{24} \cdot 2H_2O$ and NH_4VO_3 with 3-Aminbenzonitrile in aqueous solution (pH=2) at room temperature furnishes a new β-octamolybdate $[(C_7H_7N_2)_3(NH_4)]_2[Mo_8O_{26}]_2 \cdot 4H_2O$ (1). The title compound crystallizes in triclinic system, space group P-1, a = 12.0940(4) Å, b = 13.9373(6) Å, c = 15.0625(3) Å, α = 80.479(8) °, β = 83.013(2) °, γ = 66.694(5) °, V = 2295.2(2) $Å^3$, Z = 1, λ(MoKα) = 0.71073 Å. The refinement of the structure leads to a residual factor R = 0.0560 for 5010 reflections [I >3σ(I)]. The structure of 1 consist of β-$[Mo_8O_{26}]^{4-}$ with $(C_7H_7N_2)^+$ and $(NH_4)^+$ cations connected to the mineral parts by hydrogen bonds.

Keywords: octamolybdate, 3-Aminbenzonitrile, Ammonium, characterization.



View along the b axis of compound (1)

DIRECT COUPLING REACTION BETWEEN ALCOHOLS AND SILYL COMPOUNDS CATALYZED BY COORDINATED LEWIS ACID COMPOUNDS: A DFT ANALYSIS

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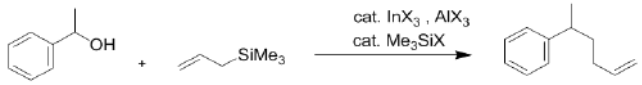
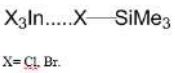
Alcohols are common and important compounds for natural products and key precursors for other functionalized compounds, such as carbonyls, ethers, and alkenes [1]. The C-C bond formation through direct substitution of their hydroxyl groups would be a quite important process to provide useful building blocks in organic synthesis [2]. However, the low leaving ability of the hydroxyl group often retards such a substitution [3]. In this works, we report on a new direct substitution method of alcohols (Schem1) catalyzed by the combination of InX_3 or AlX_3 with Me_3SiX. The catalytic activity would depend on the coordination type of InX_3 or AlX_3 to Me_3SiX "coordinated Lewis acid" (schem2). The optimal combination found with the coordination of $AlCl_3$ to Me_3SiBr, corresponds to the higher electrophilicity index f^+_k = 0.09 for Si site. It appears that electrophilicity of the Si site into coordinated Lewis acid decreases along the series: Cl_3Al---$BrSiMe_3$ > Cl_3Al---$ClSiMe_3$ > Br_3Al---$BrSiMe_3$ > Br_3Al---$ClSiMe_3$ > Cl_3In---$ClSiMe_3$ > Cl_3In---$BrSiMe_3$ > Br_3In---$BrSiMe_3$ > Br_3In---$ClSiMe_3$. This trend is maintained in solution in acetonitrile with an increase in the electrophilic capacity of the Si site. In addition, we propose a plausible mechanism using the reaction of 1-phenylethanol with allyltrimethylsilane both in the gas phase and in acetonetrile solution.



Schem1 : alkylation reaction



Schem2 : combined Lewis acid

Keywords: alkylation reaction, DFT study, Lewis acidity.

References:

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Nanocrystalline $Zr_{0.8}Y_{0.2}O_2$ oxide prepared from smoldering combustion of metal complexes of glycine and citric acid

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The solution combustion synthesis (SCS) was used to prepare zirconium oxide stabilized with a 20% of yttrium (YSZ). A precursor was prepared by combining glycine or citric acid as complexing and fuel agents with metal nitrates as oxidizer in their appropriate ratios in aqueous solution. The precursor was heated to evaporate excess water, yielding a viscous liquid. Further heating caused the precursor liquid to autoignite. Combustion was rapid and self-sustaining. The objective of this work is to find the relationship between the coordination of the organic molecule, used as a complexing and fuel agent, with metal cations and the combustion reaction and thereafter to identify optimum synthesis conditions in order to achieve a pure, crystallized and nanosized material phase. The temperature-time (T-t) profiles recorded during the combustion reaction show that the YSZ and ZrO_2 powders were obtained with a smoldering combustion reaction. However, a flaming combustion, characterized by a strong peak associated to the exothermic reaction of fuel-yttrium nitrates, was displayed with Y_2O_3 powder. The specific surface areas of the obtained cubic solid solutions YSZ are 25 and 35m²/g respectively when glycine and citric acid are used. The NMR-^{13}C spectrum showed that metallic ions were coordinated with carbonyl group. Glycine is coordinated preferentially to yttrium cations Y^{3+} which resulted in a well-crystallized powder with a specific surface area of 17 m²/g. Nevertheless, a proportion of zirconium ion in the form of ZrO^{2+} remains free in the solution which generated an amorphous product with a specific surface area of 14 m²/g

Keywords: Solution combustion synthesis, glycine, Citric acid, complex, coordination.

SYNTHESIS, CHARACTERIZATION AND STRUCTURE OF A SANDWICH TYPE TUGSTOARSENATE: $Na_{12}[As_2W_{18}Cu_3O_{66}(H_2O)_3].36H_2O$

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Over the past decades, inorganic materials based on polyoxometalates through crystal engineering have been attracting considerable interest as a promising new class of materials not only because of the structural and topological novelty of such engineered solids, but also due their potential applications in different areas such as catalysis, medicine, electrical conductivity, magnetism and photochemistry.

A new inorganic compound $Na_{12}[Cu_3(H_2O)_3(AsW_9O_{33})_2].36H_2O$ (1) have been isolated by the conventional solution method and characterized by single-crystal X-ray diffraction, infrared, ultraviolet spectroscopy and Thermogravimetric Analysis (TGA). This compound crystallized in the monoclinic system, space group P2/m, with a = 13.600(1) Å, b = 20.858 (1)Å, c = 16.790(1) Å, β = 109.359(1)°, Z = 2 and V = 4593.5(2) $Å^3$.

The crystal structures of the compounds exhibit three-dimensional supramolecular assembly based on the extensive hydrogen bonding interactions between, sodium, , water molecules and the polyanion $[Cu_3(H_2O)_3(AsW_9O_{33})_2].36H_2O]^{12-}$ which is consist of two $[\alpha\text{-}AsW_9O_{33}]^{9-}$ moieties linked by three Cu^{2+} ions resulting in a sandwich-type structure with idealized D_{3h} symmetry (Fig. 1). The infrared spectrum fully confirms the X-ray crystal structure and the UV spectrum of the title compound exhibits an absorption peak at 207 nm.

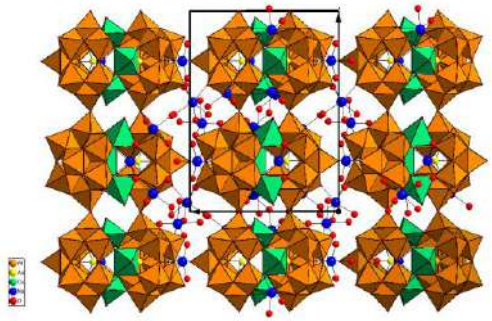

Fig. 1

A packing view of compound 1 along the a axis, showing the arrangement of the $[Cu_3(H_2O)_3(AsW_9O_{33})_2].36H_2O]^{12-}$ clusters, the sodium and water molecules.

Keywords: Chemical synthesis, X-ray diffraction, H-bonds, Polyoxometalates, Infrared spectroscopy.

PARTIAL OXIDATION OF METHANE OVER CO-PRECIPITATED Ni/Mg-Al CATALYSTS MODIFIED WITH COPPER OR IRON

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Ni/Mg-Al catalysts, prepared by Co-precipitation method and characterized by different techniques, were studied in the partial oxidation of methane (POM) to syngas (CO+H2). The catalytic performances were investigated in function of catalyst composition, Cu or Fe addition and conditions of pre-treatment. These catalysts showed a moderate activity and selectivity in the POM reaction. The results show that the activity and selectivity decreased with increasing calcination temperature and Ni content. On the other, the increase of Al amount enhanced the catalytic performances. The solid, doped with iron, constituted the best catalyst for the total oxidation of methane and for the water-gas shift reaction (WGSR). On the other hand, the addition of copper remarkably improved the catalytic performances of the Ni/Mg-Al solids in POM reaction.

Keywords: natural gas, synthesis gas, partial oxidation of methane, nickel, solid solution.

Characterization and Analytical Challenges of *Theobroma cacao*: Implications for the Water Industry

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The use of activated carbon from agricultural wastes could increase economic returns on production of such low economic value products and can also be used to reduce pollution. The main objective of this study was to prepare and to characterize activated carbons from *Theobroma* cacao an export crop produced widely in tropical Africa and used to make chocolate which is also the main source of Theobromine, a bitter alkaloid ($C_7H_8N_4O_2$). Other possible use of theobromine is in such fields as cancer prevention. This particular alkaloid (theobromine from *Theobroma cacao*) has been historically used in the past to treat circulatory problems including arteriosclerosis, certain vascular diseases, and hypertension. Activated carbons have been processed from different types of agricultural materials, such as olive stones, acorn, pecan and walnut shells as well as other stone fruits. The economics of production from these sources are relatively expensive compared to the yield resulting from the processing of *Theobroma cacao* (more than 70%). Methods of preparation involves impregnation with $ZnCl_2$ at different ratios with 50 and 75% (w/w), followed by carbonization at 350, 450 or 750°C for 3 h. The resulting granular activated carbons (GAC) were evaluated by N_2-BET (Brunauer-Emmett-Teller) adsorption. Surface characterization was performed by scanning electron microscopy. Adsorptive properties were highest in the granular activated carbons obtained at 75% $ZnCl_2$ prepared at 450^{o}C. The characteristics of the starting material, the activating agent concentration, and the carbon particle size significantly (>95%) influenced N_2-adsorption capacity.

Keywords: *Theobroma cacao*, Activated carbons, Adsorption, Wastewaters, Organic-inorganic pollutants, Analytical methods

BIOAVAILABILITY AND BIOACCUMULATION OF HEAVY METALS IN SEDIMENTS AND FISH FROM KILIDINI - PORT-REITZ SYSTEM, MOMBASA, KENYA

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Sediments and aquatic organisms in Kilindini-Port Reitz system are exposed to potential adverse effects due to heavy metal contamination from the surrounding anthropogenic activities, consequently triggering the need to conduct an assessment of bioavailability and bioaccumulation of these metals as a function of their speciation in sediments and occurrence in fish tissues. Surface sediments and fish samples were collected at georeferenced locations within the system to determine the total concentrations, bioavailability and bioaccumulation of ten heavy metals (As, Cd, Co, Cr, Cu, Fe, Mn, Ni, Pb and V). Total concentrations of metals in sediments and fish tissues, including their speciation were analyzed using ICP-MS and ICP-OES. Bioaccumulation in fish tissues was determined from calculated transfer factors (tf). X-ray diffraction was used for sediment mineralogical analysis. Sandy silt morphology dominated the sediments. Total concentrations were higher in stations around industrial areas and ship engineering works. Sediment quality assessment showed that there could be occasional cause of adverse effects to aquatic organisms according to Canadian Interim Sediment Quality Guideline (ISQG) values. Sediment speciation revealed that Mn was the highest (41 – 58%) in exchangeable fraction; hence the most available for uptake by living organisms and could lead to exposure of organisms to toxicity and decreased fitness. The rest of the metals had highest concentrations occurring in the residual fraction where they cannot be released under normal conditions, meaning that Kilindini-Port Reitz system is safe from adverse heavy metal pollution. Transfer factors (tf) indicated that As, Cd, Cr, Cu and Zn were found in fish tissues with highest concentrations and tf found in muscles, demonstrating the occurrence of bioaccumulation of these metals, posing threat to communities' health.

