Second Tunisian Chemistry Conference on Coordination Chemistry

JCC 2017

Organized by

Tunisian Chemical Society

ROYAL SOCIETY OF CHEMISTRY
TUNISIA LOCAL SECTION

11-14 May 2017

Bel Azur Hotel, Hammamet - Tunisia

Lectures and Communications Abstracts
List of Participants

Tunisian Chemical Society - Short Program of TCC 2016

Thursday 11 May 2017	
14.00	**Welcoming participants, distribution of documents and check in**
16.30	**Opening Remarks**
17.00 - 17.40	**Plenary Lecture 1 Pr. Henry CHERMETTE** *University Claude Bernard - Lyon1, France*
18.00	***RSC Welcome Reception***
19.30	***Dinner***
Friday 12 May 2017	
08.30 - 09.10	**Plenary Lecture 2 Dr. Petr KILIAN** *EaStChem School of Chemistry, Univ. St Andrews, St Andrews, U.K*
09.15 - 10.30	**Oral Communications - Session 1 - OC1 > OC5**
10.30 - 11.15	**Coffee break + Poster Session 1 (P 1 - P 38) Alphabetical Order**
11.15 - 11.55	**Plenary Lecture 3 Pr. Alessandro CASELLI**
12.00 - 13.00	**Oral Communications - Session 2 - OC6 > OC9**
13.00	***Lunch***
14.30 - 15.45	**Oral Communications - Session 3 - OC10 > OC14**
15.45 - 16.25	**Plenary Lecture 4 Pr. Jean-François NIERENGARTEN** *University of Strasbourg - France*
16.30 - 17.15	***Coffee break* + Poster Session 2 (P 39 - P 76) Alphabetical Order**
17.15 - 17.45	**Invited Speaker 1 Dr. M. Abdrerrahmane SANHOURY** *University of Tunis El Manar, FST - Tunis, Tunisia*
Oral Communications - Session 4 - OC15 > OC19	
19.30	***Dinner***
Saturday 13 May 2017	
08.30 - 09.10	**Plenary Lecture 5 Pr. Azzedine BOUSSEKSOU** *LCC/CNRS, Toulouse, France*
09.15 - 10.30	**Oral Communications - Session 5 - OC20 > OC24**
10.30 - 11.15	**Coffee break + Poster Session 3 (P 77 - P 114) Alphabetical Order**
11.15 - 11.55	**Plenary Lecture 6 Pr. Benoit CROUSSE** *University of Paris-Sud, Université Paris Saclay, France*
12.00 - 13.00	**Oral Communications - Session 6 - OC25 > OC28**
13.00	***Lunch***
14.30 - 16.00	**Oral Communications - Session 7 - OC29 > OC34**
16.00 - 16.40	**Plenary Lecture 7 Pr. Huber SCHMIDBAUER** *Technische Universität München - Garching, Germany*
16.45 - 17.15	***Coffee break***
17.15 - 17.45	**Invited Speaker 2 Dr. Thouraya BARHOUMI SLIMI** *ISSTE, Technopark of Borj-Cedria - University of Carthage, Tunisia*
17.45 - 18.45	**Oral Communications - Session 8 - OC35 > OC38**
20.30	***Closing Dinner***
Sunday 14 May 2017	
08.30 - 10.00	**Oral Communications - Session 9 - OC39 > OC44**
10.00 - 10.30	***Coffee break***
10.30 - 12.00	**Oral Communications - Session 10 - OC45 > OC50 > OC56**
12.15 - 12.55	**Plenary Lecture 8 Pr. Jack HARROWFIEL** *University of Strasbourg - France*
12.55	**Closing Remarks, Awards Distribution and JCC 2019 Announcing**
13.00	***Lunch and leaving the hotel***

FOREWORD

It is our great pleasure to welcome you in the great resort of Hammamet in Tunisia for the second edition about Coordination Chemistry Conference **JCC 2017** hosted by the Tunisian Chemical Society.

The scientific program includes 10 plenary/keynote lectures and several session talks as well as poster presentations under 6 major themes. Many thanks for all participants and for all invited speakers who firmly accepted to contribute lectures at this event.

We hope you will enjoy the conference and the stay in Tunisia, and that you will make fruitful, beneficial and friendly exchanges.

Adel MEGRICHE

President of the Tunisian Chemical Society

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

Thursday 11 May 2017	
14.00	**Welcoming participants, distribution of documents and check in**
16.30	**Opening Remarks**
17.00 - 17.40	**Plenary Lecture 1** **Pr. Henry CHERMETTE**, W. Lamine, S. Boughdiri, L. Christ, C. Morell *University Claude Bernard - Lyon1, France* **Self-interaction error in DFT calculations: Origine, importance in calculations of monoatomic anions, impact on some reaction profiles: Proposed correction**
18.00	***Welcome Reception***
19.30	***Dinner***

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Friday 12 May 2017 (morning)		
08.30 - 09.10	**Plenary Lecture 2** **Dr. Petr KILIAN** *EaStChem School of Chemistry, Univ. St Andrews, St Andrews, Fife KY16 9ST, U.K* **Coordination Chemistry with Peri-Substituted Phosphine Ligands**	
Oral Communications - Session 1		
	Com.	*communicating*
09.15 - 09.30	**OC-01**	**Jihen AJMI** *FSM - Monastir*
09.30 - 09.45	**OC-02**	**Zouhaier ALOUI** *FSB - Bizerte*
09.45 - 10.00	**OC-03**	**Leila BAHRI** *FST - Tunis*
10.00 - 10.15	**OC-04**	**Natija BARHOUMI** *FSG - Gabès*
10.15 - 10.30	**OC-05**	**Safieddine BAHLOULI** *University Abbas Ferhat - Setif, Algeria*
10.30 - 11.15	**Coffee break + Poster Session 1 (P 1 - P 38) Alphabetical Order**	
11.15 - 11.55	**Plenary Lecture 3** **Pr. Alessandro CASELLI**, G. Tseberlidis *University of Studies of Milan and ISTM - Milan, Italy* **Designing new ligands: Catalytic applications of pyridine-containing macrocyclic complexes**	
Oral Communications - Session 2		
	Com.	*communicating*
12.00 - 12.15	**OC-06**	**Takoua BEN ISSA** *FSM - Monastir*
12.15 - 12.30	**OC-07**	**Sana BEN MOUSSA** *FSM - Monastir*
12.30 - 12.45	**OC-08**	**Wissem BEN SOLTAN** *FSG - Gabès*
12.45 - 13.00	**OC-09**	**Nesrine BENAROUS** *University Frères Mentouri - Constantine, Algeria*
13.00	***Lunch***	

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Friday 12 May 2017 (afternoon)		
Oral Communications - Session 3		
	Com.	*communicating*
14.30 - 14.45	**OC-10**	**Lamia BOUBAKRI** *FSB - Bizerte*
14.45 - 15.00	**OC-11**	
15.00 - 15.15	**OC-12**	**Marwa BOUTAR** *FSB - Bizerte*
15.15 - 15.30	**OC-13**	**Ines CHNITI** *FST - Tunis*
15.30 - 15.45	**OC-14**	**Desire BIKELE MAMA** *University of Douala - Cameroon*
15.45 - 16.25	**Plenary Lecture 4** **Pr. Jean-François NIERENGARTEN** *University of Strasbourg - France* **Metal-atom impact on the self-assembly of Cup-and-Ball metalloporphyrin-fullerene conjugates**	
16.30 - 17.15	***Coffee break* + Poster Session 2 (P 39 - P 76) Alphabetical Order**	
17.15 - 17.45	**Invited Speaker 1** **Dr. M. Abdrerrahmane SANHOURY** *University of Tunis El Manar, FST - Tunis, Tunisia* **Synthesis, characterization and coordination chemistry of organophosphorus compounds**	
Oral Communications - Session 4		
	Com.	*communicating*
17.45 - 18.00	**OC-15**	**Sarra DARGOUTHI** *IPEIM - Manar*
18.00 - 18.15	**OC-16**	**Marwa DHIFI** *FSM - Monastir*
18.15 - 18.30	**OC-17**	**Nour DISSEM** *FST - Tunis*
18.30 - 18.45	**OC-18**	**Faouzi CHAHDOURA** *Université de Rennes - France*
18.45 - 19.00	**OC-19**	**Kira VOSTRIKOVA** *Nikolaev Institute of Inorganic Chemistry - Novosibirsk, Russia*
19.30	***Dinner***	

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Saturday 13 May 2017 (Morning)		
08.30 - 09.10	**Plenary Lecture 5** **Pr. Azzedine BOUSSEKSOU**, G. Molnar, L. Salmon, W. Nicolazzi *LCC/CNRS, Toulouse, France* **Molecular Spin Crossover Phenomenon at the nanoscale. Motion and Spintronic properties**	
Oral Communications - Session 5		
	Com.	*communicating*
09.15 - 09.30	**OC-20**	**Rihab DRIDI** *FST - Tunis*
09.30 - 09.45	**OC-21**	**Fatimetou EBNOU** *Faculty of Sciences and Techniques - Nouakchott, Mauritania*
09.45 - 10.00	**OC-22**	**Hichem ELOUSSIFI** *FSS - Sfax*
10.00 - 10.15	**OC-23**	**Marwa FRAY** *FST - Tunis*
10.15 - 10.30	**OC-24**	**Zayed BACCARI** *FST - Tunis*
10.30 - 11.15	**Coffee break + Poster Session 3 (P 77 - P 114) Alphabetical Order**	
11.15 - 11.55	**Plenary Lecture 6** **Pr. Benoit CROUSSE** *University of Paris-Sud, Université Paris Saclay, France* **Trifluoromethyl aldimines and fluorinated alcohols: Access to N-heterocycles**	
Oral Communications - Session 6		
	Com.	*communicating*
12.00 - 12.15	**OC-25**	**Sondes GHRAIRI** *FST - Tunis*
12.15 - 12.30	**OC-26**	**Zied GOUID** *FST - Tunis*
12.30 - 12.45	**OC-27**	**Ayoub HAJ SAID** *CRMNS - Sousse*
12.45 - 13.00	**OC-28**	**Mohamed EL ALIM** *University of Nouakchott - Al Aasriya, Mauritania*
13.00	***Lunch***	

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Saturday 13 May 2017 (afternoon)		
Oral Communications - Session 7		
	Com.	*communicating*
14.30 - 14.45	**OC-29**	**Abdessalem HAMROUNI** *ENIG - Gabès*
14.45 - 15.00	**OC-30**	**Ali HARCHANI** *FSM - Monastir*
15.00 - 15.15	**OC-31**	**Khaoula NASR** *FST - Tunis*
15.15 - 15.30	**OC-32**	**Nejib JEBLI** *FSB - Bizerte*
15.30 - 15.45	**OC-33**	**Selma KHELIFI** *FSB - Bizerte*
15.45 - 16.00	**OC-34**	**Ok-Sang JUNG** *Pusan National University - Korea*
16.00 - 16.40	**Plenary Lecture 7** **Pr. Huber SCHMIDBAUER** *Technische Universität München - Garching, Germany* **The role of coordination chemistry in platinum-based technologies**	
16.45 - 17.15	***Coffee break***	
17.15 - 17.45	**Invited Speaker 2** **Dr. Thouraya BARHOUMI SLIMI** *ISSTE, Technopark of Borj-Cedria - University of Carthage, Tunisia* **Coordination chemistry of β-chloro-α,β-unsaturated aldehydes and their derivatives**	
Oral Communications - Session 8		
	Com.	*communicating*
17.45 - 18.00	**OC-35**	**Lazhar LABIADH** *FSG - Gabès*
18.00 - 18.15	**OC-36**	**Fahima LARIBI** *FST - Tunis*
18.15 - 18.30	**OC-37**	**Sana DRIDI** *FSM - Monastir*
18.30 - 18.45	**OC-38**	**Islam Ullah KHAN** *Govt. College University - Lahore, Pakistan*
20.30	***Closing Dinner***	

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Sunday 14 May 2017 (Morning)		
Oral Communications - Session 9		
	Com.	*communicating*
08.30 - 08.45	**OC-39**	**Hajer MARZOUGUI** *FSB - Bizerte*
08.45 - 09.00	**OC-40**	**Emna MATHLOUTHI** *FST - Tunis*
09.00 - 09.15	**OC-41**	**Hanen MECHI** *FST - Tunis*
09.15 - 09.30	**OC-42**	**Alia MEJRI** *FST - Tunis*
09.30 - 09.45	**OC-43**	**Alma MEJRI** *FST - Tunis*
09.45 - 10.00	**OC-44**	**Rozina KHATTAK** *Shaheed Benazir Bhutto Women University - Peshawar, Pakistan*
10.00 - 10.30	***Coffee break***	

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Sunday 14 May 2017 (Morning continuation)				
Oral Communications - Session 10				
	Room A		**Room B**	
	Com.	*communicating*	*Com.*	*communicating*
10.30 - 10.45	**OC-45**	**Rania MEJRI** *FSB - Bizerte*	**OC-51**	**Dhouha SGHAIRI** *FST - Tunis*
10.45 - 11.00	**OC-46**	**Olfa NAOUALI** *FSB - Bizerte*	**OC-52**	**Safa THABET** *FSM - Monastir*
11.00 - 11.15	**OC-47**	**Rania OMRANI** *FST - Tunis*	**OC-53**	**Nedra TOUJ** *ISSTE - Borj Cédria*
11.15 - 11.30	**OC-48**	**Ichraf OUESLATI** *FST - Tunis / Académie Militaire, Fondouk Jedid*	**OC-54**	**Salima MOSBAH** *University Freres Mentouri - Constantine, Algeria*
11.30 - 11.45	**OC-49**	**Wafa SELMI** *FST - Tunis*	**OC-55**	**Fatiha MAHAMMEDI** *Abu Bakr Belkaid University - Tlemcen, Algeria*
11.45 - 12.00	**OC-50**	**Badreddine MAALEM** *Research Center in Industrial Technologies - Algiers, Algeria*	**OC-56**	**Afef BENGHNIA** *ENIG - Gabès*
12.15 - 12.55	**Plenary Lecture 8** **Pr. Jack HARROWFIEL**, P. Thuéry *University of Strasbourg - France* **Coordination polymers and clusters containing uranyl ion**			
12.55	**Closing Remarks, Awards Distribution and JCC 2019 Announcing**			
13.00	***Lunch and leaving the hotel***			

Speakers' Abstracts

SELF-INTERACTION ERROR IN DFT CALCULATIONS: ORIGINE, IMPORTANCE IN CALCULATIONS OF MONOATOMIC ANIONS IMPACT ON SOME REACTION PROFILES: PROPOSED CORRECTION

Henry Chermette[1],
Walid Lamine[1, 2], Salima Boughdiri[2], Lorraine Christ[3], Christophe Morell[1]

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[2]*Université de Tunis El Manar, Faculté des Sciences de Tunis, UR11ES19 Unité de recherche Physico-Chimie des Matériaux condensés, Tunis, Tunisie*
[3] *Université de Lyon, Université Lyon 1(UCBL), IRCELYON, Villeurbanne, France*
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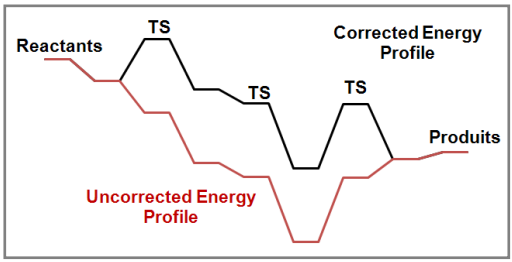
Modeling catalytic reactions involving a monoatomic anion as a co-catalyzer leads often to unrealistic reaction paths in most DFT calculations. We show that the reason is the underestimation of the anion energy. The origin comes from the fact that, on the one hand, in DFT calculations, and in general, one obtains a too much delocalization of the electronic density associated to the valence orbitals, and, in the other hand, the DFT method in its Kohn-Sham formulation (the only one used), calculates for each orbital an electronic interaction with all the electrons the total electronic density), and not with all the electrons excepted the one of the orbital in question. It results in a systematic error, so-called self-interaction error, which is the interaction energy of the electron with itself. The electronic delocalization, which, as already said is generally overestimated, allows to average and and minimize this self-interaction error in molecular systems. On the contrary, this electronic delocalization cannot be produced in systems made of a single atom. Several schemes have been proposed in the past to cure the problem, but no one has been found efficient and not computing demanding.