Key words: Bioavailability; bioaccumulation; sediments; fish tissues; heavy metals

DEGRADATION OF SYNTHETIC DYES BY A NEW ELECTRO-FENTON PROCESS USING PYRITE AS HETEROGENOUS FERROUS IRON AS CATALYST

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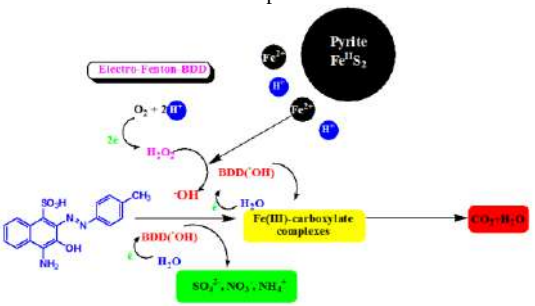
The mineralization of a new azo dye, the (4-**A**mino-3-**h**ydroxy-2-**p**-tolylazo-naphthalene-1-**s**ulfonic acid) (AHPS), has been studied by a novel electrochemical advanced oxidation process (EAOP) consisting in electro-Fenton (EF) oxidation catalyzed by pyrite as heterogeneous catalyst, and so-called "Pyrite-EF". In this process the ferrous ions as catalyst needed for the Fenton's reaction has been supplied by the continuous dissolution of solid pyrite surface instead of a soluble iron salt. The experiments were performed at constant current in an undivided cell equipped with boron-doped diamond (BDD) anode and commercial carbon felt cathode to electrogenerate in situ H_2O_2 and regenerate ferrous ions as catalyst. The effect of operating conditions such as applied current, pyrite concentration, and initial dye content were investigated. AHPS decay kinetics and mineralization efficiency was monitored during the electrolysis by HPLC and TOC measurements, respectively. The experimental results showed that AHPS was quickly oxidized by the reaction with hydroxyl radicals (•OH) produced simultaneously both on BDD surface by water discharge and in solution bulk from electrochemically assisted Fenton's reaction, with a decay kinetics following a pseudo-first-order reaction. AHPS solutions with 100 mg L^{-1} initial TOC content were then completely mineralized in 8 h applying a constant current of 300 mA in the presence of 2 g L^{-1} of pyrite as solid catalyst. Moreover the results demonstrated that the degradation of AHPS by the pyrite electro-Fenton process was more powerful than classical electro-Fenton process in the same conditions.



Keywords: Pyrite electro-Fenton, AHPS, Pyrite, Heterogeneous catalyst, BDD anode, Mineralization, Hydroxyl radical

INFLUENCE OF ANODE MATERAL ON THE ELECTROCHEMICAL OXIDATION OF SYNTHETIC DYES

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[b] *Department of Civil, Chemical and Environmental Engineering, University of Genoa, P. le J.F. Kennedy 1 – 16129 Genova, Italy*

The anodic oxidation of methyl Orange has been studied by cyclic voltammetry and bulk electrolysis, using a range of electrode materials such as Ti-Ru-Sn ternary oxide, lead dioxide and boron-doped diamond (BDD) anodes. The results show that polymeric films, which cause electrode fouling, are formed during oxidation in the potential region of supporting electrolyte stability.

While the Ti-Ru-Sn ternary oxide surface cannot be reactivated, PbO_2 and BDD can be restored to their initial activity by simple anodic treatment in the potential region of electrolyte decomposition. In fact, during the polarization in this region, complex oxidation reactions leading to the complete incineration of polymeric materials can take place on these electrodes due to electrogenerated hydroxyl radicals. Moreover, it was found that BDD deactivation was less pronounced and its reactivation was faster than that of the other electrodes.

The bulk electrolysis showed that the complete COD and colour removal were only achieved using lead dioxide and boron-doped diamond while Ti–Ru–Sn ternary oxide and platinum only permitted a partial oxidation of MO.

Keywords: Methyl Orange; voltammetry; anode materials; electrode fouling; Bulk electrolysis; oxidation.

Theoretical study of spin states of iron (III) complexes with Schiff base ligands

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Within the iron complexes, the tetradentate ligand used herein (See the figure below) was synthetized following a procedure reported in the literature [1].

In this work, Density Functional Theory (DFT) was used to analyse and explain spin state energetics of two mononuclear tetradentate complexes of an iron(III) metallic centre with N4-Schiff base ligands (N4-Fe). Satisfactory validation carried out by DFT was obtained with the OPBE exchange-correlation functional, catching the diversity of the spin state of the iron complexes studied. The importance of the calculation parameters closely associated to chemical environment (solvent…) and the choice of the used of basis set was underlined.

Furthermore, predicting Mössbauer parameters (isomer shifts and quadrupole splitting) of Fe atoms was supported by a correlation between experimental data and the corresponding DFT calculated electron densities at the Fe nuclei and quadrupole splitting. In addition, the UV absorption spectra of the two iron(III) complexes were predicted by relativistic Time-Dependent Density Functional Theory (TD-DFT) using the OPBE exchange-correlation functional and AUG/ATZ2P basis set. The calculations provided a good agreement with experimental data for the assignation of the transition types involved in the corresponding absorption spectra.

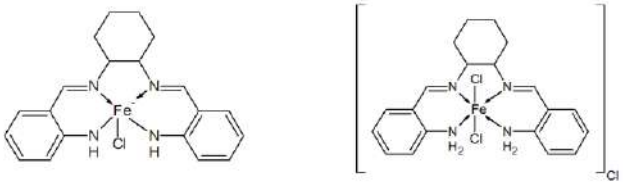

Figure: Studied iron(III) complexes

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2D-QSAR studies on flavonoids as α -glucosidase inhibitors

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Due to their huge use in traditional medicine, the flavonoids have been paying attention of researchers for several decades in order to improve their therapeutic effects. In addition to the proved biological activities such as antioxidant, antitumoral anticancer [1], recently, several researches have been focused on flavonoids and their use as antidiabetic drugs [2] and specifically as α -glucosidas inhibitors.

In order to improve the inhibition of a-glucosidase by flavonoid derivatives, we have used QSAR as efficient approach to model the inhibition of α -glucosidase using a data set composed of 56 molecules, derived from flavonoid, divided into training and test sets. We have used genetic algorithms and multiple linear regressions as features election and training algorithms respectively.

As results, the model presented good statistical parameters (R^2=0.86, Q^2 loo=0.80, Q^2 ext=0.53) and has more predictive power as requested from Tropsha [3].

Keywords: flavonoids derivatives, α -Glucosidase, Inhibitory activity, QSAR

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Preliminary identification of Citrullus Colocynthis from Togo by FT-IR and Raman Spectroscopy

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Citrullus colocynthys (L.) Schrad. (colocynthis , wild gourd, or bitter apple), is a member of the gourd family Cucurbitaceae. It is a non-hardy, herbaceous perennial vine, branched from the base. Originally from tropical Asia and Africa, it is now widely distributed in the Saharo-Arabian phytogeographic region in Africa and the Mediterranean region. Our work consist on preliminary characterization of Citrullus Colcynthis occurs in Togo. This work aims to solid Raman identification and FT-IR characterization of soxhlet extract with three solvents (Petroleum Ether, Hexane and Dichloromethane).

Keywords:
Citrullus Colcynthis, Raman spectroscopy; FT-IR spectroscopy; soxhlet extraction

Chemical characterization of Citrullus Colcynthis the base of the Togolese food

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Nutrition related problems are on rise in the under developed and developing countries and require immediate attention. The physical and mental health of a person solely linked to the consumption of nutritious food. Therefore, in this study we evaluated the chemical constitution and the antioxidant capacity of Citrullus Colcynthis the source of quotidian food of Togolese.

The total phenolic content of the methanol extract was determined according to Folin-Ciocalteu method.Citrullus colcynthis has the highest phenolic content (569, 5±0,010 mg GAE/g extract). Furthermore, the composition of Flavonoid, Procyanhidine and Carotenoid were expressed in reference with standard equivalent..Besides, the amount of minerals was established by atomic absorption spectroscopy. The mineral tested were Ca, Fe, K, Mg, Li, Na and Cu. The mineral Contents were expressed in mg per g of ash. In the current study we evaluated also the percentage of ash, protein and Fat.

For the determination of antioxidant capacity of the methanol extract we began with estimation of total antioxidant activity by phosphomolybdenum method. In addition, Four different methods were used to test the antioxidant activity of the extract, including FRAP assay (Ferric reducing antioxidant potential), DPPH radical scavenging assay (1, 1-diphenyl-2-picryl hydrazyl), ABTS (3-ethylbenzothiazoline-6-sulfonic acid) and *β*-carotene bleaching assay.

Key words: Photochemistry, Total Antioxidant Activity; ABTS, DPPH; FRAP; *β*-Carotene Bleaching Assay;

MERCURY(II) COMPLEXES WITH PHOSPHINE TELLURIDES: SYNTHESIS AND MULTINUCLEAR (^{31}P, ^{125}Te and ^{199}Hg) NMR CHARACTERIZATION IN SOLUTION

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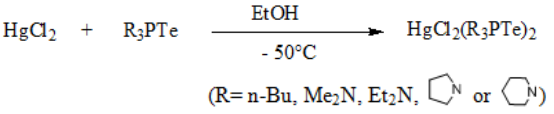
Phosphine chalcogenides of the formula R_3PE (E = O, S, Se or Te) are attracting considerable interest due to their selective complexation properties towards 'hard/soft' metal cations [1-3]. Recently, certain metal complexes of this class of compounds have shown to be suitable single-source precursors for the production of nanocrystals of metal chalcogenides, for example ME (M = Cd, Zn or Hg; E = S or Se) [4,5]. In a previous work [6], we have synthesised novel cadmium complexes with different phosphine tellurides. Herein, we describe the synthesis of new mercury(II) complexes with phosphine telluride ligands of the type $HgCl_2(R_3PTe)_2$ [R = n-Bu (**1**), Me_2N (**2**), $C_5H_{10}N$ (**3**) or C_4H_8N (**4**)]. These were characterized by IR and multinuclear (^{31}P, ^{125}Te and ^{199}Hg) NMR spectroscopy. In particular, the solution structure of these complexes was confirmed by ^{31}P NMR at low temperature, which displayed a singlet for each complex flunked by ^{125}Te satellites. These signal features were further accompanied by ^{199}Hg satellites due to corresponding two-bond P-Hg couplings, clearly showing that the ligand is coordinated to the metal through its tellurium atom. The use of these complexes as single source precursors for the preparation of HgTe nanoparticles was also investigated and results are discussed and compared with those obtained for closely related phosphine chalcogenide analogs.



Keywords: Phosphine telluride, mercury, metal complex, ^{125}Te and ^{199}Hg NMR.

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Site selective luminescence of Eu^{3+} ions in $K_2Mg(SO_4)_2 \cdot 6H_2O$ Crystal

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Eu^{3+} -doped $K_2Mg(SO_4)_2 \cdot 6H_2O$ crystal was prepared by evaporation method at room temperature. A complete structure characterization including X-Ray diffraction, Raman and infrared was carried out. The results reveal that this crystal crystallizes in a monoclinic structure and the most active phonons are associated with vibrations of molecular water and sulfate environments. On the other hand, the emission spectrum indicates that Eu^{3+} ions occupy two different sites. Therefore, a study about the luminescence from each local environment is presented. The emission spectra and luminescence decays of Eu^{3+} ions indicate than there are not energy transfer processes between both sites.

Key words: Chemical synthesis, Crystal structure, Luminescence, Infrared spectroscopy

DESIGN OF NEW BULKY BIS(ALPHA-DIIMINE) LIGANDS

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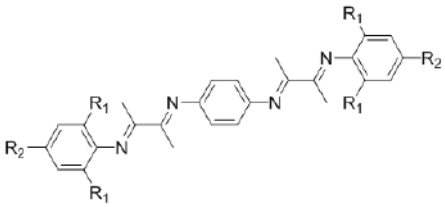
In recent years, a considerable effort has been devoted towards designing new ligand frameworks to improve catalyst performance. Especially, dinucleating ligands leading to a more efficient catalytic systems and processes benefiting from cooperative effects between adjacent active metal centers in binuclear complexes. The same electronic effects cannot be expected in their mononuclear counterparts. Subsequently, there are few works on modified α-diimine ligand systems, however, only few reports showed the use of bulky bis-α-diimine ligands in the formation of active metal complexes. In this recent work, we describe the synthesis of new bulky bis(α-diimine) ligands obtained by two successive condensation reactions between carbonyls and primary aromatic amines. Steric and electronic modulations in the ligands have been insured by the variation of the substitutions on the aryl groups.



L1 : R1 = H ; R2 = Me
L2 : R1 = Me ; R2 = H
L3 : R1 = iPr ; R2 = H

These new bis(a-diimine) ligands have been characterized by IR and RMN spectroscopy.

Keywords: dinucleating; a-diimine, adjacent metal centers

Zinc (II) complexes with bidentate orgnaphosphorus ligands: Synthesis and multinuclear NMR characterization in solution

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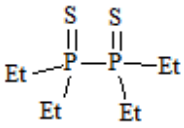
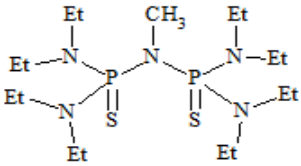
The coordination chemistry of bidentate phosphine chalcogenide ligands has become an active area of research due to their selective complexation properties towards'hard/soft' metal cations[1]. Such chelates are widely used in catalysis, metal extraction, bioinorganic chemistry and many other fields[2].
In this present work, we report on the synthesis of zinc(II) complexes with two different disulfide ligands : the tetraethyldiphosphine disulfide $Et_2P_2S_2$ and the bis(tetraetylthiophosphoramidol)methylamine $MeN[P(NEt_2)_2(S)]_2$. The spectroscopic characterizations showed that these ligands are coordinated in a bidentate fashion to the metal center via its both P=S groups.





Key words: Bidentate ligand, zinc complex , tetraethyldiphosphine disulfide, bis(tetraetylthiophosphoramidol)methylamine and NMR characterization .

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ELABORATION OF NEW OBJECTS BELONGING TO COORDINATION CHEMISTRY AND MOLECULAR MAGNETISM

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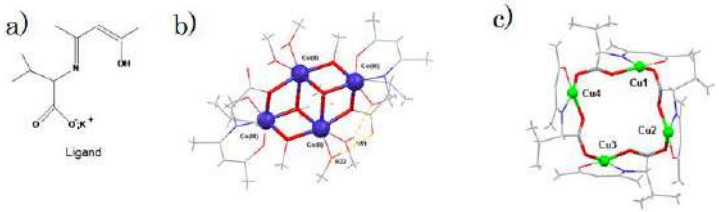
Among all the potentialities of coordination chemistry, molecular magnetism is very promising as magnetic information can be stored on one molecule. In that sense we developed in our group several strategies in order to obtain such molecular nanomagnets. One idea was to use macrocylic ligands to generate high nuclear clusters. A second approach was to put together molecular precursor bricks to generate big hetero- or homo-metallic clusters. Along this way we were able to create cubane-like complexes which can be condensed in different manners to elaborate new Single Molecule-Magnets.



Keywords: Cluster-assembled materials, magnetic compounds, Ligands, metals, Structural studies.

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Calcium Hydride as a Powerful Reducing Agent for Topotactic Oxide Deintercalation: Synthesis, Characterization and Structural Properties of Topotactically Reduced $La_{2-x}Ca_xCuO_4$ ($0 \leq x < 0.2$).

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The capability of calcium hydride as a reducing agent in oxide deintercalation reactions is explored. Reaction of the n = 1 Ruddlesden-Popper phase $La_{2-x}Ca_xCuO_4$ ($0 \leq x < 0.2$) with CaH_2 in a sealed evacuated tube at 200 $\leq T/°C \leq 300$ yields the Topotactically Reduced phase $La_{2-x}Ca_xCuO_{3.5}$ (a = 8.6071 (4) Å, b = 3.8378 (8) Å, c = 12.9964 (4) Å). The variation in the anion vacancy distribution of these reduced phases as a function of stoichiometry is discussed in relation to the coordination polyhedra of the metal cations. Structural characterization indicates the coexistence of a new oxygen-vacancy-ordered arrangement of cooperatively- distorted Cu_2O_3 planes containing 4-coordinate Cu^+/Cu^{3+} sites.

Key words: nonstoichiometric oxides, topotactic reaction mechanism, Oxygen mobility.

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Preparation of 2, 2, 2- triphenyl-1, 3, 2- dioxabismole derivatives

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Since 1951, organometallic chemistry has given birth by Pauson and Kealy [1], when combined with iron metal organic compound. This mixed combination did score a great revolution in the field of organometallic chemistry by Wilkinson and Woodward [2]. Their applications in industry have become large, and researchers have looked to their synthesis and study of their physical and chemical properties [3] and are, among others, used as catalytic agents, oxidizing arylants and in chemical reactions.

In our work, we are interested in the preparation of some derivatives of triphenylbismuth pentavalent cyclic of five-membered ring by changing the ligand between triphenylbismuth dichloride and derivatives of aliphatic dicarboxylic acids.

Moreover, the NMR spectra the proton and carbon 13 compounds obtained are due to two structural proposals five to ten membered obtained for each compound. Confirming their actual structure will be determined by the data set of X-ray diffraction.

Keywords: triphenylbismuth pentavalent cyclic, arylant agent, antioxidant agent, catalyst agent, dichloride triphenylbismuth, dicarboxylic acids.

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Electrochemical and electrochromic properties of NaV_2O_5 thin films

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Electrochromism is the reversible and visible change in transmittance and/or reflectance associated with an electrochemically induced oxidation-reduction reaction [1]. The electrochromic devices (ECDs) have promising applications in many fields, including “smart windows” in cars and buildings, reusable price labels, controllable light-reflective or light transmissive display devices (for optical information and storage) [2]. NaV_2O_5 has been investigated for a number of applications because of its layered structure with good cation intercalation ability, low voltage applied, exhibits both anodic and cathodic electrochromism properties and multicolor display. Several methods, for example, vacuum evaporation, pulsed laser, sputtering, and sol-gel, have been used to manufacture NaV_2O_5 thin films. This work deals for the first time with the NaV_2O_5 thin films prepared by "Doctor Blade" deposition. This method has already proven effective for the preparation homogeneous and porous thin films. Using the NaV_2O_5 layers on indium-tin-oxide (ITO)-coated glass as electrode, the electrochromic properties were investigated by cyclic voltammetry (CV) and optical measurements ex-situ in ionic liquid electrolyte 0.3 M (LiTFSI) in (BMITFSI). The thin films presented a better cycling stability, reversibility and multi-electrochromic behavior (orange-yellow-green) with an optical modulation of 24% in the spectral region 550-700 nm.

Key words: Vanadium oxide bronze, thin films, lithium-ion intercalation, electrochromic

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Changes in Chemical and Physical Properties of Groundnut Oil used for Frying Fish and *Falafel.*

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[c)] *U. of G., Faculty of Engineering & Technology, Dept. of Food Engineering (c)*
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Different edible oils used in frying food, are expected to have some changes in their physical and chemical properties including the production of harmful compounds. Moreover, it is now a common practice in homes and restaurants, reusing oils for frying fish or *falafel* several times. The objectives of this research were to investigate the changes in the physical and chemical qualities of groundnut (GN) oil used in frying fish and *falafel*, determine the level of Cu, Cd and Pb and study attitudes and practices done by restaurants and homes during frying process. These objectives were achieved through different methodologies; a questionnaire composed of 20 questions has been designed to 103 and 78 cooks of homes and restaurants, respectively, and depending on questionnaire findings the experiment was designed. The experiment was composed of two types of food (fish and *falafel*) which were fried separately and continuously in GN oil, for 20 cycles. Samples were taken during frying process at initial/fresh oil, 5th, 10th, 15th and 20th frying cycle number and analyzed for chemical and physical changes. The survey results showed that the process of frying in homes sector were found acceptable, except in reusing deteriorated frying oil for wiping *Kisra* pan's and cooking food. However, in restaurants, unacceptable practices were done in terms of, prolonged use of thermally deteriorated frying oils, storing remained oil in fryer, topping oil and pouring waste oil in drainage system. Color index and viscosity of the GN oil increased as the number of frying cycles increased. Peroxide, acid values and free fatty acid percent of GN oil, were increased as frying number increased. Total polar compounds (TPC) of GN oil increased as frying number increased. However, no significant differences ($p>0.05$) in physical and chemical changes were found in GN oil used for frying both types of fried food. The level of Cu, Cd and Pb change rates in GN oil used for frying fish ranged from 174-584, 0-5 and 39-638 ppb, respectively. Regarding frying *falafel*, the respective ranges were 163-222, 0-5 and 67-200 ppb, respectively. TPC and Cd didn't exceed accepted limits in studied oil, except for Cu and Pb. Thus, the study recommended that changes in chemical and physical properties of GN oil has been found acceptable in terms of quality, except for limits of Pb and Cu it is not safe.