In the present work, we have quantified this error through "Linear Transit" calculations, from a transition state towards separated fragments [1]. As example, we will describe a system modeling CO_2 insertion into epoxides catalyzed by a Zn complex with the addition of a iodide ion, introduced through the form of $Bu_4N^+ I^-$. The ligand in the Zn complex is a Schiff base.

This has permitted to correct efficiently this self-interaction error with a GGA functional. It is worth noting that the self-interaction error depends less on the amount Hartree-Fock exchange in hybrid functionals than expected. Surprisingly, no significant improvement is obtained with the "Long-Range-corrected density functionals".



[1] W. Lamine et al., Molecular Physics. **2016**,114,1066-1075.

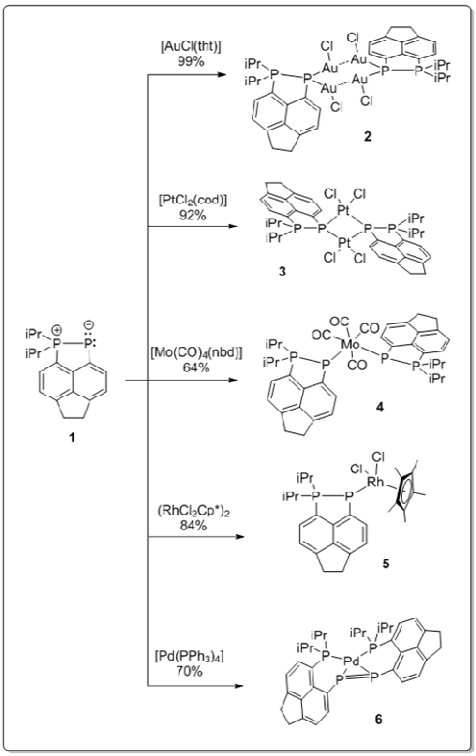
Coordination Chemistry with Peri-Substituted Phosphine Ligands

Dr Petr Kilian

EaStChem School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, U.K.

Unique geometric constraints are imposed on atoms attached to peri-positions (1,8-positions) in naphthalene. Because of the limited space available, the rigid geometry of naphthalene imposes strain on peri-atoms, promoting formation (and retention) of unusually strong bonding interaction between them.

We have used the unique peri-geometry to stabilise normally fleeting species, ranging from low coordinate (such as **1** in the scheme below) to hypervalent. In particular, using enforced proximity Lewis base coordination resulted in fundamentally new, broadly applicable method of thermodynamic stabilisation to challenge the paradigms associated with a number of reactive molecules and motifs. The (unstabilised) species in which we are interested, dissociate, disproportionate, oligomerise, or otherwise decompose well below room temperature, which severely limits their study and applicability. Our aim is to stabilise a range of normally unstable species to the point that they become bottleable. This facilitates the exploration of normally ephemeral species and thus enables the development of new reactivities and fundamentally new chemistries.



We have used coordination chemistry to gain understanding of the electronic properties of low coordinate species such as shown in the scheme.[1] In other cases we have used coordination to transition metals to probe flexibility of our multidentate ligands,[2] or to test dative properties of cationic phosphorus ligands.[3]

1. B. A. Surgenor, B. A. Chalmers, K. S. Athukorala Arachchige, A. M. Z. Slawin, J. D. Woollins, M. Bühl and P. Kilian, *Inorg. Chem.* 2014, 53, 6856-6866. DOI: 10.1021/ic500697m
2. M. J. Ray, R. A. M. Randall, K. S. Athukorala Arachchige, A. M. Z. Slawin, M. Bühl, T. Lebl, P. Kilian, *Inorg. Chem.* 2013, 52, 4346−4359. DOI: 10.1021/ic3024875
3. M. J. Ray, M. Bühl, L. J. Taylor, K. S. A. Arachchige, A. M. Z. Slawin, P. Kilian, *Inorg. Chem.* 2014, 53, 8538-8547. DOI: 10.1021/ic501142v

Designing new Ligands: Catalytic Applications of Pyridine-Containing Macrocyclic Complexes

Alessandro Caselli and Giorgio Tseberlidis

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The introduction of a pyridine moiety into the skeleton of a polyazamacrocyclic ligand affects both the thermodynamic properties and the coordination kinetics of the resulting metal complexes. These features have engender a great interest in the scientific community and the applications of pyridine-containing macrocyclic ligands ranges from biology to supramolecular chemistry, encompassing MRI, molecular recognitions, materials and catalysis. In this lecture, I will provide a perspective on the catalytic applications of metal complexes of pyridine-containing macrocyclic ligands (Pc-L's) which have been studied in our group (Figure 1), with a focus interest on the structural features relevant to catalysis.[1] The increased conformational rigidity imposed by the pyridine ring allowed for the isolation and characterization of metal complexes which show a rich coordination chemistry.[2] The very different conformations accessible upon coordination and the easy tuneable synthesis of the macrocyclic ligands have been exploited in stereoselective syntheses.[3]

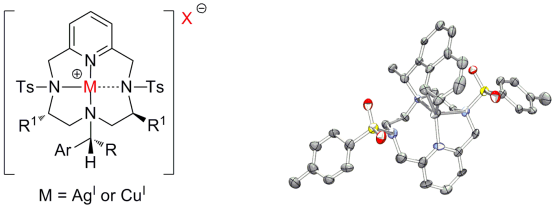

Fig. Metal complexes of Pc-L's and X-ray structure of a Cu(I) complex with a rare h^2-naphtyl moiety coordinated to the metal center.

Key words: macrocyclic ligands, homogeneous catalysis, copper, silver, C-C bond forming reactions.

References

1 B. Castano, S. Guidone, E. Gallo, F. Ragaini, N. Casati, P. Macchi, M. Sisti, A. Caselli, *Dalton Trans.* **2013**, *42*, 2451.

2 a) G. Tseberlidis, M. Dell'Acqua, D. Valcarenghi, E. Gallo, E. Rossi, G. Abbiati, A. Caselli, *RSC Adv.* **2016**, *6*, 97404; b) T. Pedrazzini, P. Pirovano, M. Dell'Acqua, F. Ragaini, P. Illiano, P. Macchi, G. Abbiati, A. Caselli, *Eur. J. Inorg. Chem.* **2015**, *2015*, 5089.

3 a) M. Dell'Acqua, B. Castano, C. Cecchini, T. Pedrazzini, V. Pirovano, E. Rossi, A. Caselli, G. Abbiati, *J. Org. Chem.* **2014**, *79*, 3494; b) M. Trose, M. Dell'Acqua, T. Pedrazzini, V. Pirovano, E. Gallo, E. Rossi, A. Caselli, G. Abbiati, *J. Org. Chem.* **2014**, *79*, 7311; c) B. Castano, E. Gallo, D. J. Cole-Hamilton, V. Dal Santo, R. Psaro, A. Caselli, *Green Chem.* **2014**, *16*, 3202.

Metal-Atom Impact on the Self-Assembly of *Cup-and-Ball* Metalloporphyrin-Fullerene Conjugates

Jean-François Nierengarten

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Construction of artificial photoactive devices capable of mimicking photosynthesis by transforming sunlight into chemical potential is one of the most sought objectives in the quest for new sources of energy.[1] For this purpose, chemists have developed a wide variety of donor-acceptor systems where photon energy is used to produce a photoinduced electron transfer from the donor to the acceptor moiety.[2] Among them, porphyrins and fullerenes have extensively been combined due to their respective notable electron-donor and electron-acceptor properties.[3]As part of this research, a fullerene-ammonium derivative has been combined with different metalloporphyrin-crown ether receptors to generate very stable supermolecules.[4] The combination of fullerene-porphyrin and ammonium-crown ether interactions leads to a strong chelate effect as evidenced by a high effective molarity (3.16 M). The different parameters influencing the stability of the supramolecular ensembles, in particular the nature of the metal in the porphyrin moiety, have been rationalized with the help of theoretical calculations thus providing new insights into fullerene-porphyrin interactions. The latest developments in this field will be presented.

References

[1] V. Balzani, A. Credi, M. Venturi, in *Molecular Devices and Machines*, Wiley-VCH Verlag GmbH & Co. KGaA, **2008**, pp. 171-207.

[2] a) S. Berardi, S. Drouet, L. Francas, C. Gimbert-Surinach, M. Guttentag, C. Richmond, T. Stoll, A. Llobet, in *Chem. Soc. Rev.*, The Royal Society of Chemistry, **2014**; b) M. D. Kärkäs, E. V. Johnston, O. Verho, B. Åkermark, *Acc. Chem. Res.* **2013**, *47*, 100-111.

[3] a) K. M. Kadish, K. M. Smith, R. Guilard, *Handbook of porphyrin science*, World Scientific Publishing, **2010**; b) F. Langa, J. F. Nierengarten, *Fullerenes: Principles and Applications*, Royal Society of Chemistry, **2011**; c) S. Fukuzumi, in *Functional Organic Materials*, Wiley-VCH Verlag GmbH & Co. KGaA, **2007**, pp. 465-510.

[4] a) L. Moreira, J. Calbo, B.M. Illescas, J. Arago, I. Nierengarten, B. Delavaux-Nicot, E. Orti, N. Martin, J.-F. Nierengarten, *Angew. Chem. Int. Ed*. **2015**, *54*, 1255-1260. B) L. Moreira, J. Calbo, J. Arago, B. M. Illescas, I. Nierengarten, B. Delavaux-Nicot, E. Orti, N. Martin, J.-F. Nierengarten, *J. Am. Chem. Soc.***2016**, *138*, 15359-15367.

Synthesis, characterization and coordination chemistry of organophosphorus compounds

Med Abderrahmane Sanhoury

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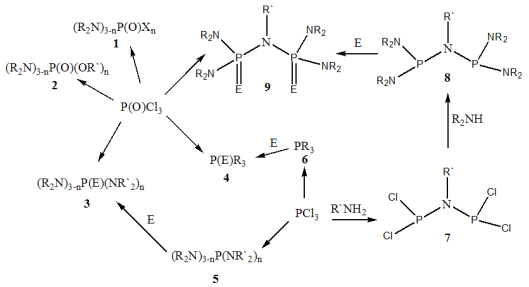
Organophopshorus compounds (OPs) represent an important and versatile class of compounds that have are useful in many areas of chemistry [1]. In addition to being used as prodrugs and intermediates in organic synthesis, OPs are widely used as ligands for transition metal catalyzed reactions due to their chemical versatility [2]. For instance, phosphine chalcogenides have been used extensively as transfer agents yielding a reactive source of chalcogenides [3]. In some cases the OP ligands can be removed under heat and vacuum to produce solid metal chalcogenides. These studies have allowed for a better understanding of the growth of extended metal chalcogenide semiconducting solids [4]. In this presentation we will give an overview of the different approaches for the synthesis of various phosphoramides, phosphoamidates, phophine chalcogenides and corresponding diphosphoryl derivatives (**1-9**). Specifically in this context and as a continuation of our interest in organophosphorus chemistry [5,6], we will also describe their coordination chemistry towards both soft and hard metal ions. These products were fully characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR, IR and in some cases by X-ray analyses. In addition, the effect of the nature of different phosphorus substituents on the reaction yield and complex stability will be compared and discussed.



Keywords: Phosphoryl chloride, secondary amines, phosphine chalcogenides, phosphoramidates, metal complex, NMR.

References

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Molecular Spin Crossover Phenomenon at the nanoscale Motion and Spintronic properties

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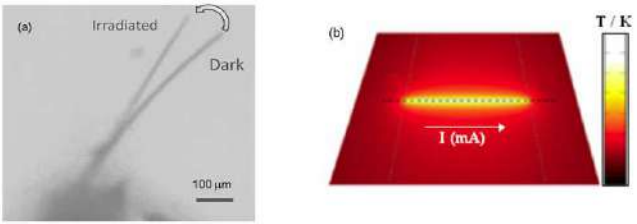
The spin crossover phenomenon in inorganic materials is one of the most spectacular examples of molecular bistability, which means that these molecules may exist in two different electronic states within a certain range of external perturbations. Most notably, the existence of a thermal hysteresis in certain complexes (in the solid state) confers a memory effect on these systems.[1-4] 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]
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 sensors, nano-electronic, photonic, motion and nano-mechanical 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 nano -mechanical and spintronic properties.



(a) Comparison of the cantilever bending in the photo-induced high spin (HS) and low spin (LS) states for a {Fe(3-CNpy)[Au(CN)2]2}.2/3H2O based single crystal actuator.[12,13]
(b) Luminescence modulation by high spin, low spin optical absorptions.[9]

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Trifluoromethyl Aldimines and Fluorinated Alcohols: Access to *N*-Heterocycles

Benoit Crousse

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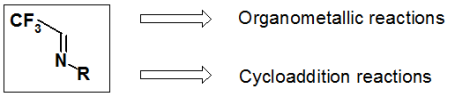
✓ The development of asymmetric methodology, allowing for preparing stereochemically defined and structurally varied amino compounds, has been one of the major goals of synthetic organic chemistry. Considering the unique consequences of fluorine substitution for hydrogen in organic molecules, such as an opportunity for the rational modification of physical, chemical, steric and thus, biological properties of the parent compounds, the synthesis of selectively fluorinated and enantiomerically pure amino compounds, as biological relevant targets, might be of particular interest.[1] We developed the access of new fluorinated synthons by cycloaddition reactions and organometallic additions on fluorinated aldimines,[2] and we were interested in applying these methodologies to the asymmetric synthesis of fluoroalkyl amines.



✓ Fluoroalcohols such as trifluoroethanol (TFE) and hexafluoroisopropanol (HFIP) have emerged as powerful media to perform organic reactions.[3] The presence of trifluoromethyl groups brings very specific properties to fluorinated alcohols with regards to their hydrogenated analogues. Thus, trifluoroethanol (TFE) and hexafluoroisopropanol (HFIP) exhibits unique features (high acidity (pKa (TFE) = 12.4, pKa (HFIP) = 9.3), hydrogen bond donor ability, high ionizing power and very polar solvents, poor nucleophilicity).[3] Due to these particular properties, fluoroalkyl alcohols have been used as "reaction-promoter" solvents. Indeed, they have been successfully involved in a wide variety of reaction which normally requires an external assisting agent (Lewis or Brønsted acids).
Here we would like to present our contribution in the synthesis of *N*-heterocycles in these alcohols, and of fluorinated *N*-heterocycles from CF_3-aldimines.

Key words: N-heterocycles, amines, fluorine, aldimines, fluorinated alcohols.

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The Role of Coordination Chemistry in Platinum-based Technologies

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Platinum plays an essential role in many industries. Owing to its many unique physical and chemical properties, it is the metal of choice for many applications, even though its low abundance in nature, the demanding mining technologies practiced for its recovery from ores or for recycling from waste materials, and finally the sophisticated techniques required for its separation from other precious metals make it one of the highest-priced elements. The lecture will summarize current data on production, demand and applications of the metal and its compounds.

All platinum chemistry starts from one key compound, hexachloroplatinic acid, which is converted in a large number of down-stream processes into a wide range of other complexes which allow for efficient and safe production of high-performance materials and chemicals.

The focus will be on the main processes employed in those industries which account for the highest consumptions of platinum, i. e. catalysts for automotive exhausts and organic transformations such as hydroforming and hydrosilylation, but also for electro- and electroless plating etc. The routes to platinum complexes used in medicine and other niche applications are also considered, and environmental problems associated with the usage of platinum complexes are illustrated by selected examples.

Coordination chemistry of α β-chloro-α,β-unsaturated aldehydes and their derivatives

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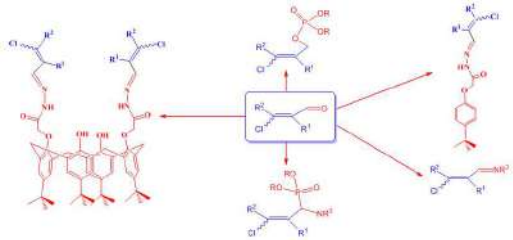
α,β-Unsaturated aldehydes constitute an important class of compounds due to their presence in biological systems as well as their utility as synthetic intermediates in organic synthesis. They are potential precursors of Schiff bases, N-acylhydrazones, calixarenes and organophosphorus compounds [1,2]. These types of compounds have been widely studied in literature and are considered as attractive molecules in medical and pharmaceutical fields because of their broad spectrum of biological activities such as antibacterial, antifungal and antitumor effects [1-3]. They are also explored in different areas including catalysis, metal extraction and science materials [4,5]. In this presentation, an overview of the synthesis of a range of new variously functionalized ligands [6-8], starting from β-chloro-α,β-unsaturated aldehydes is reported. Specifically, their metal binding properties are investigated. All the target ligands and their corresponding complexes were fully characterized by multinuclear (^{1}H, ^{13}C, ^{31}P and ^{119}Sn) NMR, IR, UV-Vis, HRMS and elemental analyses. In addition, the effect of different substituents on the complex formation and stability as well as stereochemical outcome in particular will be presented and discussed.



Keywords: β-chloro-α,β-unsaturated aldehydes, Schiff bases, N-acylhydrazones, calixarenes, organophosphorus compounds, metal complex, NMR.

References:

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Coordination Polymers and Clusters containing Uranyl Ion

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[b] *NIMBE, CEA, CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*

The capacity of uranyl ion to act as a photo-oxidant is a property of interest in relation to the incorporation of uranyl ion in three-dimensional coordination polymers containing cavities possibly enabling selective absorption of reducing substrates. The coordination geometry of uranyl ion is, however, such as to favour the formation of two-dimensional arrays giving rise to layered solids lacking significant space for substrate binding. We have endeavoured to overcome this tendency by the formation of mixed uranyl/(transition or main group) metal ion species, the intent being that the transition or main group metal should induce three-dimensional connectivity. This has resulted in the characterisation of various 3D coordination networks as well as some novel uranyl ion cluster species,[1] work which is reviewed in the present discussion.

Reference

1. For recent publications containing references to preceding work, see: (a) P. Thuéry, J. Harrowfield, *Inorg. Chem.* **2017**, *56*, 1455-1469; (b) P. Thuéry, J. Harrowfield, *Cryst. Growth Des.* **2017**, *17*, 963-966.

Oral Communications' List

(alphabetically authors' name)

Name	Ref
J. Ajmi, I. Nagazi, A. Haddad *FSM - Monastir* Crystal structure of a new Strandberg-type sodium selenomolybdate Na_4 $[Se_2Mo_5O_{21}].5H_2O$	**OC 01**
Z. Aloui, M. Rzaigui, C. Ben Nasr *FSB - Bizerte* Synthesis, crystal structure, and spectroscopic studies of a new Bi(III) halide complex: $[C_7H_{10}NO]_2BiBr_5$	**OC 02**
Z. Baccari, M.A. Sanhoury, B. Crousse, T. Barhoumi-Slimi *FST - Tunis* Synthesis, characterization and coordination chemistry of new α-hydroxyphosphonates	**OC 24**
S. Bahlouli, N. Haddaoui, R. Doufnoune *University Abbas Ferhat - Setif, Algeria* Elaboration and characterization of nanocomposite (Polypropylene_ethylene-diene-monomer)/silica	**OC 05**
L. Bahri, T. Barhoumi-Slimi, M.A.K. Sanhoury, B. Crousse, M.T. Ben Dhia *FST - Tunis* New allylic phosphate and phosphoramidate tin(IV) chloride complexes : Synthesis and multinuclear (^{1}H, ^{19}F, ^{31}P and ^{119}Sn) NMR characterization	**OC 03**
N. Barhoumi, S. Ammar, A. Gadri *FSG - Gabès* Decay kinetics and mineralization of the antibiotic sulfamethazine from water by electro-Fenton using natural chalcopyrite as heterogeneous catalyst	**OC 04**
T. Ben Issa, H. Ghalla, S. Marzougui, A. Romerosa, L. Benhamada *FSM - Monastir* Crystal structure and theoretical studies on a new organic-inorganic compound	**OC 06**
S. Ben Moussa, K. Kaaroud, M.Gruselle, Patricia Beaunier, Bechir Badraoui *FSM - Monastir* Combined effect of magnesium and Amino glutamic acid on hydroxyapatite structure	**OC 07**

Name	Ref
W. Ben Soltan, S. Ammar, O. Babot, T. Toupance *FSG - Gabès* Textural and structural properties of SnO_2 nanoparticles prepared by the polyol method for photocatalytic activity	**OC 08**
N. Benarous, A. Cherouana, E. Aubert, P. Durand, S. Dahaoui *University Frères Mentouri, Constantine - Algeria* Synthesis, characterization, crystal structure and DFT study of two new polymorphs of a Schiff base (E)-2-((2,6-dichlorobenzylidene) amino)benzonitrile	**OC 09**
A. Benghnia, A. Benito, R. Ben Slama, B. Chaouachi *ENIG - Gabès* Metal-organo-graphite oxyde matrices as efficient sorbents for hydrogen storage	**OC 56**
D. Bikele Mama , E. Younang *University of Douala - Cameroon* Structural and bonding properties of complexes obtained from first-row transition metal chelation by 3-alkyl-4-phenylacetylamino-4,5-dihydro-1H-1,2,4- triazol-5-ones and its derivatives : DFT, NBO and QTAIM	**OC 14**
L. Boubakri, S. Yasar, V. Dorcet, C. Bruneau, I. Özdemir, N. Hamdi *FSB - Bizerte* Palladium *N*-heterocyclic carbene complexes: Synthesis, structure and their catalytic application in Suzuki-Miyaura and Sonogashira coupling reactions	**OC 10**
	OC 11
M. Boutar, M.H. Noamane, N. Mattoussi, C. Desroches, R. Abidi, D. Luneau *FSB - Bizerte* Metal organic frameworks MOF's based on diacid calix [4]arenes complexes: Synthesis, characterization and Application	**OC 12**
F. Chahdoura, C. Pradel, M. Gómez *Université de Rennes - France* Glycerol as innovative medium for immobilization of metal nanocatalysts	**OC 18**

Name	Ref
I. Chniti, M.A.K. Sanhoury, I. Chehidi *FST - Tunis* Synthesis of new highly fluorinated imidothio(dithio)carbonate ligands: *S*-alkylation of perfluoroalkylthio-and dithiocarbamates	**OC 13**
S. Dargouthi, C. Minot, B. Tangour *IPEIM - Manar* A theoretical study of H_2O adsorbed and dissociated on TiO_2 nanotube	**OC 15**
M. Dhifi, S. Thabet, A. Haddad *FSM - Monastir* A novel organic-inorganic hybrid based on $[As_2W_{18}O_{62}]_2^{6-}$ polyanion: $[C_4H_7N_2]_6[As_2W_{18}O_{62}].4H_2O$	**OC 16**
N. Dissem, B. Artetxe, J. M. Gutiérrez-Zorrilla, L. San Felices, L. Lezama, A. Haddad *FST - Tunis* A robust framework formed by polymeric octamolybdates and copper(II) complexes of tetradendate N-donor ligands	**OC 17**
R. Dridi, S. Cherni Saoussen, M.F. Zid, N. Boudjada *FST - Tunis* Synthesis, crystal structure and physico-chemical charecterization of a new chromium complex	**OC 20**
S. Dridi, A. Mechria, M. Msaddek *FSM - Monastir* Novel structure of cationic nickel difluoride complexe: Synthesis and characterization	**OC 37**
F. Ebnou, K. Sidi, M. Elalim, M.T. Ben Dhia, M.A.K. Sanhoury *Faculty of Sciences and Techniques - Nouakchott, Mauritania* Cadmium and mercury complexes with organochalcogenophosphorus ligands containing piperidinyl, morpholinyl or diethylamino groups: Synthesis and multinuclear NMR characterization	**OC 21**
M. El Alim, F. Ebnou, M.T. Ben Dhia, M.A.K. Sanhoury *University of Nouakchott, Al Aasriya - Mauritania* Synthesis and characterisation of Zn^{+2}, Cd^{+2} and Al^{+3} complexes with phosphoramides containing diffetent cyclic amino groups	**OC 28**

Name	Ref
H. Eloussifi, J. Farjas, P. Roura, M. Dammak *FSS - Sfax* Chelating agents effect on morphology of YBCO thin films prepared from fluorinated solution	**OC 22**
M. Fray, R. Abidi, T.Barhoumi-Slimi *FST - Tunis* Synthesis and characterization of cadmium complexes of α, β-unsaturated N-Acylhydrazones	**OC 23**
S. Ghrairi, T. Ben Dhia, T. Barhoumi-Slimi *FST - Tunis* Synthesis, characterization of new tin tetrachloride complexes of β-chloro-α, β-unsaturated aldehydes	**OC 25**
Z. Gouid, M.A.K. Sanhoury, M.T. Ben Dhia, S. Boughdiri *FST - Tunis* Synthesis and characterization of zinc and cadmiumselenide nanoparticles capped with different phosphine oxide ligands	**OC 26**
A. Haj Said, M. Mahfoudh *CRMNS - Sousse* Metal-organic frameworks for surface functionalization of electrodes	**OC 27**
A. Hamrouni, F. Ajala, H. Lachheb, F. Parrino, L. Palmisano, A. Houas *ENIG - Gabès* Synthesis and physicochemical study of doped Al-ZnO nanoparticles: application in heterogeneous photocatalysis	**OC 29**
A. Harchani, A. Haddad *FSM - Monastir* Hirshfeld surfaces analysis and Theoretical properties of Polyoxometalate compound	**OC 30**
N. Jebli, M.A.K. Sanhoury, C.V. Stevens, S. Touil *FSB - Bizerte* Synthesis and characterization of new tin(IV) chloride complexes with α,α'-bis(diphenylphosphoryl)-cycloalkanones	**OC 32**
O.K. Jung *Pusan National University - Korea* Tailor-made synthesis of multilayered trimetallocyclophanes via transannula p-p interactions	**OC 34**

Name	Ref
I.U. Khan, Shahzad Sharif *Govt. College University - Lahore, Pakistan* Use of pyridine-2, 4, 6-tri carboxylic acid for assembling of lanthanide coordination frameworks	**OC 38**
R. Khattak, I. I. Naqvi *Shaheed Benazir Bhutto Women University - Peshawar, Pakistan* Kinetics and mechanism of the redox reactions between dicyanobis(phen/bpy)iron(III) and hexacyanoferrate(II)	**OC 44**
S. Khelifi, F. Ayari, A. Choukchou Braham, D. Ben Hassan Chehimi *FSB - Bizerte* Removal of anionic acid dye from aqueous solution by Fenton-like process using pillared bentonite as heterogeneous catalyst	**OC 33**
L. Labiadh, A. Gadri, S. Ammar *FSG - Gabès* Degradation of Acid Orange 7 by a novel electro-Fenton process using chalcopyrite as heterogeneous source of iron and copper catalysts	**OC 35**
F. Laribi, M.A.K. Sanhoury, I. Chniti, I. Ben Chehida *FST - Tunis* Synthesis, characterization and coordination chemistry of new highly fluorinated phosphoramidates	**OC 36**
B. Maalem, A. Balaska, A. Hamouda, S. Djemili *Research Center in Industrial Technologies - Algiers, Algeria* Characterization of the mill scale of Hot rolling Mill IMETAL-El Hadjar	**OC 50**
F. Mahammedi *Abu Bakr Belkaid University - Tlemcen, Algeria* Modification d'amidon par voie seche- Retention des polluant organique	**OC 55**
H. Marzougui, S. Attia-Essaies, D. Ben Hassen-Chehimi *FSB - Bizerte* Synthesis, structural and optical properties of Nd^{3+} ions in $K_2Mg_2(SO_4)_3$ langbeinite salts	**OC 39**
E. Mathlouthi, J. Larinova, N. Amdouni, Y. Guari, J. Long *FST - Tunis* Synthesis and characterization of core-shell Prussian blue nanoparticles for biomedical applications	**OC 40**