Keywords: (Groundnut oil – Frying – *Falafel* – Fish – Restaurants and home - TPC – Heavy metals)

REMOVAL OF CHLORINE SECONDARY POLLUTANTS FROM AQUEOUS MEDIA USING SUBSTRATE ANCHORED ZERO VALENT BIMETALS

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The focus of this study was to immobilise zero valent bi-metals on a solid substrate and apply if for degradation of chlorine disinfectation compounds from water. This involved the synthesis of a solid material on which metal ions could be complexed reaction followed by reduction to zero valent state. Polystyrene material contains no functional groups capable for metal ions complexation, but was modified through the nitration of the aromatic rings followed by a subsequent reduction to form an amino compound upon which metal ion were complexed. The resulting material in each step was characterised with FTIR .The results after nitration showed the presence of a peak at 1523.71 cm^{-1} which could be due to a nitro group within the ring structure which is characteristic of a nitrogen substituted ring, a peak observed at 1600.8 cm^{-1} could be due to NO_2 attached to the ring. Signals at 1226.6 cm^{-1} and 1651.0 cm^{-1} could be due to N=O stretch. After the reduction of the nitro compound, the peaks observed at1523.71 cm^{-1}, 1651.0 cm^{-1} and 1226.0 cm^{-1} disappeared due to the formation of an amine group. A strong band at 3425.3 cm^{-1} is attributed to -NH group. After anchoring the metals the strong band at 3425.31 cm^{-1}, 2935.5 cm^{-1} , 1604.7 cm^{-1} , 1647 cm^{-1}, 2455.2 cm^{-1}, 1527.5cm^{-1}, 1697.2 cm^{-1} , 3425.3 cm^{-1} and 3109 cm^{-1} disappeared and new bands observed at 1110.9 cm^{-1},1190 cm^{-1},1384.8 cm^{-1} and 1645.2 cm^{-1}. This may be due to the metal ion co-ordinated with the substrate. The bands observed at 518 and 617.2 cm^{-1} region, may be due to the formation of metal-nitrogen bonds.

Keywords:
Polystyrene, Chlorination, Zero-valent bimetals, Degradation, Complexation, Reduction, Secondary pollutant.

Characterisation by electrochemical impedancespectroscopy of a pet membrane electrode basedon zeolithe

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A polyethylene terephthalate membrane electrode based on clinoptilolite as the ionophore was prepared and was deposited on a gold electrode. This one was characterised with electrochemical impedance spectroscopy and modelled with an equivalent electric circuit. The detection of ammonium at low concentrations and the interaction with the other cations were made by impedance measurements. The study of the interaction of ammonium ions in presence with the cations such as Na^+,Ca^{2+} and K^+ in the same concentration showed that the electrode is selective and sensitive for very low concentrations 10^{-7} mol/l, but the membrane is saturated for concentrations greater than 10^{-2}M. The life expectancy of the membrane exceeded 50 days when we changed the PBS solution after 44 days.

Key words: Impedance spectroscopy , Clinoptilolite , Ammoniumdetection

INCLUSION PROPERTIES BY SOME PYRANOPYRIDOTHIAZOLE DERIVATIVES

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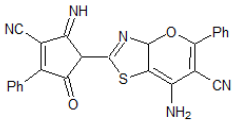
Pyranopyridothiazole derivatives are biologically interesting molecules that have established utility in the pharmaceutical compounds with these ring systems have a wide application range of biological activities and pharmacological actions,[1] antibacterial[2] inhibitory activity.[3]

The binding properties of a Aminothiazole (**1**) and Cyanopyranopyridothiazole (**2**) derivatives toward the alkali, alkaline earth and some transition metal cations, have been investigated in methanol, followed by UV Spectrophotometry Absorption and conductivity. Thus, the stoichiometries of complexes formed and their stability constants were determined by digital processing of data.



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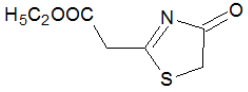

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Key words:. Thiazole, Stoichiometries, Stability, constants, Inclusion properties

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SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL ACTIVITIES OF NEW AZO LIGANDS AND THIER METAL COMPLEXES 4: 3-[(E)-(1,5-DIMETHYL-3-OXO-2-PHENYL-2,3-DHYDRO-1H-PYRAZOLE-4-yl)DIAZENYL] PENTANE-2,4-DIONE AND ITS Co(II), Fe(III), Ni(II) and Cu(II) COMPLEXES

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Aminoantipyrine was diazotized and coupled with pentane-2,4-dione to derivatize **3**-[(E)-(1,5-dimethyl-3-oxo-2-phenyl-2,3-dhydro-1H-Pyrazole-4-yl)diazenyl] pentane-2,4-dione) (DOPDPD). The Co(II),Fe(III) and Cu(II) and Ni(II) complexes of Ligand were also synthesized. DOPDPD was characterized based on the UV, IR, 1H and 13C NMR Spectroscopy, Elemental analysis and X-Ray crystallogragh. However, the structures of the complexes were determined on the basis of conductance studies, stoichiometric determination, IR and Electronic spectra. The ligand was tridentate coordination through oxygen and nitrogen and formed complexes of octahideral geometry with all the metal ions with general formula ML_2 .The Ligand at 20mg/cm^3 concentration showed no activity against all the micro organisms. However, the Co(II) complex was very active against all the micro-organisms up to concentration .0.625 mg/cm^3 when compared to ampicillin.

WATER-FILLED PSEUDO-NANOTUBES CARRYING PROTONS IN THE SILVER SALT: $Ag_{2.50}H_{0.50}[Cr(C_2O_4)_3]\cdot 5H_2O$ (1)

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The family of materials with a variable Ag-Cr-oxalate channel lattice, formulated generally as $[(M_xAg_{0.50-x})(H_2O)_3]@[Ag_{2.50}Cr(C_2O_4)_3]$ ($0 \leq x \leq 0.50$; M = K, Cs, Ag), has been at the focus of interest in contemporary research and development [1]. These silver salts generally crystallize in a nonmolecular polymer framework preferentially with flexible deficiencies x of Ag^+ ions, thus generating a negatively charged lattice grid. They share in their crystal structures the one-dimensional channel lattice as their characteristic feature. Recently, we reported a closely related channel lattice network with chemical composition $[Ag_{2.90}Cr(C_2O_4)_3]^{0.1-}$ [2], where the silver charge deficit is compensated solely by protons embedded amongst water clusters within the channels. In the present work, we describe compound **1** as another member of this family of silver-deficient oxalatometalates with the lattice grid $[Ag_{2.50}Cr(C_2O_4)_3]^{0.5-}$, where the silver charge deficit (0.50) is offset by the equivalent charge from 0.50 H^+ - the highest observed so far. Evidence of the protonic charge allowed to migrate very fast up and down within the "water-streams" in the channels, pretty much like this usually happens in acidic aqueous media, opens the door into the fascinating family of materials that may be dubbed *Nanochannelled Onedimensional Proton Conducting Solids (1D-PCS)*. Experimental results will be presented and discussed.

Keywords: Crystal structure; Nanochannels; Silver-deficient coordination polymers; Water clusters; Proton conducting solids.

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Laser Flash Photolysis studies of *o*-hydroxyacetophenone and its derivatives

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Photoremovable protecting groups (PPG) have undergone a renaissance in recent years. They offer the means to deliver rapidly bioactive materials, such as neurotransmitters, ATP, or simply Ca^{2+} ions, to small, addressable target sites, and thereby they enable biologists to follow the ensuing physiological events in real time [1].

Raising interest in the applications generates demand for more efficient and faster releasing the target molecules. Recently, a clean bifurcation between two important photochemical reactions – a competition between the Type II hydrogen abstraction and photo-Favorskii rearrangement for *o*-hydroxyphenacyl-*o*-methylphenacyl derivatives has been carried out [2]. The knowledge of the release mechanism and identification of the intermediates formed during the course of this photoinduced reaction could help us to design a new PPG system. The photochemistry of *o*-hydroxyphenacyl chromophore and its respective derivatives have been investigated using laser flash photolysis, and the possible mechanism is proposed along with the reported observed rate constants.

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Synthesis and photophysical properties of novel fluorescent sensors for the highly selective Zn (II) detection

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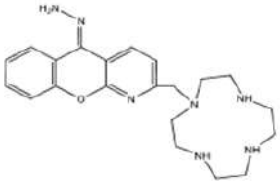
The synthesis of optical probes presents several promising approaches, especially in the field of biology analysis, medical imaging and commercial devices.
Their principle is based on the complexation of the metal ion, giving rise to a specific optical response, either through CHelation-Enhanced Fluorescence (CHEF) or CHelation-Enhanced Quenching (CHEQ) effect.
This process can be used to detect metal cations such as Zn (II), which is involved in many biochemical functions e.g., vision and immune reactions.

For this aim we have developed potential sensors for Zn^{2+} ions, based on novel derivatives of methyl-chromeno-pyridinyliden hydrazone[1]. We studied its photophysical properties and its coordination behaviour towards this intrinsically spectroscopic silent ion. The fluoroionophore wherein the complexing unit is the cyclen and the fluorescent unit, an original azaxanthone-hydrazone (Scheme1). Then, by monitoring selectivity fluorescence tests with various divalent cations we have confirmed the good ability of our ligand to sense Zn^{2+}.



Scheme1: A new mono-*N*-functionalised fluorescent chemsensor

Keywords : Transition metal, Zinc, fluorescent probe, fluorescence.

Reference

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Chemical Composition and Anti-inflammatory Activity of the Essential Oil of *Foeniculum Vulgare (Fennel)* from South Africa (Eastern Cape)

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Foeniculum vulgare is a medicinal and aromatic wild-growing plant found in the Eastern Cape region of South Africa. This study evaluates comparatively the volatile components of different morphological parts of the plant and their anti-inflammatory activity.

Fresh leaf, root and seed as well as dried leaves of the plant were separately processed by hydrodistillation for 4 h and their essential oils ((EOs) collected. Extracted EOs were further subjected to GC/GC-MS analysis. The oils were later evaluated for anti-inflammatory activity on the egg albumin-induced oedema model in rats.Rats pretreating orally with EOs 1h before subplantar injection with 0.1 ml of 50% (V/V) fresh egg albumin and paw sizes measured with digital caliper hourly over a period of 5 h.

Chemical analysis of EOs showed that the number of compounds detected and identified were 22, 19, 21 and 18 for fresh seed, fresh leaf, fresh root and dried leaf respectively. The oils obtained were light-yellow in colour and aromatic. The percentage yield was in this order: fresh seed>fresh leaf>fresh root>dried leaf. The chemical compositions of obtained EOs also varied among the oils while the major compounds identified included; anethole, fenchone, limonene, α-pinene and methyl chavicol. The results of the anti-inflammatory test showed that all the oils caused significant ($P<0.05$) reduction in oedema size compared to the negative control group mainly at 2-3 h post induction. However, fresh and dried leaf oils showed better activity compared to the standard drug (Ibuprofen, 100 mg/kg).