Name	Ref
H. Mechi, M.A. Sanhoury, M.T. Ben Dhia, H. Ben Romdhane *FST - Tunis* Binuclear complexes of tin, mercury, zinc and iron with N2S ligand derived from 1,3,4-thiadiazole-2,5-dithiolate dipotassium using click chemistry	**OC 41**
A. Mejri, B. Tangour, F. Picaud *FST - Tunis* Theoretical study of chemical reaction and drug confinement inside single walled carbon nanotubes	**OC 42**
A. Mejri, Outaf Fliss, Khaled Alouani *FST - Tunis* Bis(aminophosphine) diselenides as chemosensors for heavy metal cations: An electrochemical, spectroscopic and theoretical study	**OC 43**
R. Mejri, J.C. Dias, S. Besbes Hentati, C.M. Costa, S. Lanceros-Mendez *FSB - Bizerte* Effect of anion type in the performance of ionic liquid/poly(vinylidene fluoride) electromechanical actuators	**OC 45**
S. Mosbah, L. Bencharif *University Freres Mentouri - Constantine, Algeria* Synthesis of new materials for use as organic active layers characterization of Z (2, 3-diAryl) acrylonitrile by cyclic voltammetry and impedance spectroscopy	**OC 54**
O. Naouali, R. Medyouni, W. Elgabsi, L. Baklouti, N. Hamdi *FSB - Bizerte* Synthesis and cation biding of a new peripherally functionalized phthalonitrile and their Co metallophthalocyanines	**OC 46**
K. Nasr, M.A.Sanhoury, K. Essalah, M.T. Ben Dhia *FST - Tunis* Experimental and theoretical study of tin(IV) chloride complexes with organophosphorus ligands	**OC 31**
R. Omrani, M.A.K. Sanhoury, T. Ben Dhia, M. L. Efrit, A. Ben Akacha *FST - Tunis* Synthesis and characterization of tin tetrachloride complexes with phosphonothioamidates	**OC 47**

Name	Ref
I. Oueslati *FST - Tunis / Académie Militaire, Fondouk jedid* Kinetics study of gas phase reactions of atomic hydrogen with tetramethylsilane, methylsilane and formaldehyde	**OC 48**
W. Selmi, J. Abdelhak, M. Marchivie, M.F. Zid *FST - Tunis* Synthesis, crystal structure, spectroscopic characterization and Hirshfeld surface analysis of iron cyanide complex	**OC 49**
D. Sghairi, M.A. Sanhoury, M. Romdhani Younes *FST - Tunis* New β,β'-aminodiols: Synthesis and reactivity towards phosphoryl chloride	**OC 51**
S. Thabet , B. Ayed, A. Haddad *FSM - Monastir* Synthesis, crystal structure and physico-chemical characterization of a new inorganic compound: $K_{0.5}Na_4[H_{2.5}SbMo_6O_{24}].18H_2O$	**OC 52**
N. Touj, S. Yaşar, I. Özdemir, N. Hamdi *ISSTE - Borj Cédria* Highly active palladium catalysts containing N-heterocyclic carbene for room temperature Suzuki-Miyaura cross-coupling of aryl bromides with arylboronic acids	**OC 53**
K. Vostrikova *Nikolaev Institute of Inorganic Chemistry, Novosibirsk - Russia* Design of low-dimensional molecular magnets based on anisotropic cyanometallates	**OC 19**

Oral Communications' Abstracts

Program of
Friday
12 May 2017

Crystal Structure of a New Strandberg-Type Sodium SelenomolybdateNa_4 $[Se_2Mo_5O_{21}].5H_2O$

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Université de Monastir, Faculté des Sciences de Monastir
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Polyoxometalates (POMs) as early-transition-metal oxide clusters have received much attention in various fields such as catalysis, ion exchange, electrochemistry, magnetism and medicine for their enormous variety of structures and unique properties **[1-4]**.

Because of this importance, it was of interest to synthesize a new member of SelenopentamolybdatesNa_4 $[Se_2Mo_5O_{21}].5H_2O$ and to investigate its structural characterization by single crystal X-ray diffraction, IR,UV and thermogravimetric analysis.

The title compound was crystallized in the triclinic system, space group P-1 with a =11.1600Å, b = 14.3948Å, c = 14.9613Å, α= 89.963 °, β= 76.072°, γ = 86.640 °, Z = 2.

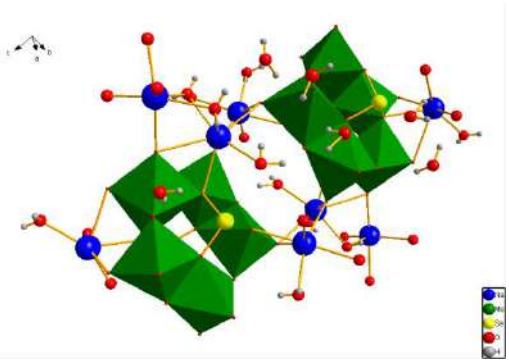

Fig : Asymmetric unit of compound 1

Keywords: X-ray diffraction, Selenopentamolybdates , Crystal Structure.

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Synthesis, crystal structure, and spectroscopic studies of a new Bi(III) halide complex: $[C_7H_{10}NO]_2BiBr_5$

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A new organic-inorganic hybrid compound, 2-methoxyanilinium pentabromobismuthate(III), $[C_7H_{10}NO]_2BiBr_5$, was synthesized and its structure determined by means of single crystal X-ray diffraction studies at room temperature. This compound crystallizes in the orthorhombic $C222_1$ space group with cell parameters a = 11.8870(4), b = 23.4775(8), c = 8.1232(3) Å, V = 2267.0(1) $Å^3$ and four molecules in the unit cell. The structure of the title compound is built up from one-dimensional $[BiBr_5]^{2n-}_n$ polyanionic zig-zag chains composed of deformed $BiBr_6$ octahedra share Br(2) and 2-methoxyanilinium cations. The assignment of the vibrational bands was based on comparison with vibrational mode frequencies of homologous compounds. Theoretical calculations were performed using density functional theory (DFT) for studying the vibrational spectrum of the investigated molecule in its ground state. The ^{13}C CP-MAS NMR spectrum is in agreement with the X-ray structure.

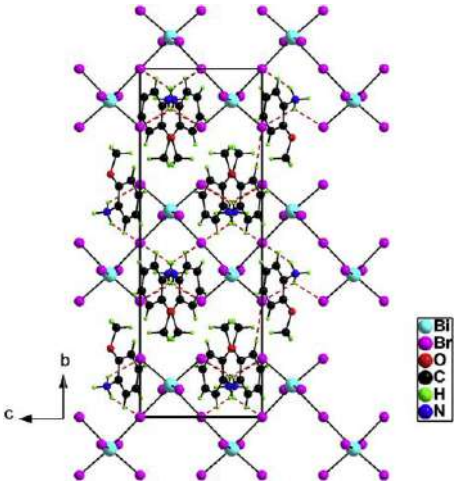

Figure Projection of the structure of $[C_7H_{10}NO]_2BiBr_5$ along the c-axis.

Keywords: X-ray diffraction; Crystal structure; IR spectroscopy; CP-MAS NMR; DFT calculations

New allylic phosphate and phosphoramidate tin(IV) chloride complexes: Synthesis and multinuclear (^{1}H, ^{19}F, ^{31}P and ^{119}Sn) NMR characterization

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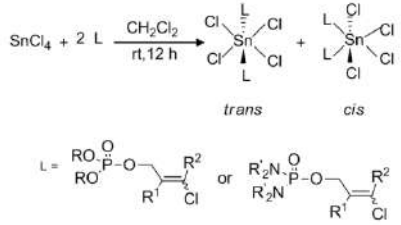
Octahedral tin(IV) complexes of the general formula [SnX_4L_2] (X = halide and L is the phosphoryl ligand), readily accessible via reaction between SnX_4 and various neutral donor ligands, have attracted much interest [1-3]. The stereochemistry of [SnX_4L_2] adducts depends considerably on the substituents directly bound to the phosphorus atom. In these compounds two isomers, with the ligand L in *cis* or *trans* mutual orientations, are possible [4,5]. In this work, we show that allylic phosphates and phosphoramidates (L) bearing different vinyl substituents readily form stable octahedral complexes with tin(IV) chloride to yield new tin complexes. These adducts have been characterized by multinuclear (^{1}H, ^{31}P and ^{119}Sn) NMR and elemental analyses. In dichloromethane solution at room temperature, the NMR data showed the presence of a mixture of *cis* and *trans* isomers for the phosphate tin complexes whilst only the *trans* form was observed for the phosphoramidate derivatives. The difference between the two types of phosphoryl ligands could be interpreted in terms of the electronic effects of the substituents on the phosphorus atom of the ligand.



Keywords: Tin(IV) chloride, allylic phosphates, allylic phosphoramidates, ^{119}Sn NMR, $^{2}J(^{119}Sn–^{31}P)$ coupling constant.

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Decay kinetics and mineralization of the antibiotic sulfamethazine from water by electro-Fenton using natural chalcopyrite as heterogeneous catalyst

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The chalcopyrite-electro-Fenton (chalcopyrite/EF) treatment of 230 mL of 0.20 mM sulfamethazine in sulfate medium of pH 3.0 has been made upon addition of 1.0 g L^{-1} of natural chalcopyrite that self-regulated soluble Fe^{2+} concentration, Cu^{2+} concentration and pH. The electrolytic cell was equipped with either a boron-doped diamond (BDD) or Pt anode and a carbon-felt cathode. Using a BDD anode, a pseudo-first-order kinetics was found for the antibiotic abatement, which was accelerated with raising the applied current. The sulfamethazine decay in EF/chalcopyrite was faster than in classical EF with 0.20 mM Fe^{2+} by the larger generation of $^{\bullet}OH$ from Fenton's reaction. The concentration of carboxylic acids like oxalic, oxamic, formic, maleic and fumaric was determined by ion-exclusion HPLC. All these acids were completely removed at the end of EF/chalcopyrite with BDD.

Keywords: Sulfamethazine, Boron-doped diamond; electro-Fenton; EF/chalcopyrite; Wastewater treatment

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[2] Kinetics of oxidative degradation/mineralization pathways of the antibiotic tetracycline by the novel heterogeneous electro-Fenton process with solid catalyst chalcopyrite. Natija Barhoumi, Hugo Olvera-Vargas, Nihal Oturan, David Huguenot, Abdellatif Gadri, Salah Ammar, Enric Brillas, Mehmet A. Oturan. Applied Catalysis B: Environmental (2017).

Elaboration and characterization of nanocomposite (Polypropylene_ ethylene-diene-monomer)/silica

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University ABBAS Ferhat Setif, Departement of Technology,
Laboratory Physical Chemistry of High Polymers LPCHP, Algeria

The work developed in my study focuses on elaboration and characterization of a new class of polymers..Blends polypropylene / ethylene-diene-monomer have been studied for many years. Mixes polypropylene matrix have attracted the attention of academic and industrial researchers, because of the commercial interest is improving the impact resistance of the polymer at low temperatures.
To this end, the way which comprises mixing the polypropylene with a compound of lower glass transition temperature or higher ductility(elastomer, PE…..). in our case it is particles elastomeric EPDM to remedy the incompatibility problem between PP and EPDM, two compatibilizers were used: block copolymer 'PEP' and copolymer 'PP-g-MAH' to improve the interfacial adhesion between the two phase, and to improve the rigidity of the material, inorganic particles of silica has been added. These lead to materials with high mechanical properties both in terms of rigidity in terms of ductility and impact resistance. The study of mechanical properties such as tensile strength and impact strength show typical as hybrid materials. The introduction of the modified and not modified filler has allowed to improve rigidity of composites. In addition, the use of compatibilisants has allowed to improve interfacial adhesion of the phases in presence by giving mechanical properties higher than those of the pure mixtures.

Key words: Blend, elastomer, compatibilizer, interfacial adhesion

Crystal structure and theoretical studies on a new organic-inorganic compound

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The crystal structure of a new organic phosphate was determined from single crystals obtained by slow evaporation methods (space group; a=7.5508(3) Å, b=7.9705(3) Å, c=8.6849(3) Å; α =77.3725(18)°, β = 82.6225(19)°, γ = 74.9829(19)°). The crystal structure of this is built up from infinite hydrogen bonding inorganic chains of $(H_3PO_4)_n$ lay parallel to the axis, which are also connected to the quinoline rings through hydrogen bonds in a 3D arrangement. The structure was examined through atoms in molecules (AIM) topological [1] and Hirshfeld surface (HS) analyses [2] and its molecular structure optimized by theoretical density functional (DFT) calculations. The QP observed IR absorptions between 4000-400 cm-1 were assigned on the basis of the calculated theoretical vibrational modes.

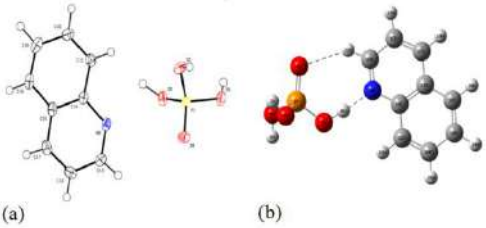

Fig.: (a) Asymmetric unit of the QP molecule.
(b) Optimized molecular structure of QP optimized at DFT-B3LYP\6-311++G(d,p) level of theory.

Key words: organic phosphate, X-ray single-crystal determination, DFT, Hydrogen bond, Vibrational analysis, AIM and HS analyses.

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Combined effect of magnesium and Amino glutamic acid on hydroxyapatite structure

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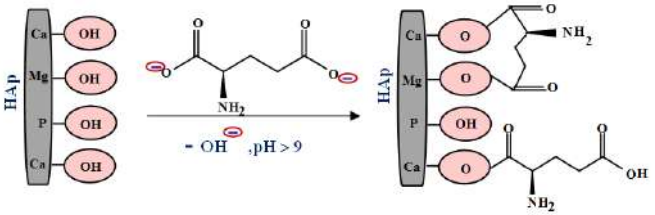
Magnesium modified calcium hydroxyapatite of different Mg/Ca compositions have been synthesised using the hydrothermal method in the presence of glutamic acid [1]. The resulting materials have been characterised by X-ray powder diffraction, chemical analysis, IR Spectroscopy and Transmission Electron Microscopy (TEM). X-ray diffraction analysis shows that the obtained materials consists of a single phase having an apatitic structure. IR spectroscopy highlights the presence of carboxylic groups for the organic moieties grafted onto the apatitic surface [2,3]. The results of the TEM analysis confirm the apatite structure is preserved with a modification of size of the crystals in accordance with the analysis of XRD pattern.



Scheme. Formation of Ca carboxylate salt leading to the grafting of glutamic on the HAp surface

Keywords: Hydrothermal method, Apatitic surface, Glutamic acid, Hybrid compound

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Textural and structural properties of SnO_2 nanoparticles prepared by the polyol method for photocatalytic activity

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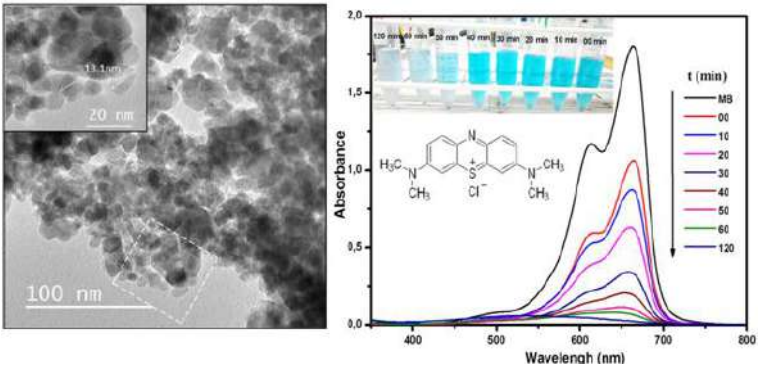
Nanocrystalline mesoporous SnO_2 nanoparticles were synthesized by the polyol method followed by thermal annealing. The composition, texture, structure and morphology of the samples treated at 90, 500 and 700°C in air were determined by X-ray diffraction (XRD), transmission electron microscopy (TEM), Fourier transform infra-red spectroscopy (FTIR), thermogravimetry coupled to mass spectrometry (DTA/TGA/MS) and Nitrogen Sorption Porosimetry. FTIR and TGA–MS data indicate that tin oxide species were obtained with a complete removal of polyol residues after thermal treatment above 500°C. 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 temperature of the thermal post-treatment. Moreover, TEM and N_2 sorption porosimetry show that the calcined samples are composed of an aggregated network of almost spherical nanoparticles, the mesoporosity observed being related to the interparticle space. On the other part, the photocatalytic test of SnO_2 nanoparticles was studied using methylene blue (MB) as model organic pollutants. The SnO_2 nanoparticles revealed that the discoloration of MB reached 98% after irradiation of 120 min.



Keywords: nanoparticles; SnO_2; photocatalytic; polyol;

Synthesis, characterization, crystal structure and DFT study of two new polymorphs of a Schiff base (E)-2-((2,6-dichlorobenzylidene) amino)benzonitrile

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Schiff base compounds are well-studied area of research, having remarkable biological activities[1,2] and able of forming stable complexes developing new applications in the area of solvent extraction of f-elements [3].

In this work, crystal structures of two new polymorphs of the title compound, prepared by the reaction of 2,6-dichlorobenzaldehyde with 4-amino-benzonitrile in ethanol are reported.

The crystal of the first polymorph (I), crystallizing in the monoclinic space group $P2_1/c$, was obtained by slow evaporation of solution reaction, however, the crystal of the second one (II), who crystallize in the orthorhombic space group Pbca, was obtained in high temperature condition. The dihedral angles between the two aromatic rings are 4.81º in (I) and 82.26º in (II), respectively. Theoretical calculations on isolated molecules at the MP_2cc-pVDZ level show that the two polymorphs correspond to two molecular conformations that are within less than 1 kJ mol^{-1} and DFT periodic calculations indicate that (II) is more stable than (I) by 4.1 kJ mol^{-1} of formula unit.

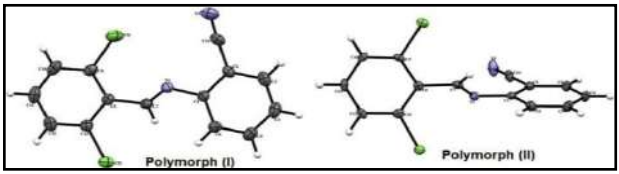

Fig. ORTEP view of the asymmetric unit of (I) and (II).

Key words: Schiff base, Polymorphs, FT-IR, UV–Vis, X-ray diffraction and DFT.

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PALLADIUM *N*-HETEROCYCLIC CARBENE COMPLEXES: SYNTHESIS, STRUCTURE AND THEIR CATALYTIC APPLICATION IN SUZUKI-MIYAURA AND SONOGASHIRA COUPLING REACTIONS

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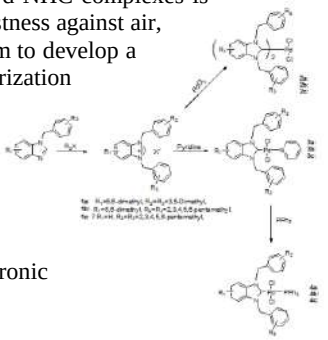
N-heterocyclic carbenes (NHCs) and phosphines have been among the most remarkable ligands for homogeneous catalysis with transition metals towards medical applications and industry.[1] The use of different metal complexes have led to important innovation in homogeneous catalysis.[2] Although there are numerous metal-carbene complexes, the prominence of Pd-NHC complexes is likely due to their catalytic efficiency and robustness against air, moisture and high temperature.[3]. Herein, we aim to develop a simple procedure for the synthesis and characterization of a new palladium complex series with *N*-heterocyclic carbene (NHC) (2a-c), pyridine (3a-c) and phosphine ligands (4a-c). **Scheme1** The catalytic activities of these complexes were screened for the Sonogashira and Suzuki reactions between aryl halides and phenylacetylene, and phenylboronic acid, respectively under mild conditions.[4]



Scheme1: Synthesis of benzimidazolium salts **1a-c** and Palladium Complexes **3-4**.

Key words: Palladium complex, N-heterocyclic carbene (NHC), pyridine, phosphine, Sonogashira, Suzuki reactions.

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Metal organic frameworks MOF's based on diacid calix [4]arenes complexes: Synthesis, characterization and Application

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Our goal is to develop porous materials by forming coordination polymers with calix[n]arene. The porous coordination polymers known as the Metal Organic Framework (MOF) are currently a very active field of research in the field of chemistry and inorganic materials[1]. MOFs have a wide range of potential applications including selective gas storage (H2, NO, CO2, CH4), catalysis and biomedical[2]. For their part, calixarenes have macrocyclic structures capable of forming a hydrophobic cavity which can trap an apolar guest[3]. In the solid state it is well known that calix [4] arenes can act as porous entities capable of absorbing solvent gas molecules or alternatively capable of separating a gas mixture. The formation of ligand-based MOFs such as calixarenes opens up the possibility of forming new porous materials using two levels of porosity associated with both the ligand and the coordination framework.

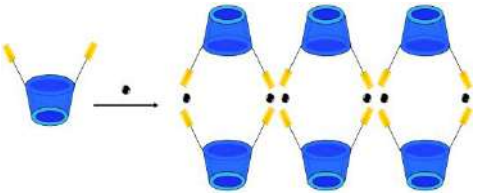

Fig. diacid calix[4]arene's complexes

Key words: diacid calix[4]arene, synthesis, complexation, MOF.
Acknowledgement: we thank the PHC Utique program for the financial support.

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Synthesis of new highly fluorinated imidothio(dithio)carbonate ligands: *S*-alkylation of perfluoroalkylthio-and dithiocarbamates

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The functionalization of the [-NH-(C=X)-X] motif, through alkylation, offers an attractive method for the generation of derivatives which may have interesting technological applications [1], medicinal and biological properties [2]. More interestingly, these derivatives have proven to be potent antiviral and antitumor agents [3] as well as drug intermediates [4]. In our previous work, we have described the synthesis and conformational study of highly fluorinated thio- and dithiocarbamates [5,6] as well as their complexes with mercury(II) [7]. As a continuation of this work, we report herein on the selective *S*-alkylation of these thio(dithio)carbamates. The highly fluorinated *S*-methyl imidothio-(dithio)carbonates thus obtained were characterized by different spectroscopic NMR, IR and HRMS techniques. In addition, the coordination chemistry of these carbonates as ligands towards $SnCl_4$ is already under investigation and will be presented with further details.

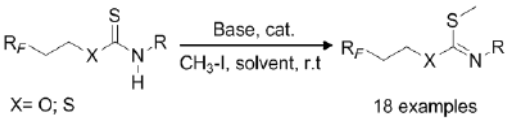

Fig.

Keywords: *S*-alkylation, thio(dithio)carbamates, imidothio(dithio)carbonates, highly fluorinated ligands, NMR spectroscopy.

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STRUCTURAL AND BONDING PROPERTIES OF COMPLEXES OBTAINED FROM FIRST-ROW TRANSITION METAL CHELATION BY 3-ALKYL-4-PHENYLACETYLAMINO-4,5-DIHYDRO-1H-1,2,4-TRIAZOL-5-ONES AND ITS DERIVATIVES : DFT, NBO and QTAIM

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Extensive DFT calculations were used to explore the complexation of 3-alkyl-4-phenylacetylamino-4,5-dihydro-1h-1,2,4-triazol-5-one (ADPHT) derivatives by first-row transition metal cations (Fe^{2+}, Ni^{2+}, Cu^{2+}, Cu^{+}, Zn^{2+}). Two different cases were performed: neutral ADPHT ligand and mono deprotonated ligands. Geometry optimizations have been performed in gas-phase and solution-phase (water, benzene and N,N-dimethylformamide (DMF)) with B3LYP/Mixed I (LanL2DZ for metal atom and 6-31+G(d,p) for C, N, O, H atoms) and with B3LYP/Mixed II (6-31G(d) for metal atom and 6-31+G(d,p) for C, N, O, H atoms) levels. Our results indicates that the M^{2+}-ligand bond distances yielded by B3LYP/ Mixed II are shorter than that relative to B3LYP/Mixed I. This fact can be attributed to the fact that the valence orbitals are not properly described by the latter one. Single points have also been carried out at CCSD(T) level. The comparison of thermodynamic energies of the formation (energies, enthalpies and Gibb energies) of the 28 complexes, obtained from these three different calculations. CCSD(T) complexation energy values for deprotonated ADPHT $–M^{2+}$ complexes are higher than their B3LYP homologs. Such a similar larger difference predicted by Constantino et al [1] in computational study on interactions of Co^{+} and Co^{2+} with glycine is attributed to a bad annulment of self-interaction term by the exchange functional that leads to overstabilization of molecular systems by density functional methods. The metal ion affinities (MIA) have shown to be influenced by the nature of the ligand and the retained NBO charge of the metal ion. The topological parameters yielded from Quantum Theory of Atom in Molecules (QTAIM) [2] indicate that metal-ligand bonds are partly covalent. The significant reduction of the proton affinity (PA) observed when passing from ligands to complexes in gas-phase confirms the notable enhancement of antioxidant activities of neutral ligands in this medium. But, the solvation of the complexes diminishes this enhancement. The positive values of the proton affinity free energy (PAFE) obtained exhibit the spontaneity of the deprotonation of metal- neutral ligand complexes.

Key word: Metal chelation, ADPHT, Metal affinity, QTAIM, antioxidant activity.

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A theoretical study of H_2O adsorbed and dissociated on TiO_2 nanotube

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This work presents a theoretical study of the interaction of H_2O with a single-walled TiO_2 anatase nanotubes. The calculation are performed using the density functional theory (DFT) study based on the periodic method to provide this interaction. Both surface (101) of anatase and (n,0) TiO_2 nanotubes, with diameters ranging from 10.827Å to 16.623 Å, are considered for the study of adsorption process. Two modes for the adsorption are investigated, molecular and dissociative adsorption. Our calculated results show that the molecular and dissociative adsorption of H_2O are exothermic. However, molecular water adsorption is more favorable than dissociative water adsorption. comparably with the adsorption on the surface (101) of anatase, molecular and dissociative adsorption of the outer surface are energetically favorable.

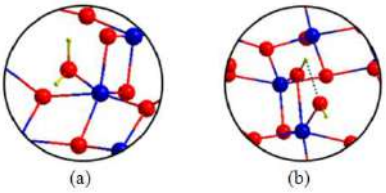

Fig. The optimized structures for H_2O adsorbed and dissociated on (9,0) nanotube.

Key words: Titanium dioxide, TiO_2 nanotube, adsorption, dissociation.

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A Novel Organic-Inorganic Hybrid Based On $[As_2W_{18}O_{62}]_2^{6-}$ Polyanion: $[C_4H_7N_2]_6[As_2W_{18}O_{62}].4H_2O$

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The remarkable chemical and physical properties of polyoxometalate anions have been of interest for many years due to their large variety of applications such as medicine, biology, catalysis, material sciences and chemical analysis [1]. In this context a new arsenotungstates based on Dawson polyanions $[C_4H_7N_2]_6[As_2W_{18}O_{62}].4H_2O$ (1) have been isolated by conventional solution method and characterized by single-crystal diffraction, IR and UV–visible spectroscopies. Compound 1 crystallizes in hexagonal system, space group P-3 with a=20.2904 Å, b=20.2904 Å, c=16.8246 Å, V=5998.38 $Å^3$ and Z=2.

Single-crystal X-ray analysis shows that compound (1) possesses a 3D framework, which is built up of polytungstoarsenate clusters $[As_2W_{18}O_{62}]_2^{6-}$, organic cations and water molecules; the extensive net hydrogen bonds between cations and anions contribute to the crystal packing.

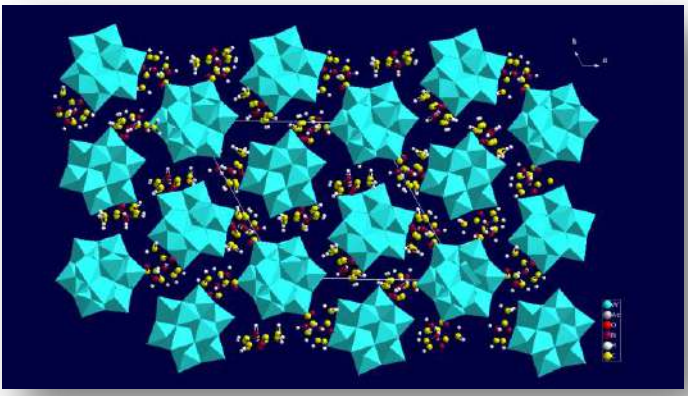

Fig. A Projection along the [001] direction of the title compound.

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A robust framework formed by polymeric octamolybdates and copper(II) complexes of tetradendate N-donor ligands

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The combination of polyoxometalate (POM) anions with copper(II) complexes of tetradentane N-donor ligands has resulted in hybrid structures that can undergo thermally triggered crystal-to-crystal transformations [1]. Following this approach a new phase has been hydrothermally synthesized, namely $[Cu(cyclam)]_{2n}[Mo_8O_{26}]_n \cdot 1.5nH_2O$ (**1**) (cyclam: 1,4,8,11-tetraazacyclotetradecane). Compound **1** shows a POMOF-like (POM Open Framework) 3D covalent network structure formed by $[Mo_8O_{26}]_n^{4n-}$ chains running along the [100] direction which are linked to each other through the coordination spheres of $\{Cu(cyclam)\}^{2+}$ complexes. This structural assembly generates square-like channels parallel to the *y* axis where the hydration water molecules are hosted. The robust structure of **1** remains virtually unaltered upon thermal evacuation of guest solvent molecules, resulting in the anhydrous phase (**1a)** with accessible micropores as demonstrated by single-crystal X-ray diffraction measurements.