It can be concluded that various morphological parts of *F. vulgare* contain volatile oils which varied in their yield and chemical compositions. All the oils demonstrated significant anti-inflammatory activity. The sweet aroma and biological activity showed by these oils may be useful in cosmetic and pharmaceutical industries.

Keywords: *Foeniculum vulgare*, Essential oil, Anti-inflammatory.

GREEN ROUTE SYNTHESIS OF ZNO NANOPARTICLES, CHARACTERIZATION AND APLLICATION IN ETHANOL SENSING

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Nanotechnology is currently occupying the minds of researchers due to the fact that nanoparticles have most of their constituting atoms on their surfaces. In addition, the nanoparticles are similar to biomolecules and can thus penetrate a cell. These two properties make nanoparticles have unique and noble properties compared to their bulk counterparts. Nanoparticles thus have tremendous applications in sensors, medicine, cosmetics, optoelectronics, environmental protection, information storage and in catalysis.
Chemical and physical methods used for synthesis of nanoparticles suffer from many drawbacks like the use of toxic chemicals, high energy consumption and expensive equipment. Biological methods specifically the use of plants is currently under exploitation due to the fact that they are cost effective and environmentally friendly way of synthesizing nanoparticles. In the present study, zinc oxide nanoparticles (ZnO NPs) were successfully synthesized using zinc nitrate and aqueous bio components of leaves extract of *Spathodea campanulata* as the reducing as well as stabilizing agent. The medicinal value of *Spathodea campanulata* fascinated me to utilize it for biosynthesis of zinc oxide nanoparticles (ZnO NPs).
The nanoparticles were characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Visible spectroscopy, attenuated total reflection Fourier transform infrared (ATR-FTIR), energy dispersive X-ray spectroscopy (EDX) and X-ray diffraction (XRD). Formation of nanoparticles was monitored using UV-Visible spectroscopy and absorption peak in the range of 320-330nm was observed. The band gap of the ZnO nanoparticles was calculated from absorption spectra and found to be 3.4eV. From the transmission electron microscope (TEM) images, the fashioned ZnO nano crystallites were of average size range of 20-50nm. XRD, SEM and EDX characterization revealed the face-centered cubic of highly crystalline nanoparticles with spherical shape and presence of elemental zinc and oxygen. Attenuated Total Reflection Fourier Transform infra-red was used to study the groups of biomolecules involved in the reduction of Zn ions as well as stabilization of the ZnO nanoparticles.
Cyclic voltammetry was used to study the electrochemical properties of the ZnO nanoparticles based ethanol sensor. The surface area of glassy carbon electrode (GCE) was modified using ZnO nanoparticles and this enhanced the current response for the electrochemical nanosensor with a detection limit of 0.1112×10^{-6}M being achieved. The study shows that the ZnO nanoparticles have potential applications as new generation ethanol sensors.

MATERIALS AND BIODEGRADABLE BIOSORBENTS BASED LOCAL RESOURCE APPLICATION TO FIXING DYE AQUEOUS SOLUTION.

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Laboratoire de Chimie Appliquée et Génie Chimie, Département de chimie, Faculté des Sciences Université Mouloud Mamemeri, Tizi Ouzou, Algérie

Pomegranate peels studied within the frame work constitute a locally abundant and law const resources. The aim of study is to illustrate the valorization of these fruits peels and their use for processing of waste chaste changed in textiles dyes. The purpose of our study is the adsorption of the textile dye BS (Blue Solophenyl GL, CI Direct Blue). The experiments were performed in batch under contact agitation after determining the parameters influencing the phenomena such as the equilibration time, the pH, the mass of adsorbent, the initial concentration of dye.

Key words: Pomegranate peels, biosorption, textile dye, wastewater.

NEW INORGANIC-ORGANIC HYBRID: SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF $(NH_4)_3K_3[Fe_2(HAsO_4)_2(C_2O_4)_4].2H_2O$

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According to the literature, many researches on metal–oxalate coordination compounds are carried out due to their original structures and potential applications in co-precipitation precursor [1], in heterogeneous catalysis [2] and in magnetism [3]. However, few iron oxalate-phosphates have been reported to date. The oxalate anion is a key bridging element in several molecular magnetic materials. To our knowledge only two iron arsenate-oxalate with organic cation, was recently synthesized [4-5]. In the present work, we report the preparation andX-ray crystal structure of a new open-framework structure of iron arsenate-oxalate $(NH_4)_3K_3[Fe_2(HAsO_4)_2(C_2O_4)_4].2H_2O$. It has been prepared by slow evaporation, and characterized by single-crystal X-ray diffraction methods. It was crystallized in the triclinic space group *P*-1, with a = 10.154(4)Å, b = 10.430(4)Å, c = 15.085(7)Å, α = 96.81(3)°, β= 105.04(43)°, γ = 93.93(3)°, V = 1523.7(11)Å^3 and Z = 2. Its crystal structure, consists of two crystallographically independants bishydrogenarsenato tetraoxalato diiron (III) anions, both located on centres of inversion, while the potassium and ammonium cations and water molecules are located in general positions.These moieties are connected through N–H…O and O–H…O hydrogen bonds to form infinity of layers parallel to (101) plane leading thus to a two-dimensional open framework.

Key words: Iron arsenate-oxalate, X-ray diffraction, Crystal structure.

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SYNTHESIS AND CRYSTAL STRUCTURE OF A NEW OPEN-FRAMEWORK IRON OXALATOARSENATE $Li(NH_4)_4[Fe_2(HAsO_4)(H_2AsO_4)(C_2O_4)_4].6H_2O$

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Many research activities have focused on the synthesis of hybrid inorganic–organic open-framework materials to their enormous structural varieties and the accompanying multitude of potential applications. The oxalato-bridged networks continue to receive much attention, because the oxalato ligand has high degrees of freedom of the bridging modes, allowing a large variety of structure. Recently, metal oxalato-phosphate open frameworks, such as $K_{2.5}[(VO)_2(HPO_4)_{1.5}(PO_4)_{0.5}(C_2O_4)].4.5H_2O$[1], have been reported to show reversible Li-ion intercalation/extraction, suggesting that the oxalato-bridge is robust against ion intercalation. Particular, alkali oxalato-phosphate shown promise as electrode materials for LIBs [2-3]. Aim of this work is the synthesis and crystal structure of a new open-framework structure of iron arsenate-oxalate $Li(NH_4)_4[Fe_2(HAsO_4)(H_2AsO_4)(C_2O_4)_4].6H_2O$. The crystal structure is characterized by single-crystal X-ray diffraction methods. It was crystallized in the triclinic space group *P*-1. Its crystal structure consists of two crystallographically independants dihydrogenarsenato hydrogenarsenato tetraoxalato diiron (III) anions, both located on centres of inversion, while the lithium, ammonium cations and water molecules are located in general positions. These moieties are connected through N–H…O and O–H…O hydrogen bonds to form infinity of layers parallel to (101) plane leading thus to a two-dimensional open framework.

Key words: Iron arsenate-oxalate, Synthesis, Single crystal X-ray diffraction.

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SYNTHESIS AND CHARACTERIZATION OF A NEW COMPLEXES $[Ni(C_{10}H_{24}N_4)](H_2O)_4(SO_4)$

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More attentions have been paid to metal-organic coordination compounds because of their potential applications in several areas [1, 2]. In particular, the coordination chemistry of nickel (II) complexes with multidentate ligands has always been a subject of much attention due to its diverse nature and their applications catalytic, magnetic and biological properties in addition to the structural aspects. Up to now, there is a limited number of nickel (II) complexes containing mesocyclic diamines like 1,4-diazepane or its derivatives. This work reports synthesis and study of new nickel (II) complex, $[Ni(C_{10}H_{24}N_4)](H_2O)_4(SO_4)$ **(Fig.1),** by x-ray diffraction, thermal analysis, IR and optical characterization.

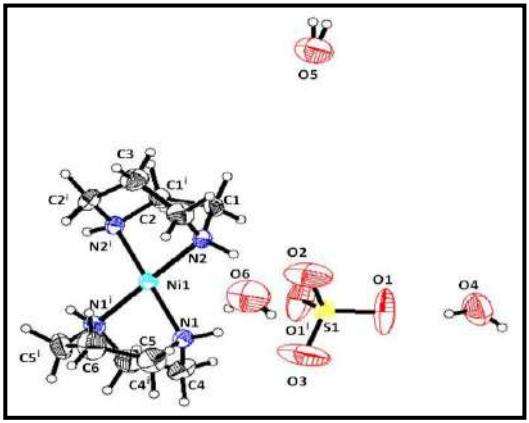

Figure 1: ORTEP view of $[Ni(C_{10}H_{24}N_2)]SO_4.(H_2O)_4$ showing 50% probability ellipsoids.

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Electronic Structure and Coordination chemistry of Mono- and Binuclear Transition Metal Sandwich complexes of Triphenylene

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Polycyclic arenes known as polycyclic aromatic hydrocarbons (PAH) constitute a large class of organic compounds [1] have attracted a great deal of interest in material science due to their shapes and other properties resulting from their extended delocalized π-systems [2-6], because they permit the introduction of one or more transition metals on the discrete aromatic rings [7] and have played an important role as potential ligands in sandwich complexes since the discovery of ferrocene. Full geometry optimization has been carried out for all the low-energy isomers of $M(Tphn)_2$ (Tphn = Triphenylene; M = Ti, Cr, Fe, Ni) sandwich complexes. Singlet and triplet spin state structures have identified as energy minimum. Depending on the electron richness of the molecule and the nature of the metal a complete rationalization of the bonding in triphenylene complexes has been provided. The sandwich complexes, both triphenylene ligands as PAH prefer to behave differently regarding the coordination mode for satisfying the metal electron need. The population or the depopulation of the antibonding metal-ligand orbitals leads to coordination or decoordination of bonds, thus conducting to various hapticies from η^2 to η^6. The findings show that the energy barrier of the rotation between both ligands is neglected. The coordination of the central ring was revealed to be unfavorable compared to that of the terminal one. The binuclear sandwich complexes offer the possibility of the M-M bonding depending on the nature and the valence electrons of the metal.

Keywords:
Bonding Analysis, Orbital interactions, Spin states, Density functional theory, metal-metal bonding.

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METHANOL COMPLEXES AND CLUSTERS DETECTION THROUGH THE VISCOSITY ARRHENIUS DERIVED PROPERTIES IN METHANOL + N,N-DIMETHYLACETAMIDE BINARY MIXTURES FROM 298.15 K TO 318.15 K

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Physical and chemical properties of solvent mixtures are important for understanding their thermodynamic behavior. One of the most important considerations is that these properties may provide information about molecular interactions. Excess molar volumes, viscosity deviations and excess molar Gibbs energy of activation of viscous flow in methanol + N,N-dimethylacetamide binary mixtures at (298.15, 308.15, and 318.15) K. were calculated from experimental density and viscosity data presented in previous work. Here these experimental values were used to test the applicability of the correlative reduced Redlich-Kister, Herráez and Belda equations as well as their corresponding relative properties. The relative functions are important to reduce the effect of temperature and, consequently, to reveal the effects of different factors and types of interactions. Values of limiting excess partial molar thermodynamic properties at infinite dilution were deduced from different methods. We can add that the As-values' transition between local minima and maxima at the compositions (x_1 = 0.125, 0.50 and 0.75) shows the intensities' difference of molecular interaction forces governing in the existing clusters or complexes {(1Met:7DMA), (1Met:1DMA) and (3Met:1DMA)} in liquid phase. We note that the composition (x_1 = 0.501) corresponds to the formation of the complex (DMA:Met) confirmed by 1H-NMR spectroscopy.