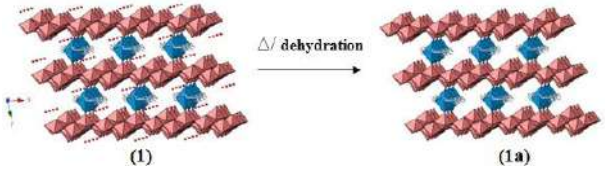

Fig. View along the [001] direction of the open framework of **1** that remains virtually identical upon dehydration.

Key words: Polyoxometalates, robust porous structure, hybrid framework.

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Glycerol as innovative medium for immobilization of metal nanocatalysts

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At present in which a major emphasis is being placed on the design of eco-friendly processes, solvents are a key factor from both an economic and environmental point of view (the global market for solvents is forecast to reach ca. 20 million metric tons by 2015).[1] Accordingly, the design of green solvents is becoming ever more crucial for the chemical industry; such solvents should fulfil specific criteria: i) use of a renewable feedstock, ii) low VOC emission, iii) low flammability, and iv) functional group compatibility.[2] In this context, glycerol represents an innovative solvent coming from biomass and produced in high amounts as a by-product in the production of biodiesel. Its low-cost, non-toxicity, high boiling point, high solubilising ability for organic (except those fully apolar) and inorganic compounds, and low miscibility with other organic solvents, constitute notable properties that make it especially appropriate for catalytic applications, in particular those involving metal-catalysed processes.[3]
In our team, we could recently prove the ability of glycerol to efficiently contribute to the stabilization and immobilization of nanometric species (mainly Pd- and Cu-based nanoparticles), which, in turn, allows a straightforward recycling of the catalytic phase.[4-7]
In the present communication we go to underline the versatility of metallic nanoparticles immobilized in a glycerol phase (molecular- and surface-like behaviour), being successfully applied in multi-step syntheses by a one-pot approach, without isolation of intermediates, using one recyclable catalytic precursor and obtaining metal-free target products.

Scheme 1 One-pot coupling/cyclisation/cycloaddition multi-step processes catalysed by PdNPs@Cu_2ONPs in glycerol.

Key words: glycerol / metal nanoparticles / palladium / copper / C-C and C-heteroatom cross couplings / hydrogenation /cycloaddition / recycling / multi-step reactions / synthesis of heterocyclic compounds.

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Design of Low-Dimensional Molecular Magnets Based on Anisotropic Cyanometallates

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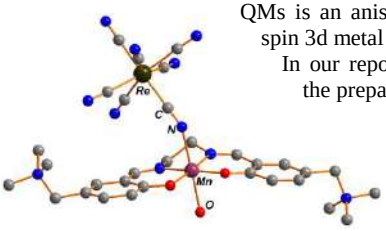
During last decades an interest in discrete 0D/1D polynuclear complexes behaving as single molecule or chain magnets (SMM or SCM) is increased considerably due to their possible application in the high density information storage devices, spintronics and quantum computing [1]. Magnetic behavior of such quantum magnets (QMs) is determined by an energy barrier *U* that has to be surmount to reverse magnetization. The value of *U* for SMM depends on the uniaxial anisotropy energy and total spin of the molecule. For a chain of ferromagnetically coupled spins ability to a slow magnetic dynamics at finite temperatures was predicted by Glauber [2]. Contrary to SMMs, the *U* of SCMs depends not only on the magnetic anisotropy energy but also on the intrachain magnetic interaction [3], hence, it should be easier to rise *U* for SCMs compared to SMMs. Thus, for the design of the 0D or 1D molecular magnetic materials, a set of key parameters must be considered: high total spin, axial magnetic anisotropy and strong exchange interaction between the magnetic centers. If the first two define the height of *U* separating molecule spin projections, the critical temperature (T_b) depends mostly on the last option. The stronger exchange interactions, the better ground spin state is isolated from excited one. It was shown that 4d and 5d cyanometallates with a strong spin-orbit coupling are very promising syntones [4] in design of such systemes [5]. The origin of slow magnetic relaxation in QMs is an anisotropic exchange interaction between high spin 3d metal complexes and heavier cyanometallates [6]. In our report we present the synthetic approaches for the preparation of 0D and 1D coordination bimetallic assemblies involving cyanide complexes of Fe, Ru, Os and Re and displaying slow magnetic dynamics and hysteresis, Re and Os based chains being the first examples of SCMs.



Key words: quantum magnets, ruthenium, osmium, rhenium, cyanometallates

Acknowledgements: this work was partially supported by RFBR, grant 16-03-00880-a.

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13 May 2017

SYNTHESIS, CRYSTAL STRUCTURE AND PHYSICO-CHEMICAL CHARECTERIZATION OF A NEW CHROMIUM COMPLEX

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Over the last three decades, coordination chemists have acquired high control and expertise in the design of supramolecular architectures.
One of the current trends in this area is the search of tri(oxalato) chromium (III) compounds. In fact, these systems has attracted intense interest not only because of their appealing structural novelty, but also due to their fascinating properties and applications, such as catalysts, luminescence, NLO and magnetic [1].
Following these lines of investigation, we have focused our work on the synthesis and the characterization of a new compound of formula $(C_7H_7N_2)(H_2C_2O_4)[Cr(C_2O_4)_3].3H_2O$.
This compound crystallizes in the orthorhombic Pbca space group with a = 18.029 (4)Å, b = 19.123 (4)Å, c = 19.479 (4)Å , V= 6809 (2)Å^3 and Z= 8.
The resolution of the structure leads after several cycles of refinement followed by some Fourier-Differences to reliability factors R(F) = 3.6 % and wR(F^2) = 10.50%.
The structure is made up of one $[Cr(C_2O_4)_3]^{3-}$ anion, three $(C_7H_7N_2)^+$ cations, one oxalic acid molecule and three crystallization water molecules, which are held together by hydrogen bonds and π-π stacking interactions.
The structure of the title compound consists of layers formed by $[Cr(C_2O_4)_3]^{3-}$ and free water molecules intercalated by organic cations $(C_7H_7N_2)^+$ (Fig. 1).
The crystal packing is stabilized by N—H...O and O—H...O hydrogen bonds [3,4] between $(C_7H_7N_2)^+$, $[Cr(C_2O_4)_3]^{3-}$ and the uncoordinated water molecules. These interactions link the layers together forming a three-dimensional network and reinforcing the cohesion of the ionic structure.
The structure was characterized by various experimental techniques including IR, UV–visible spectroscopies and thermogravimetric analysis. Magnetic properties was also studied in order to find out the types of interactions existing between the metal centers.

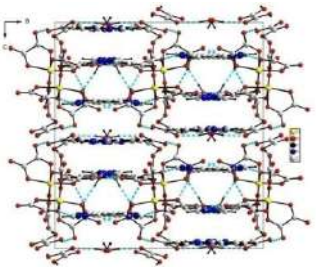

Fig. 1 Projection of the $(C_7H_7N_2)(H_2C_2O_4)[Cr(C_2O_4)_3].3H_2O$ structure along the *b* axis

Key words: Chromium(III) complex, Crystal structure, spectroscopic characterization, magnetic properties

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Cadmium and mercury complexes with organochalcogenophosphorus ligands containing piperidinyl, morpholinyl or diethylamino groups: Synthesis and multinuclear NMR characterization

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Organophosphorus compounds are well-known for their use as pesticides, insecticides and recently as prodrugs due to their activity as acetylcholinesterase inhibitors [1]. In particular, phosphine chalcogenides of the formula R_3PE (E = O, S or Se) are attracting considerable interest owing to their biological activity and selective affinity towards metal ions [2]. In a previous work [3,4], we have synthesized a series of new organochalcogenophosphorus compounds bearing different cyclic amino groups. In this presentation, we will describe the synthesis of new complexes of metal cations such us Cd^{2+}, Hg^{2+} and Zn^{2+} with these ligands. These complexes were fully characterized by multinuclear (^{1}H, ^{13}C, ^{31}P, ^{77}Se, ^{113}Cd and ^{199}Hg) NMR and IR spectroscopic techniques.

$$MX_2 + n((R_2N)_{3-i}P(E)(NR'_2)_i) \xrightarrow{\text{Ehanol/acetone}} [MX_2((R_2N)_{3-i}P(E)(NR'_2)_i)_n]$$

(M = Cd, Hg or Zn; X = Cl or NO_3, n = 2 and X = ClO_4, n = 4; R_2N = Pip, Mor or NEt_2; E = S or Se and i = 0, 1 or 2)

Keywords: Organophosphorus, piperidinyl, morpholinyl, Cd and Hg complexes, NMR spectroscopy.

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Chelating agents effect on morphology of YBCO thin films prepared from fluorinated solution

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We present our work in the preparation of metalorganic precursor solutions with reduced triethanolamine (TEA) and/or diethanolamine (DEA) content, able to fulfil the requirements for high-performance superconducting YBCO epitaxial layers as a promising approach to low cost and scalable coated conductors. It has been proposed to add DEA or TEA chelating agents to accelerate the decomposition and to improve film morphology. Stable YBCO precursor solution with 20% TEA or with 20% DEA have synthetized. Since TFA groups are very electronegative TEA does not coordinate with the metal, and hence the solutions are stable. Different flowing atmospheres are used: The results regarding the kinetics and the morphology with wet N_2 are discouraging, while with wet O_2, results are very promising. The morphology is better than that observed in layers without TEA.

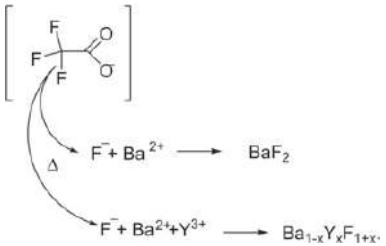

Fig. Formation of fluorine compounds during thermal decomposition of metalorganic salts.

Key words: superconducting YBCO, triethanolamine (TEA), diethanolamine (DEA).

Synthesis and characterization of cadmium complexes of α, β-unsaturated N-Acylhydrazones

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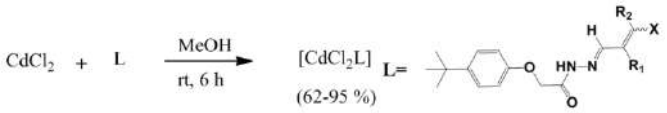
N-Acylhydrazones (NAHs) are very useful azomethines in many areas. They have found applications in medicine as antimicrobial and antitumor agents; in commerce as dyestuffs and agrochemicals and in environment as analytical agents [1-3]. Recently, they are attracting considerable attention as potential systems for information storage and optoelectronic devices [4]. Particularly, they have been used as highly effective extractants of several metals [5]. In this work, we describe the synthesis of new tetrahedralcadmium complexes of N-acylhydrazones of β-chloro-α,β-unsaturated aldehydes. These adducts $[CdCl_2L]$ (L= p-tBuPhOCH$_2$(CO)NHN=CHCR^{1}C=CR^{2}Cl) were fully characterized by NMR, IR, and UV-Vis spectroscopies. The magnitude of the metal-ligand interaction was estimated on the basis of the carbonylvalence vibration values and used to classify the NAHs according to their Lewis basicity. In addition to the effect of the substituents on the complexing properties, the difference in behavior between solid and liquid states will be also discussed.



Keywords: β-chlorovinylaldehydes, N-acylhydrazones, cadmium complexes, NMR spectroscopy.

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Synthesis, characterization and coordination chemistry of new α-hydroxyphosphonates

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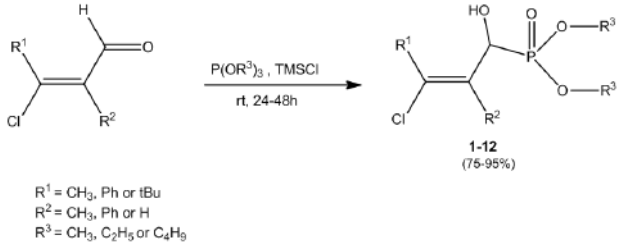
α-Hydroxyphosphonates constitute an important class of compounds owing to their biological and physical properties as well as their utility as synthetic intermediates. Thus their synthesis has received an increasing attention due to their potential biological activities, such as antiviral, antibacterial, anticancer, pesticidal, HIV protease as well as enzyme and renin inhibitory properties [1-4]. In the present work, we describe the synthesis of new α-hydroxyphosphonates from β-choloro-α,β-unsaturated aldehydes. These new biologically interesting hydroxyphosphonates (**1-12**) were obtained through the two-component reaction of aldehydes and trialkyphosphites using TMSCl as catalyst. The compounds were prepared and characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR, HRMS and IR spectroscopy. The coordination chemistry of these **α**-hydroxyphosphonates as new ligands towards tin tetrachloride will be also presented.



Keywords: β-Chlorovinyl aldehydes, α-hydroxyphosphonates, NMR spectroscopy.

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Synthesis, characterization of new tin tetrachloride complexes of β-chloro-α, β-unsaturated aldehydes

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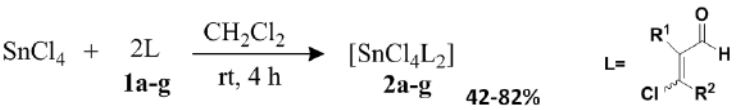
The study of metal complexes with carbonyl compounds is important in organic and bioorganic chemistry. In addition to the ability of the formation of new C-C bonds, they may allow the control of the stereochemistry of a reaction [1,2]. In this work, we report the synthesis of new octahedral tin tetrachloride complexes of β-chlorovinylaldehydes with the general formula $[SnCl_4L_2]$ (L= $(CHO)R_1C=CR_2Cl$) [3]. The adducts have been characterized in solution using NMR, IR and UV-Vis spectroscopies. All the results showed that complexation occurred through the carbonyl oxygen atom and the number of carbon atoms in the alkyl chain of the substituents R_1 and R_2 have a significant effect on complexation formation [4]. The magnitude of the metal-ligand interaction was estimated on the basis of the values of the carbonyl valence vibrations in IR spectroscopy and used to classify the aldehydes according to their Lewis basicity.



Keywords: β-Chlorovinylaldehydes, tin octahedral complexes, Lewis basicity, NMR spectroscopy.

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Synthesis and characterization of zinc and cadmiumselenide nanoparticles capped with different phosphine oxide ligands

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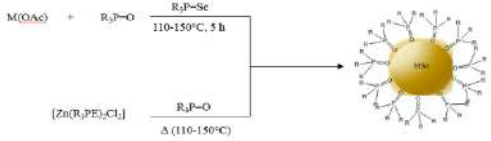
In the recent years, studies on nanoparticles have generated a greater interest due to their unique properties andtheir various applications. For instance, they are used as window layer of solar cells [1] in the production of hydrogen blue green LEDs, EL displays, anti-reflection coatings for infrared devices and other nonlinear optical device [3] and especially in lasers and photovoltaic's [2]. There are many processes for the preparation of semiconductor nanoparticles such as simple chemical method. In our research work, we focused on the preparation of CdSe and ZnSe nanoparticles capped with different phosphine oxideligands from different sources or from metal complexes of the type of $[MCl_2(R_3PE)_2]$ (R = Oct, Bu with E = O, S or Se) as single source precursors.The complexes have been synthesized and characterized by multinuclear (^{1}H, ^{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 spectroscopic data show that the ligand is coordinated to the zinc center through the chalcogenide atom of the P=E group. The MSe nanoparticles (M=Cd, Zn) have been synthesized and characterized by UV-visible and PL spectrophotometry, IR spectroscopy and XRD analyses.



Keywords: Phosphine chalcogenide, zinc complexe, ZnSe, CdSe nanoparticles.

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Metal-Organic Frameworks for surface functionalization of electrodes

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Metal-Organic Frameworks (MOFs), a subclass of Coordination Polymers, are hybrid mesoporous materials resulting from supramolecular self-assemblies of metal ions/clusters with polydentate organic linkers [1]. They are multifunctional materials having potential applications in gas storage and separation, catalysis, drug delivery systems, energy storage and sensors elaboration [1]. Although more than 20 000 MOFs structures have been reported and studied to date, the structuring of metal–organic frameworks at the mesoscopic/macroscopic scale and the elaboration of MOFs-coated surfaces are still challenging problems [2-4]. In fact, elaborating MOFs as thin films is a crucial point to spur their use in optoelectronic devices, sensors and electrodes for energy storage and conversion.
In this work, we describe our recent research endeavors devoted to electrodes modification by MOFs. Firstly, we report a mild synthesis, by coordination modulation, of MOFs particles with submicron size and negative surface charge. The resulting crystals were characterized by powder XRD, FT-IR spectroscopy, granulometry and ζ potential measurements. Then, the negatively charged MOFs were successfully deposited, as thin films, onto an Indium Tin Oxide electrode using electrophoretic deposition and LbL methodology.

Key words: Coordination polymers, MOFs, SURMOFs, Electrophoretic deposition, LbL methodology, Coordination modulation

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SYNTHESIS AND CHARACTERISATION OF Zn^{+2}, Cd^{+2} and Al^{+3} COMPLEXES WITH PHOSPHORAMIDES CONTAINING DIFFETENT CYCLIC AMINO GROUPS

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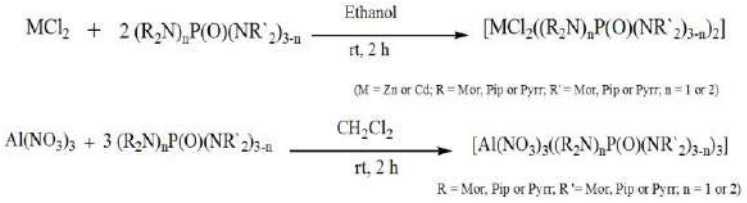
Phosphoramides are increasingly attracting considerable attention due their potential applications in industry as flame retardants, in medicine as prodrugs, in catalysis and synthesis as chiral ligands [1,2]. Interstingly, certain metal complexes of this class of compounds have shown to be suitable single-source precursors for the production of monocrystals of metal chalcogenides of the type ME (M= Zn or Cd, E= O) [3,4]. In this work, we will report on the synthesis of the zinc cadmium and aluminum complexes with phosphoramides containing different cyclic amino groups of the type $(R_2N)_nP(O)(NR`_2)_{3-n}$. These complexes were fully characterized by multinuclear (^1H, ^{13}C and ^{31}P) NMR, IR spectroscopy and conductimetry. The effect of the substituents of the phosphophorus atom on the stability of the complex formed will be also presented.



Keywords: Phosphoramides, aluminium, zinc, cadmium complex, ^{31}P NMR.

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Synthesis and physicochemical study of doped Al-ZnO nanoparticles: Application in heterogeneous photocatalysis

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Heterogeneous photocatalysis is considered as a promising technique in several applications. Currently, the photocatalysts applied in the environmental remediation under natural solar light had not reached a high performance yet. In this research, doped Al-ZnO photocatalysts were synthesized by sol-gel method and were examined by XRD, DRS, BET and FTIR. The photocatalytic activity was evaluated on the degradation of Indigo Carmin under artificial UV light (8 w). The band structure, the structural, and optical properties were studied in order to understand the correlation between the physicochemical properties and the photocatalytic activity of the samples. The photcatalytic activity was found to be enhanced by the incorporation of Al into the ZnO lattice. Particularly, the doped Al-ZnO photocatalyst with the Al/ZnO molar ratio equals to 0.01/1 showed the highest efficiency. The surface properties and the potential of the valence band had a significant role to the enhancement of photocatalytic activity.

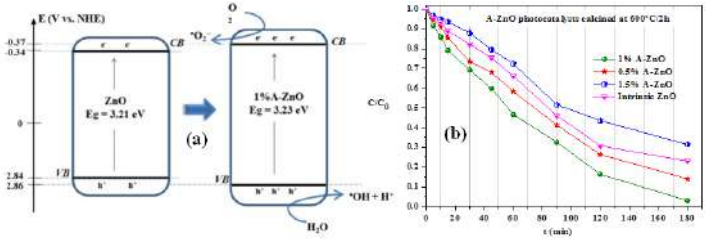

Fig. (a) Estimated bands position of the ZnO before and after Al doping and (b) photodegradation of the IC in the presence of the ZnO and doped Al-ZnO.

Keywords: Al-doped ZnO, sol-gel, nanoparticles, photocatalysis, Indigo Carmin.

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Hirshfeld surfaces analysis and Theoretical properties of Polyoxometalate compound

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Hirshfeld surfaces analysis and Semi-empirical calculations were performed to study the intermolecular interactions and theoretical properties of polyoxometalate compound $(C_6H_{14}N)_4(NH_4)_2[P_2Mo_5O_{23}]\cdot H_2O$ (1). In generally the theoretical achievements were found in a good agreement with the experimental data. The calculated results of the crystal structure and molecular geometry for this compound provided helpful information for the study of electronic structure and molecular properties of polyoxometalate compounds. Furthermore, the current study indicated that the Hirshfeld surfaces analysis and fingerprint plots revealed that the closest contacts of this compound were dominated by different types of H bonding interactions.

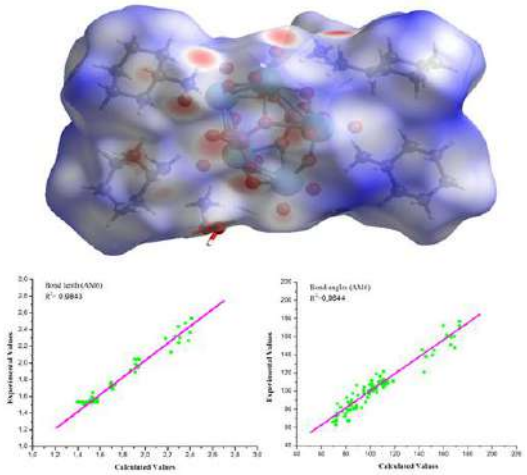

Fig. Hirshfeld surfaces and Correlation graphics of calculated and experimental molecular bond lengths and bond angles of (1)

Key words: Hirshfeld surfaces; Polyoxometalate; Theoretical study.

Experimental and theoretical study of tin(IV) chloride complexes with organophosphorus ligands

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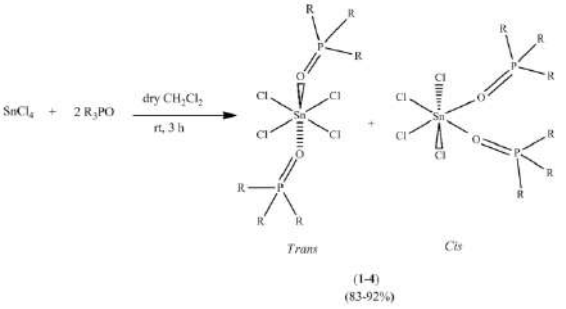
Investigations on tin(IV) adducts continue to provide to provide fundamental information about both the Lewis acid–base model and the reactivity of tin(IV) species [1–5]. In this work we report on the preparation of tin tetrachloride complexes of the type $[SnCl_4(R_3PO)_2]$ (R = Et_2N (**1**), *n*-Bu_2N (**2**), *n*-Bu (**3**) or *n*-BuO (**4**)) have been prepared. These adducts were fully characterized by multinuclear (^1H, ^{13}C, ^{31}P and ^{119}Sn) NMR and IR spectroscopy. The NMR data show that while the ligands $(Et_2N)_3P(O)$ and $(n\text{-}Bu_2N_3)P(O)$ form exclusively *trans* complexes with tin the ligands $n\text{-}Bu_3P(O)$ and $(n\text{-}BuO)_3P(O)$ form a mixture of *cis* and *trans* isomers in solution. These ligands were therefore classified according to their donor ability (complex stability) in the order: $(Et_2N)_3P(O) \approx (n\text{-}Bu_2N_3)P(O) > n\text{-}Bu_3P(O) > (n\text{-}BuO)_3P(O)$. This could be explained in terms of steric hindrance for the first two ligands and electronic effects for the last two. ^{31}P and ^{119}Sn NMR experimental thermodynamics and DFT/B3LYP theoretical studies were carried out on the complexes **1**-**4**. The results show good agreement between experimental and theoretical data.



Keywords: Tin (IV), Phosphoryl ligands, Tin tetrachloride, 119Sn NMR, DFT/B3LYP

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Synthesis and characterization of new tin(IV) chloride complexes with α,α'-bis(diphenylphosphoryl)-cycloalkanones

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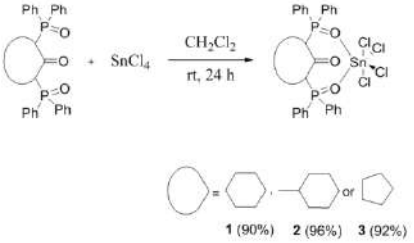
The synthesis and characterization of phosphorus chelating ligands continues to be an attractive field of research in the past few decades due to their metal cation affinity [1,2]. The interest for these compounds is due to their well-known useful applications, such as in the high-performance extraction of various metals [3,4], in the preparation of ion-selective electrodes [5,6], or as light-emitting components in light-emitting diodes [7]. More recently, we have reported on the synthesis of α,α'-bis(diphenylphosphoryl)-cycloalkanones [8]. Herein we describe the coordination chemistry of these diphosphoryl compounds as bidentate ligands towards the strong Lewis acid tin tetrachloride. Therefore, three new tin(IV) complexes of the type [SnCl4(Ph2P(O)CH(R)C(O)CH(R)P(O)Ph2)] [R = CH_2-CH_2-CH_2 (**1**), CH_2-$CH(CH_3)$-CH_2 (**2**), CH_2-CH_2 (**3**)] were prepared by the reaction of $SnCl_4$ with the ligand, α,α'-bis(diphenylphosphoryl)-cycloalkanones in anhydrous dichloromethane. These new adducts were characterized by multinuclear (^{31}P, ^{1}H) NMR and IR spectroscopy.



Keywords: Bidentate phosphoryl ligand, Tin tetrachloride, ^{119}Sn NMR, ^{31}P NMR, tin complexes.

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Removal of anionic acid dye from aqueous solution by Fenton-like process using pillared bentonite as heterogeneous catalyst

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Advanced oxidation processes (AOP) have been extensively used in the treatment of wastewater from the textile industry[1], as it has been seen that dye degradation and removal is very hard to be carried out. Among these AOPs, heterogeneous Fenton-like catalyst[2] and several attempts have been made using supporting materials. So, in this work especially, Al-Fe-Pillared clay has also been reported to be an efficient catalyst for Fenton-like processes[3]. Then, we describe the synthesis and characterization of the heterogeneous catalyst Fenton Fe-Al-PILC prepared by pillaring process of natural Tunisian clay used in heterogeneous Fenton reaction to degrade the Congo red dye. In order to optimize reaction conditions, effects of pH, initial catalyst concentration and amount of H_2O_2 were investigated. The results showed that the degradation yield could reach 95.75% with a solution of CR (10^{-4}M), 0,1g of catalyst and 10mM H_2O_2 at 25°C, pH3 at the end of 30 min. The kinetic studies revealed that the degradation profile is well fitted by the first-order kinetic model.

Key words: Al-Fe-Pillared, catalyst, Fenton-like process, Congo red dye

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Tailor-made Synthesis of Multilayered Trimetallocyclophanes via Transannula π–π Interactions

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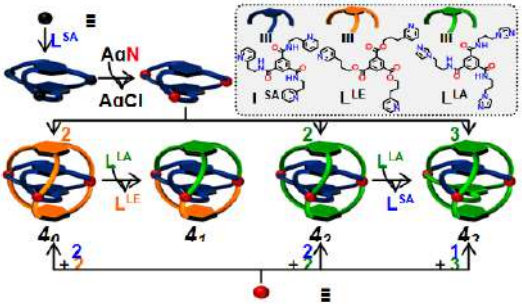
Synthesis and operation of a nano-demension 24 × 24 × 15 $Å^3$ "left and right ball-joint-type host-guest system" via one π···π interaction and three NH···O=C hydrogen-bonds along with the combined helicity are described. The system consists of unprecedented conglomerate aggregates of two distinct helical metallacyclophanes, chiral isomer (*P*)-$[Pd_3X_6(L_1)_2]$@(*M*)-$[Pd_3X_6(L_1)(L_2)]$ and its enantiomer (*M*)-$[Pd_3X_6(L_1)_2]$@(*P*)- $[Pd_3X_6(L_1)(L_2)]$ are described. Successive reactions afford desirable four-layered metallacyclophanes via tailor-made procedure. Synthesis and operation of a nano-demension size multilayered metallacyclophane system via one π···π interaction along with the combined helicity are described. A synthetic strategy of generation of new molecular species utilizing a provision of nature has been reported: nano-dimensional (23(2) × 21(1) × 16(1) $Å^3$) hetero four-layered trimetalla-cyclophanes via the proof-of-concept experiments that utilize a suitable combination of π···π interactions between the central aromatic rings, tailor-made short/long spacer tridentate donors, and the combined helicity are constructed. The unprecedented four-layered metallacyclophane system's behavior offers a landmark in the development of new molecular system.



Scheme 1. Construction of four-layered tripalladium(II)cyclophanes through consecutive, substitution, and direct reactions.