Key words: Binary liquid mixture, viscosity, Reduced Redlich-Kister equation, Molecular interaction, Complex, Cluster.

NEW ORGANIC-INORGANIC HYBRID SALTS BASED ON *TRANS*– DIAQUABIS(OXALATO)CHROMATE(III) ANIONS

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Mbarki Mohammed[b] and Fokwa P. T. Boniface[b]

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Recently, a great attention has been paid to organic-inorganic hybrid materials due to their varied structures and physical properties [1,2]. In line with this research area, we present therein, two novel organic-inorganic hybrid salts, 2-Aminopyridinium *trans*–diaquabisoxalato(2–)chromate(III), $(C_5H_7N_2)$-$[Cr(C_2O_4)_2(H_2O)_2]$ **(1)**, and Pyridinium *trans*–diaquabisoxalato(2−) chromate(III) urea monosolvate, $(C_5H_6N)[Cr(C_2O_4)_2(H_2O)_2].OC(NH_2)_2$ **(2)**. These salts have been synthesized *via* one-pot reaction and characterized by elemental, EDX, IR, UV-Vis and thermal analyses. Both compounds crystallize in a monoclinic system with space groups *C2/c* for **(1)** and *I2/a* for **(2)**. Hydrogen bonding interactions of the type N–H···O and O–H···O together with coulombic forces help to consolidate the three-dimensional packing. The isolation of compound (**2)** with urea as the solvent molecule lends good grounds to anticipate that, predictable and consistent formation of networks involving the anionic building block $[Cr(C_2O_4)_2(H_2O)_2]^-$ is still in its infancy.

Keywords: Hybrid salts, bis(oxalato)chromate(III) anion, organic cations, crystal structure, hydrogen bonds.

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ALUMINUM SALTS AS ALTERNATIVE CATALYSTS FOR PREPARATION OF BIODIESEL FROM TRAP GREASE (HIGH FREE FATTY ACID FEEDSTOCKS)

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Fatty acid methyl esters (FAMEs) (biodiesel) can be derived from both vegetable and animal fats. Currently, commercial production of biodiesel relies on converting triglycerides to FAMEs using base-catalyzed transesterification, but the high cost of virgin-oil feedstock is a economic deterrent. One approach to making biodiesel economically competitive with petroleum diesel is to use less-expensive feedstock's such trap greases (food establishment septage). Unfortunately, the high free fatty acid (FFA) content of waste feedstock's, particularly so-called trap grease, makes base-catalyzed chemistry problematic, so a two-step process, acid–catalyzed esterification of the FFA followed by base-catalyzed transesterification of any remaining glycerides, is often employed. Sulfuric acid is the most common acid used in the first step compounds of this process.

$$RCOOH + CH_3OH \overset{\text{Cat.}}{\rightleftharpoons} RCOOCH_3 + H_2O$$

In this study, we examined the use of aluminum salts as alternative catalysts for the esterification of high FFA feedstock's to FAMEs. A comparison of the relative rates of esterification by the aluminum compounds and sulfuric acid are presented. The catalytic mechanism is examined by Al-27 NMR.

SYNTHESIS, CHARACTERIZATION, AND CRYSTAL STRUCTURE OF A NEW COPPER CYCLOHEXAPHOSPHATE COMPLEX, $Cu_{1,5}Li(C_2H_{10}N_2)P_6O_{18}.7H_2O$

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Transition metal-phosphates constitute a well explored type of compounds, which, despite their long-term studies, they continue to attract the attention of structural chemists because of their unpredictable structural diversity. Besides their traditional applications in catalysis, adsorption and separation based on the porosity in the structures, these new materials have shown great promise for applications in optics, electronics and magnetism **[1, 2]**. An overview on the metal cyclohexaphosphate associated with organic cations suggests that only limited examples are known. As a contribution to the elaboration of this compound family, we report in the present work, the synthesis and the characterization of the second copper-lithium cyclohexaphosphate with organic cations: $Cu_{1,5}Li(C_2H_{10}N_2)P_6O_{18}.7H_2O$(**1**) **[3]**. Single-crystal X-ray diffraction analysis revealed that the complex crystallizes in the triclinic system with $P\bar{1}$ space group. The structure consists of vertex-linking of CuO_6 octahedral, LiO_4 and P_6O_{18} rings, forming macroanionic layers. Protonated ethylenediammonium cations are located in the inorganic framework cavities. Additionally, the thermal behavior and the antibacterial activities of the elaborated complex has been investigated.

Keywords: Copper(II) cyclohexaphosphate; Crystal structure; Thermal analysis; X-ray diffraction; Antibacterial activities.

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Synthesis and physico-chemical studies of a novel layered structure with a heptanuclear Cd complex: $(C_9N_4H_{28})Cd_7(H_2O)_2Cl_{18}.nH_2O$ (n = 5.89)

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Supramolecular chemistry based on metal-ion-directed assembly of organic molecular building blocks is receiving extensive attention owing to its potential application in the fields of catalysis, nonlinear optics, magnetism and molecular recognition [1–2].

Herein, we report the synthesis and physico-chemical characterization of a novel heptanuclear Cd complex $(C_9N_4H_{28})Cd_7(H_2O)_2Cl_{18}.nH_2O$ (n = 5.89). This inorganic–organic hybrid compound features an unusual cadmium chloride structure, it adopts a layered structure consisting of double-chains and tetramers of [Cdϕ6] (ϕ= Cl, O) octahedra. Each octahedron, within a unit of one $[CdCl_5O]$ and four $[CdCl_6]$, shares four cis-edges with neighboring octahedra to form an octahedral double-chain running along the direction of [101]. The octahedral double-chains are connected together by tetramers $[Cd_4Cl_{14}(H_2O)_2]$ via corner-sharing to form a corrugated layer parallel to (10-1). This compound has also been investigated by FT-IR and solid-state ^{13}C, ^{15}N CP-MAS and 2D ^{13}C-H NMR spectroscopies.

Keywords: X-ray diffraction, double-chains, IR spectroscopy, CP-MAS NMR, DFT calculations.

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SHEETS OF TETRANUCLEAR Ni(II) [2 × 2] SQUARE GRIDS STRUCTURE WITH INFINITE ORTHOGONAL TWO-DIMENSIONAL WATER−CHLORINE CHAINS

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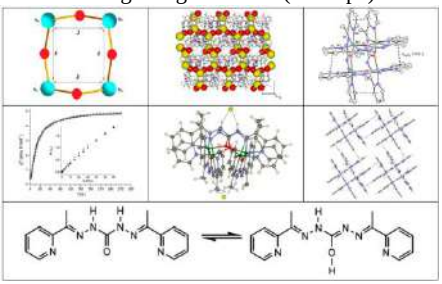
The tetranuclear nickel(II) complex $[Ni_4(HL)_4]Cl_4 \cdot 4H_2O$ {H_2L = 1,5-bis[1-(pyridin-2-yl)ethylidene] carbonohydrazone} has been prepared by reaction in methanol of nickel(II) chloride and H_2L in 2:1, (M:L) molar ratio. The single crystal X-ray diffraction analysis revealed a [2 × 2] square grid of tetramer units with the metal ions joined in pairs by the alkoxide oxygen atom in the μ_2 mode with octahedral geometry around each nickel ion. The supramolecular structure shows that the tetramer units are linked through edge to-face (T shape) C−H···π interactions, forming sheets with hydrophobic (occupied by infinite 2D water−chlorine chains) and hydrophilic (occupied by chlorine anions) channels. Variable temperature magnetic studies suggest an antiferromagnetic coupling between the adjacent Ni(II) centers with a coupling constant of $\boldsymbol{J} = -6.6\ cm^{-1}$.



Schemas related to structural and magnetic data of the complex

Key words: Tetramer, nickel(II) complex, magnetism molecular

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RUTHENIUM-CATALYZED CLEAVAGE OF A CARBON-CARBON TRIPLE BOND: TRANSFORMATION OF ALKYNYL ALCOHOL INTO ALKENE AND CARBON MONOXIDE

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The coordinated metal catalyzed oxidative cleavage of carbon-carbon triple bonds is an important producer of alkene and alcohol intermediates for the chemical and pharmaceutical industries, however only a few of the catalytic examples are found in the literature. This could be probably due to the triple bond functionality which generally results in unwanted products containing unstrained C=C or C-C bonds during catalytic transformations. At times the catalyst compounds involved could be unstable or less active resulting into a mixture of products. This study reports on a new system of a ruthenium catalyst which is based on pyridyl/quinolylimine ligands. These compounds were synthesized and characterized by NMR, FTIR, TGA, UV-vis, elemental analysis. The obtained pure compounds were tested for the carbon-carbon triple bond oxidative cleavage of alkynyl alcohols. The results will be discussed.

Key words: Ruthenium (II) complexes, schiff bases, triple-bond cleavage, catalysis.

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SYNTHESIS AND BIOLOGIC EVALUATION OF THE FIRST GENERATION OF GLYCOCLUSTERS COMBINING BOTH IRON COMPLEXING PROPERTIES AND INTERACTION WITH LecB AT CELL WALL LECTINE OF *PSEUDOMONAS AERUGINOSA*

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Pseudomonas aeruginosa (*PA*) presents an important threat to human health especially in immunocompromised patients (AIDS, cystic fibrosis …).[1] We have been interested in developing some biocides agent targeting this gram (-)–pathogenic bacterium. Our approach is driven by two main considerations: the use of lectins such LecB by *PA* in its selective recognition of wall fucoglycane of host cells and neighboring bacteria receptors to form biofilms. The inhibition of this process is a possible target to stop infection by *PA*. The second is its dependence to iron, an essential nutrient for *PA*. *PA* involves Fe^{2+} witch play an essential role as enzymes cofactor and impact the formation of biofilms.[2]This ferrous cation is formed in the periplasm and transported to cyctoplasm space after reduction of ferrique form Fe^{3+} that is available in exogenous environment.[3] To purchase Fe^{3+}, PA involves Pyoverdine I as the main natural chelator (siderophore).[4] The use of artificial chelators of Fe^{3+} that compete efficiently with pyoverdine I could induce iron deprivation and consequently bacterial death.
In the present work, we describe the synthesis, the iron complexation and the interaction study with LecB of the first generation of glycoclusters designed for both Fe^{3+} complexation and LecB interaction inhibition.[5]

Key words: Calixarene, L-Fucopyranose, Fe(III), Pseudomonas aeruginosa, lectins, biofilms.

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ASSESSING THE IMPACT OF SOCIO-ECONOMIC ACTIVITIES IN FORT PORTAL TOWN ON THE WATER QUALITY OF RIVER MPANGA

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The impact of socio-economic activities on water quality was investigated along River Mpanga within Fort Portal town. Samples of water were analyzed for Turbidity, Ammonia, Nitrite, Nitrate and Phosphate. Temperature, pH, electrical conductivity and total dissolved solids were measured onsite.

Electrical conductivity (EC) values ranged between 388.75±5.15 µs/cm, and 252.75±36.19 µs/cm at S7and S2 respectively. Total dissolved solids (TDS) followed the same trend with the highest at S7 (. 196.00±3.51 mg/l) and lowest at S2 (127.65±18.52 mg/l). High mean values of EC and TDS at S7 are attributed to accumulation of pollutants from various socio-economic activities into the river. The pH mean values were between 7.02±0.04 and 7.22 ± 0.09. Mean temperature values ranged from 18.95±0.52oC to, 19.92±0.53oC.

High phosphate values at S3 (1.18±0.28 mg/l) were associated with the outflows from the sewage treatment plant along Mugunu stream joining River Mpanga and high values at S7 (1.21±0.18mg/l) could be due to cumulative inputs of pollutants. Mean Nitrate ranged between 0.04±0.00 and 0.09± 0.03 mg/l. A significant difference between the undisturbed stream (S1) and the sampled points along the river as it flows through the town was noticed.

Results show increased levels of pollution along the river though the results are within limits of National Environment (Standards for discharge of effluent into water and land) Regulations, 1999. The study calls for close monitoring of socio-economic activities to minimize deterioration of water quality.

Key words: Socio-economic activities, water quality, River Mpanga

AN ALTERNATIVE PATH FOR CLEAN SYNTHESIS OF ADIPIC ACID CATALYZED BY AN HETEROPOLYACID DRIVED COMPLEXE

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Adipic acid (AA) is of great importance commercially in that it is used in the manufactures of nylon 6,6 and many other products. Currently nitric acid is used in the oxidation of cyclohexanone and/or cyclohexanol to AA in most industrial processes. However, the use of this oxidant generates environmentally harmful materials. It is, therefore, highly desirable to develop more environmentally friendly methods for the manufacture of AA [1].

Various methods including biosynthesis have been elaborated recently for the clean synthesis of adipic acid [2,3]. However, they were too expensive or too complicated to apply to industrial processes. Heteropolycompounds are widely used in several catalytic reactions because of their excellent oxidizing ability and strong acidity [4,5].

The purpose of this study is to find the optimal conditions for the production of adipic acid through oxidation of cyclohexanone and cyclohexanol over $H_3PMo_{12}O_{40}$ heteropolyacid using H_2O_2 as oxidant. Several factors have been studied such as the effect of the weight of catalyst, the stirring rate, the mode of addition of H_2O_2, the amount of the substrate and the reaction time.

The most important result showed that the best yield of adipic acid > 33% is obtained at 20hours of reaction time with only 0.03g of catalyst and <9ml of hydrogen peroxide.

Keywords:adipic acid, polyoxometalate, oxidation, Hydrogen peroxide, free solvent, heterogeneous catalysis

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TRANSITION METAL-SUBSTITUTED POLYOXOMETALATES AS CATALYSTS IN THE OXIDATION OF CYCLOHEXANONE TO ADIPIC ACID WITH H_2O_2

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Polyoxometalates (POMs), have received much attention in various fields such as catalysis, photochemistry, nonlinear optics, biology and medicine [1]. Their physico-chemical, acidic and oxidative properties can be adjusted according with the nature of constituent elements [2]. In the field of catalysis, the most studied POMs are those with the Keggin. They were tested in wide variety of reactions in homogeneous and heterogeneous phases. In the redox processes, the nature of counter- cation in the $[PMo_{12}O_{40}]^{3-}$ system can play a significant role. Thus, it has been shown that using Fe(III), vanadyl(VO^{2+}), antimony (Sb^{3+}) or cobalt (Co^{2+}) ion as counter-cation develop of a more favourable distribution of both reduced Mo(V) and oxidized Mo(VI) sites[2,3,4].

In the present work transition metal monosubstituted heteropoly anions in cationic position with formula of $MPMo_{12}O_{40}$ (M=Ni, Co, Mn, Cu and Zn) have been studied for the catalytic oxidation of cyclohexanone to adipic acid in friendly conditions. The heteropolysalts have been synthesized by a cationic exchange method in two steps.

After synthesis the salts have been characterized by several analysis methods as FTIR, DRX and thermal analysis TG.

Finally the catalytic activity of the as prepared and characterized compounds have been tested in the reaction of production of adipic acid through cyclohexanone oxidation using hydrogen peroxide as oxidant at 90°C in free solvent conditions. The effect of some reaction conditions and the nature of transition metal have been examined too.

Keywords: transition metal**,** adipic acid, polyoxometalate, oxidation, H_2O_2, free solvent, catalysis**.**

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SYNTHESIS, CHARACTERIZATION AND PRELIMINARY ANTIMICROBIAL STUDIES OF THREE SCHIFF BASES DERIVED FROM INDOLE-2, 3- DIONE AND THEIR Co(II) AND Ni(II) COMPLEXES.

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Three Schiff bases; 3-(o-aminophenyl)imino-2H-indol-2-one, Lo, N, N^1-m-phenylbis(3-imino-2H-indol-2-one), Lm, and N, N^1-p-phenylbis(3-imino-2H-indol-2-one), Lp, were synthesized via the condensation reactions of 1, 2-diaminobenzene, 1, 3-diaminobenzene and 1, 4-diaminobenzene with indole-2, 3-dione respectively. The ligands formed complexes with Co(II) and Ni(II) yielding complexes of the form $[Co(Lo)_2]$, $[Ni(Lo)_2]$, $[Co(LpCl_2]$, $[CoLm]Cl_2$, $[NiLm]Cl_2$ and $[NiLp]Cl_2$. The ligands and complexes were characterized based on melting point, stoichiometric data, elemental analysis, molar conductance, electronic, infrared, nuclear magnetic resonance and mass spectroscopic studies. Ni(II) and Co(II) combined with Lo(o-phenylenediamine ligand) in a 1: 2 ratio but formed complexes of 1:1 mole ratio with Lm(m-phenylenediamine ligand) and Lp(p-phenylenediamine ligand). Lo ligated as tetradentate ligand with Co(II) using $–NH_2$, C = O and C= N groups, but coordinated as a bidentate ligand to Ni(II). Lm and Lp were tetradentate in their coordination to Co(II) via two C=O and C=N, but ligated to Ni(II) using two C=O, two C=N and two N-H groups, thereby acting as hexadentate ligands. Octahedral geometry has been assigned to $[Co(Lo)_2]$, $[NiLm]Cl_2$, $[CoLpCl_2]$ and $[NiLp]Cl_2$ whereas $[Ni(Lo)_2]$ and $[CoLm]Cl_2$ are square planar in geometry. Preliminary antibacterial screening based on agar well diffusion method showed the complexes to have mild to strong activity against some bacteria strains with $[CoLm]Cl_2$ and $[NiLp]Cl_2$ being the most potent. The ligands were not very active.

Keywords: Schiff bases, indole-2, 3-dione, benzenediamines, antibacterial activity.

NOVEL BIMETALLIC NICKEL AND PALLADIUM COMPLEXES

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The heterogeneous Ziegler-Natta catalysts have been dominant in the ethylene oligomerization/polymerization reactions. However, these compounds show serious limitations of oxidation and instability. Late transition metals are less oxidized and show reasonable stability. Brookhart et al. have reported homogeneous α-diimine catalysts for ethylene oligomerization with great success. The monometallic α-diimine Ni(II) and Pd(II) catalysts are known. However, none of them are bimetallic in nature. Bimetallic catalysts would show possible cooperative effect due to their potential differences. In this study, tetrahydrophenyl linked iminopyridine ligands were synthesized using Schlenk techniques[2-3]. Six new homobimetallic complexes synthesized from these ligands[4]. Two of them are Ni(II) type while four of them are of Pd(II).
These complexes will then be screened for catalytic activity of ethylene oligomerization/polymerization using gas-chromatography profile. All these results will be discussed.

Keywords: Iminopyridine, ethylene polymerization, nickel, palladium

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Kinetic and Mechanistic Studies of 1,3-Bis(2-pyridylimino)isoindolate Pt(II) Derivatives. Experimental and new Computational Approach.

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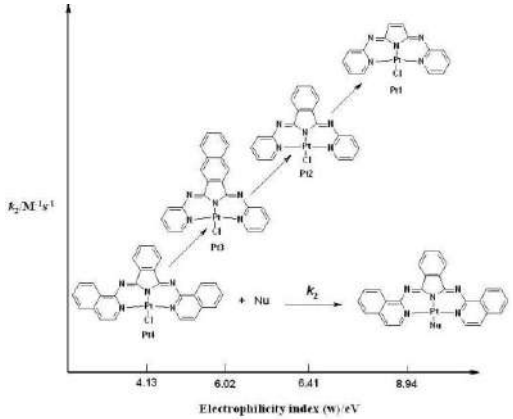
The rate of substitution of chloride ligand by three bio-relevant nucleophiles; thiourea (**Tu**), N,N-dimethylthiourea (**Dmtu**) and N,N,N,N-tetramethylthiourea (**Tmtu**) in the complexes: 1,3–bis(2-pyridylimino)isoindoline platinum(II) chloride**(Pt2)**, 1,3-bis(2-pyridylimino)benz(f)isoindoline platinum(II) chloride (**Pt3**) and 1,3-bis(1-isoquinolylimino)isoindoline platinum(II) complex (**Pt4**) was investigated under *pseudo* first-order conditions as a function of concentration and temperature using Stopped-Flow and UV-Visible spectrophotometry. Computational modeled data of bis (pyridylimino) 3,4-pyrrolate platinum(II) chloride(**Pt1**) was incorporated in the study for comparison. The observed *pseudo* first-order rate constants for substitution reactions obey the rate law $k_{obs} = k_2[Nu]$. High negative activation entropies and second-order kinetics for the displacement reactions all support an associative mode of activation. The reactivity is dependent on stabilization of the LUMO energy and inversely proportional to the number of phenyl rings added irrespective of the site of attachment. The electron density on the ligand moiety plays a significant role in substitution behavior of the platinum(II) complexes, as supported by DFT descriptors {electrophilicity index(ω) and chemical hardness (η)}.



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ENCAPSULATION OF CO (II) COMPLEX WITH A SCHIFF BASE LIGANDS DERIVED FROM 1,10-PHENANTROLINE-5,6-DIONE AND O-PHENYLENE DIAMINE IN ZEOLITE Y.

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The encapsulation of Co (II) with the ligand derived from 1,10 phenantroline 5,6 dione(PD) and o-phenylene diamnie(OPD) (Guest-host) catalyst was accomplished by ship-in bottle method by assembling the ligand and the metal complex inside the zeolite super cage. The metals were first incorporated in the zeolite Y by standard ion exchange method in distilled water as a solvent. The neat metal complex of Co(II) was synthesized by direct method by condensing the metal chloride with ligand derived from 1,10-phenantroline 5,6-dione(PD) and o-phenylene diamine(OPD). The host guest materials obtained and the neat complexes have been characterized by FTIR, Termogravimetric (TGA), elemental analysis (CHN) and Inductive Coupled Plasma (ICP). Analysis of the data shows that the metal exchanged process as well as the immobilization of metal complexes in the super cages of zeolite Y took place in the expected stoichiometry**.**

Keywords: Encapsulation, 1,10PD, 1,10PDOPD, Schiff base ligand, Immobilization, Ship-in bottle synthesis.

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Enantioselective synthesis of some benzylic acetates precursors of drugs *via* enzymatic kinetic resolution

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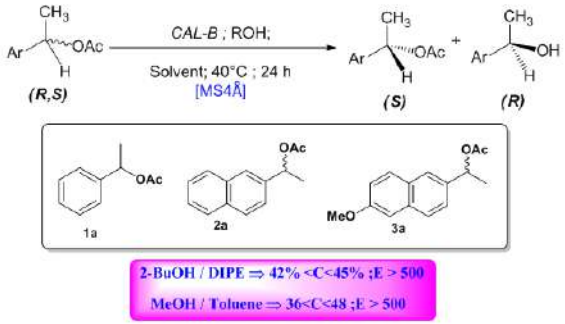
The optically active benzylic acetates are widely used as synthetic intermediates in pharmaceutical and agrochemical industries. They are also, exploited as powerful ligands in asymmetric synthesis.

For their conception, several methods have been described, and one of them and the most practical is the enzymatic kinetic resolution. These methods employed lipases for their high level of efficiency, under mild conditions respectful of some green chemistry criteria [1].

Herein we describe an efficient pathway mediated by lipase to achieve the both enantiomers of some benzylic acetates precursors of drugs in non aqueous media, with high optic purities up to 99% and reach 50% of conversion [2].



Key words: Enzymatic kinetic resolution, Lipases, Benzylic acetates, pharmaco-therapeutics.

References:

[1] P. T. Anastas, N.Eghbali, *Chem. Soc. Rev.*, **2010**, 39, 301-312.
[2] A. Zaïdi, M. Merabet-Khelassi, L. Aribi-Zouioueche, *Catal Lett*., **2015**, 145, 1054–1061.

CAL-B catalyzed tranesterification as key step to deracemization of benzylic alcohols through combined *CAL-B*/ Ruthenium catalysis.

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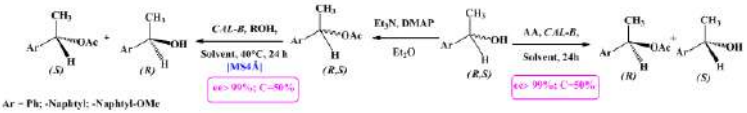
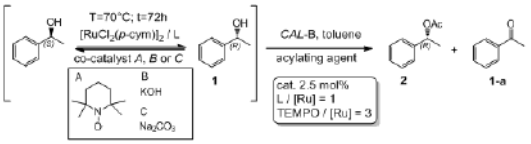
The use of Lipases as powerful catalysts contributes to the development of greener processes for the production of enantioenriched intermediates for organic synthesis. The enzymatic kinetic resolution trough transesterification (Alcoholysis / Acetylation) is the most practical methods for the efficient production of enantiomerically enriched building blocks [1].



Herein we describe our results of both enantio-complementary reactions Alcoholysis / Acetylation of some benzylic alcohols. Both enantiomers were obtained at high optical purities at 50% of conversion.[2]
The high level of the enzymatic acetylation was successfully combined to a Ruthenium catalyzed racemization of those benzylic alcohols to elaborate a deracemization process called dynamic kinetic resolution. [3]



Key words: Enzymatic kinetic resolution, Dynamic kinetic resolution, *CAL-B*, Ruthenium, Benzylic acetates.

References:

[1] P. T. Anastas, N.Eghbali, *Chem. Soc. Rev.*, **2010**, 39, 301-312.
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VALORISATION DES PHOSPHOGYPSES PAR LEUR INTEGRATION DANS LES MATERIAUX DE CONSTRUCTION

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This work deals with the valorization of phosphogypsum by its integration in building materials. Clayey raw materials used in this study originate from Agareb (Sfax) and phosphogypsum from Tunisian Chemical Group (Sfax).
The raw materials were first characterize chemical, mineralogical, granulometric and textual analyses were carried out. Them, the effect of incorporating different percentages of clay and phosphogypsum on the cylindric experiments was investigated and physico-mechanical characteristics were analyzed. The resultats showed that sun-dried phosphogypsum integration in clay to make cylindrical eprouvette would give the material a better resistance to compression in comparison to others phosphogysum treatments. The optimization of the composion exhibited that the mixture of 25% phosphogypsum improves compression resistance **(2,55 MPa)**, porosity **(19,52 %)** and density **(1,88 g/cm3)**.

Keywords : Phosphogypsum, building materials, compression resistance.

SYNTHESIS AND CARACTERISATION OF A NEW STRANDBERG-TYPE POLYOXOMOLYBDATE $(NH_4)Rb_3[Se_2Mo_5O_{21}].H_2O$

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The Strandberg family of compounds is very interesting. It is considered one of the polyoxometalates (POMs) which represents an outstanding class of molecular building blocks for the preparation of this kind of material, which give rise to a variety of applications in different fields such as catalysis, medical chemistry, magnetism, and optics **[1–3]**. That's why a new strandberg-type polyoxomolybdate formulated as $(NH_4)Rb_3[Se_2Mo_5O_{21}].H_2O$ (1) has been isolated by conventional solution method and structurally characterized by single-crystal X-ray diffraction methods, IR, UV–vis spectra, and thermogravimetric analysis. This compound crystallizes in the orthorhombic system, space group $Pbc2_1$ with unit a = 9,8546 (2) Å ˚, b = 12,6747 (15) Å, c = 17,474 (5) Å, $\alpha = \beta = \gamma = 90$ °, Z = 4. The crystal structure of (1) is built up from a Strandberg clusters connected through hydrogen-bonding interactions into a three-dimensional supramolecular network (figure1).

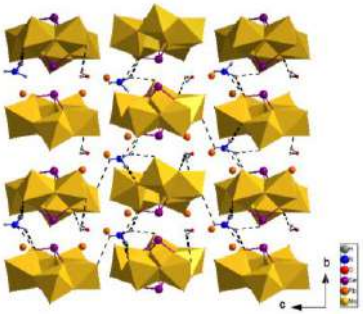

Figure1:
A packing view of compound 1 along the a axis, showing the arrangement of the $[Se_2Mo_5O_{21}]^{4-}$ clusters, the rubidium cations and the lattice water molecules in the crystal structure. The dashed lines denote the hydrogen interactions.

Keywords: Polyoxomolybdate, Strandberg, crystal structure.

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SYNTHESIS AND CARACTERISATION OF A NEW WAUGH-TYPE POLYOXOMETALATE $K_{1.5}(NH_4)_{4.5}[MnMo_9O_{32}].4.2H_2O$

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Polyoxometalates (POMs) as early-transition-metal oxide clusters, have received much attention in fields such as catalysis, ion exchange, electrochemistry, magnetism and medicine for their enormous variety of structures and unique properties **[1-4]**. Because the Waugh-type polyanions have multiple coordination active centers, it was of interest to synthesize a new polyoxomanganomolybdate $K_{1,5}(NH_4)_{4,5}[MnMo_9O_{32}].4.2H_2O$ (1) and to investigate its structural characterization by single crystal X-ray diffraction, IR, cyclic voltammetry measurements and thermogravimetric analysis.
The title compound was crystallized in the trigonal system, space group R3 with a = 15.950 Å, b = 15.950 Å, c = 12.447 Å, γ = 120 °, Z = 3. Single-crystal X-ray diffraction analyses reveals that compound **(**1**)** consists of one $[MnMo_9O_{32}]^{6-}$ cluster anion, 1.5 cation K^+, 4.5 cations NH_4^+ and 4.2 lattice water molecules. The Waugh-type clusters are connected with ammonium ions through hydrogen-bonding interactions which ensure the cohesion of the structure into a three-dimensional network.

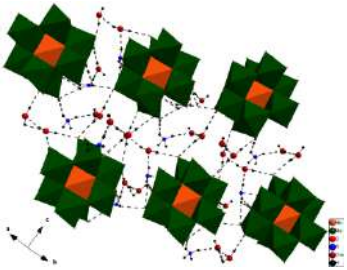

Figure 1
A packing view of compound, showing the arrangement of the $[MnMo_9O_{32}]^{6-}$ clusters, ammonium cations and the lattice water molecules in the crystal structure. Potassium atoms have been omitted for clarity. The dashed lines denote the hydrogen interactions.

Keywords: polyoxometalate, Waugh-type polyanions, Crystal Structure.

References

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Corrosion inhibition of carbon steel A 283 C using the acetylsalicylic acid

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Carbon steel is used in mass amounts in marine applications, chemical processing, petroleum production and refining. These applications usually induce serious effect on equipments, tubes and pipelines [1-3]. The protection of these materials are generally secured by inhibitors used for their rapid action. Particularly organic compounds containing heteroatoms are usually employed. Generally, they act by adsorption on the metal surface which takes place through heteroatoms such as: nitrogen, oxygen, phosphorus, sulphur, triple bonds or aromatic rings…. The interactions between an organic inhibitor and a metal surface are principally physical adsorption and/or chemisorptions [4-5].

Recently, many studies are interested at the investigation of pharmaceutical compounds. In fact, these compounds offer interesting possibilities for corrosion inhibition and are of particular interest because of their safe use, high solubility in water and containing electronegative atoms in their molecules. These compounds should be good corrosion inhibitors [6-7].

Based on the foregoing points, the aim of this work is to study the inhibition efficiency of the acetylsalicylic acid in decanted water from a tank bottom hydrocarbon storage (East Region Transport: Skikda Algeria) using chemical (polarization and impedance) measurements. The mode of adsorption and the corrosion inhibition, mechanism are also discussed. Results showed that: The inhibition efficiency increased with increasing inhibition concentrations, but decreased with increasing temperature. Polarization studies showed that this compound is an anodic inhibitor for carbon steel in decanted water. The inhibition occurs through adsorption of the inhibitor molecule on the metal surface. The adsorption of the inhibitor on the metal surface is found to obey Langmuir's adsorption isotherm. The values of thermodynamic parameters, such as K_{ads}, ΔG°_{ads}, ΔH°_{ads} and ΔS°_{ads} are calculated.

Keywords: Corrosion, Carbon Steel, Acetylsalicylic Acid, Inhibition, Decanted Water, Adsorption.

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