Key words: Pd(II) complexes, Metallacyclophanes, π–π Interactions

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Degradation of Acid Orange 7 by a novel electro-Fenton process using chalcopyrite as heterogeneous source of iron and copper catalysts

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The mineralization of Acid Orange 7 (AO7) has been studied by a novel electrochemical advanced oxidation process (EAOPs) consisting in electro-Fenton (EF) oxidation by chalcopyrite as heterogeneous catalyst, so-called "EF-chalcopyrite", in which chalcopyrite powder was the source of Fe^{2+} and Cu^{2+} as metal co-catalysts instead of a soluble iron salt used in classical EF. Trials were performed with a stirred boron-doped diamond (BDD)/carbon-felt cell under O_2 bubbling for cathodic H_2O_2 generation. Hydroxyl radicals formed from water oxidation at the BDD anode and in the bulk from Fenton's reaction between Fe^{2+} and H_2O_2 were the main oxidizing agents. The effect of current on kinetic decay, mineralization rate, mineralization current efficiency and specific energy consumption was examined under comparable EF and EF-chalcopyrite conditions. An almost total mineralization was achieved for a 0.28 mM AO7 solution operating at 300 mA for 6 h. The kinetic decay of the dye was followed by reversed-phase HPLC and obeyed a pseudo-first-order reaction. Ion chromatography analysis confirmed the release of NO_3^- and NH_4^+ ions during AO7 mineralization.

Key words: heterogeneous catalyst, electro-Fenton, Acid Orang 7, carbon felt, catalysis.

Synthesis, characterization and coordination chemistry of new highly fluorinated phosphoramidates

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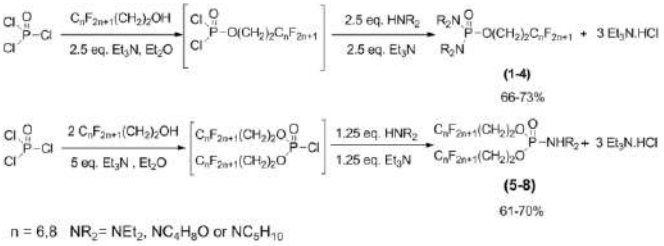
Phosphoramidates are a class of organophosphorus compounds which have great potential and applications as a pesticides [1], flame retardants [2] and prodrugs [3]. For instance, they have been developed into clinically useful chemotherapeutic agents used in the treatment of prostate cancer [4] and HIV infection [5]. They are also used as potential ligands due to their high metal affinity [6]. In the present work, a one-pot synthesis of new highly fluorinated phosphordiamidates (**1**-**4**) and phosphoramidates (**5**-**8**) was performed through phosphorylation of corresponding alcohols followed by aminolysis with various secondary amines. The compounds were obtained in 61-73% yield. They have been characterized by multinuclear (^{1}H, ^{13}C, ^{19}F and ^{31}P) NMR and IR spectroscopy. The preliminary coordination chemistry study of these phosphoramidates as potential ligands towards metal cations will be also presented.



Keywords: Phosphoramidate, fluoroalkyl, alcahool, ^{31}P NMR spectroscopy.

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NOVEL STRUCTURE OF CATIONIC NICKEL DIFLUORIDE COMPLEXE: SYNTHESIS AND CHARACTERIZATION

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A new family of paramagnetic cationic fluorine nickel(IV) complexes was prepared in good yields. The compounds have the general formula $[Ni(L)_2F_2](PF_6^-)_2$ are synthesized by decomposition of the salt methallyloxytris(dimethylamino)phosphonium hexafluorophosphate $[C_4H_7OP(NMe_2)_3]^+ PF_6^-$ in the dichloromethane in the presence of $Ni(COD)_2$ and the pyridinylimine ligands.
These new complexes C1–C3 have been characterized by IR spectroscopy and elemental analysis, as well as X-ray crystal structure analysis for compound C2.

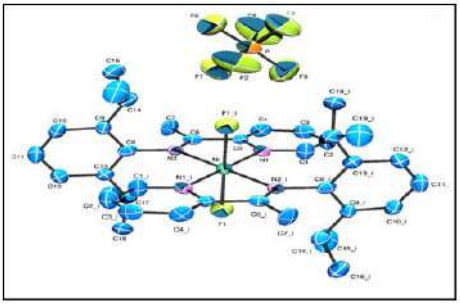

Fig. cationic Nickel(IV) difluoride complexe

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

Use of Pyridine-2, 4, 6-tri Carboxylic acid for assembling of Lanthanide Coordination Frameworks

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Pyridine-2, 4, 6-tricarboxylic (PTA) provides various coordination modes and may serve as terminal or bridging building blocks to assemble higher-dimensional lanthanide coordination frameworks. Single X-Ray Diffraction technique, FTIR spectroscopy, Elemental Analysis, Thermal and SQUID analysis were used to explore their coordination behavior. In view of the excellent coordination capability of this ligand, we have reported number of coordination polymers [1-2]. In three-dimensional Ce(III) mixed ligands coordination polymers, Ce(III) ions show three different coordination numbers of seven, eight and ten while PTA adopts four kinds of coordination modes [1]. Another, series of 1-D and 2-D coordination polymers of cerium (III) with PTA was reported [2] whereas, zero dimensional (0D) Praseodymium (III) Complexes is under review [3]. Herein, we are reporting the synthesis of Lanthanide complexes derived from highly connective PTA by heating in an autoclave under autogenous pressure. X-Ray structural analysis reveals the asymmetric unit of the frameworks consists of two Ln(III) ions, the Ln1 atom is nine-coordinated while Ln2 atom is ten-coordinated showing 3D coordination polymers (Fig. 1) $[Ln_4(PTAH)_6(H2O)_9(NH_3)]_n.(H_2O)_6$. Two types of coordination modes having one novel mode are observed for each of three polymers possessing 17 % voids volume. Due to void volume and prominent porosity these 3D polymers may show potential applications in gas storage and separation. These studies reveal that PTA is versatile organic linker to generate poly functional porous coordination polymers by reflux, hydrothermal, solvothermal and mild hydrothermal conditions.

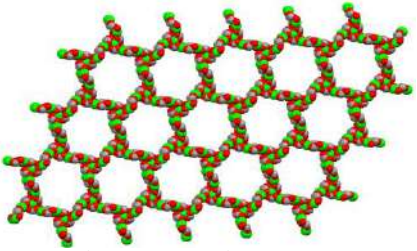

Fig. 1 An infinite 3D layer of Lanthanide complexes

Key words: Pyridine-2, 4, 6-tri Carboxylic acid, Lanthanide Metal-Organic Framework, Gas Storage and separation

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14 May 2017

Synthesis, structural and optical properties of Nd^{3+} ions in $K_2Mg_2(SO_4)_3$ langbeinite salts

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The Nd^{3+}doped langbeinite salts were prepared by the solid state diffusion method. A complete structural characterization has been carried out by means of powder X-ray diffraction (XRD) confirming a crystallization in cubic system $P2_13$.The Raman spectroscopy have showed the internal vibrations due to SO_4^{2-} ion, external vibration, Nd^{3+} ion incorporation on the Matrix. Also, the EDS and SEM has confirmed the elemental composition of the langbeinite salts. Absorption spectrum of this compound was investigated in the wavelength range of 300–3000 nm and the optical properties have been discussed. The emission spectroscopy at 532nm showed the $^4F_{5/2} \rightarrow {}^4I_{9/2}$, $^4F_{3/2} \rightarrow {}^4I_{9/2}$, $^4F_{3/2} \rightarrow {}^4I_{11/2}$ transitions. The results indicate the potentially use of this system to carry other research and endeavor the use of sulfate as easy manufacturing material for high technological applications.

Key words: Langbeinite salts, rare-earth, structural analysis, luminescence properties.

Synthesis and characterization of core-shell Prussian blue nanoparticles for biomedical applications

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Prussian Blue Analogues (PBA) nanoparticles attract a great deal of attention due to their interesting magnetic, optical, catalytic and intercalation properties, which can be tuned by variation of the composition, size and morphology. Among different applications, they have been proposed for the employment in biology and medicine as contrast agents for several types of imaging, including Magnetic Resonance Imaging, (Catala et al., 2014 and JL et al., 2015) photoacoustic imaging, (Huang et al.., 2013) scintigraphy, (JL et al., 2014) and as therapeutic agents for phototherapy, (*Chem.Commun.*, 2012). In this work we present the synthesis and characterization of PBA core@SiO_2 shell nanoparticles carried out by two step procedure: (i) the synthesis of the PBA nanoparticles, and (ii) the silico-shell growth by the sol-gel method.

Keywords: Prussian blue, nanoparticles, silica, core-shell.

Binuclear complexes of tin, mercury, zinc and iron with N2S ligand derived from 1,3,4-thiadiazole-2,5-dithiolate dipotassium using click chemistry

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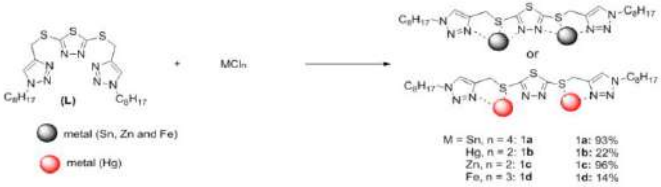
In order to reduce the impact of heavy metals on environmental pollution, research works have focused on the use of polymers with complexing properties as a method of metallic decontamination. Ligands containing more than one donor atom such as Nitrogen and sulfur are widely used for the complexation of transition metals such as 2,5-dimercapto-1, 3,4-thiadiazole (DMTD) which is well known for certain transition metals [1-3] and can constitute the repetitive unit of a polymer with complexing properties. Thus, we were inspired by the ligand containing an N2S donor set of atoms which can be easily prepared using click chemistry from the reaction of 1,3,4-thiadiazole-2,5-dithiol dipotassium salt with propargyl bromide followed by the addition of the product formed from the reaction of sodium azide and octyl iodide, using Cu(I) as catalyst [4]. The coordination properties of this ligand towards different metals considered as soft, intermediate or hard acids such as Sn^{4+}, Zn^{2+}, Fe^{3+} and Hg^{2+} were investigated. The corresponding Sn(IV), Zn(II), Fe(III) and Hg(II) complexes were characterized by FT-IR, UV-Vis, ^{1}H and ^{13}C NMR spectroscopy as well as conductivity. In the case of complexes obtained with tin and zinc, the results show a more significant change of the ligand upon coordination with metal center compared to those of mercury and iron consistant with an octahedral structure of complexes around the Sn and Zn, while the Hg and Fe derivatives have rather distorted tetrahedral structures.



Keywords: Thiadiazole, click chemistry, tin, mercury, zinc, iron complexes, NMR spectroscopy.

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Theoretical study of chemical reaction and drug confinement inside single walled carbon nanotubes

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Carbon-based nanostructures now occupy a prominent place in many research areas, including health-related fields since their functionalization properties open the doors of biocompatibility. In addition, the internal volume offered by these structures allows considering a high confinement conditions. Among the most studied structures, carbon nanotubes (or CNTs) are extensively used in the fields of chemistry, physics and biology.
As part of our research, we studied first, a one-step chemical reaction confinement inside SWCNT of varying diameters (from 10.20 Å to 14.82Å) and presenting the same chirality.
In a second part of the study, we studied a conventional anticancer molecule (the molecule of Cisplatin (or CPT) inside the same CNTs to find the ideal diameter favoring the containment of more drug molecules **[1]**.
The easy functionalization of these CNTs opened the very important question of the saturation of dangling bonds at the ends of the nanotubes. To study the role of these connections, we conducted several studies to estimate the role of various chemical functions on the NTC encapsulation ability to simulate up the experimental conditions of synthesis of CNTs.
For this, the CNTs were saturated or by functions -H, or -OH functional groups or COOH functions. For each case studied, the confinement of one, two, three and finally four molecules of Cisplatin was then considered.

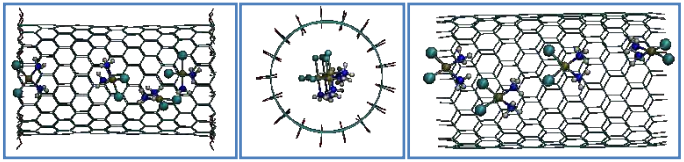

Fig. Four CPT molecules confined within tubes of different endings

Several observables were extracted from our molecular dynamics simulations. The drug retention time in each case and the interactions between the molecule and its environment are considered as the most pertinent.

Keywords CNTs, CPT, drug confinement.

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Bis(aminophosphine) diselenides as chemosensors for heavy metal cations: An electrochemical, spectroscopic and theoretical study

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The development of new electrochemical sensors for metallic cations has been receiving a huge interest. Ferrocene-based sensors were widely used to the electrochemical sensing by variation in the oxidation potential of ferrocene/ferrocenium redox couple [1-2]. In contrast, a little attention has been devoted to the organophosphorus chalcogenide-based chemosensors. In this work, we present the synthesis, spectroscopic and electrochemical characterization of bis(aminophosphine) diselenides-based chemosensors. The electrochemical studies reveal that bis(tetraethylselenophosphoramidoyl)-methylamine, $MeN[P(Se)(NEt_2)_2]_2$ (**L1**) is able to bind various heavy metallic cations (M^{2+}: Zn^{2+}, Cd^{2+}, Pb^{2+}, Hg^{2+} and Fe^{2+}) forming very stable complexes. The addition of each cation led to important oxidation potential shifts up to 1070 mV. However, the cyclodiphosphazane ligand $[MeNP(Se)(NEt_2)]_2$ (**L2**) exhibited no sensitivity for any of the reported cations.In addition, DFT/ B3LYP theoretical study was carried out and that unlike to the cyclic ligand L2, L1 is potentially able to chelate metal ions.

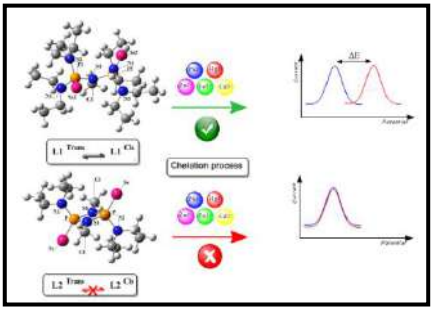

Fig. Chelation process of bis(aminophosphine) diselenides based-chemosensors

Key words: Chelation process, bis(aminophosphine) diselenides, heavy metal cations , voltammetry, theoretical study

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Kinetics and Mechanism of the Redox Reactions between Dicyanobis(phen/bpy)iron(III) and Hexacyanoferrate(II)

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We observed a complex kinetics during the redox reactions between dicyanobis(phen/bpy)iron(III); $[Fe^{III}(phen/bpy)_2(CN)_2]^+$, and hexacyanoferrate(II); $[Fe^{II}(CN)_6]^{4-}$. The study was performed in aqueous medium at 60 mM ionic strength through spectrophotometric procedures. The spectrophotometric analysis in UV-Vis region helped to identify the formation of corresponding Fe(II)/(III) complexes as the products of the reaction(s). Our results showed that each reaction completed in three phases. In each phase, we observed a different kinetic order. The zeroth order in the first phase, an overall second order in the second phase of the reaction until the end of the reaction. A third phase close to the end of the reaction, which was termed as a competition phase between the rate of redox reaction(s) and the rate of precipitation of the neutral iron(II) product species. Around 72% and ~69% fractions of the two reactions respectively, followed zeroth order kinetics in the first phase. The results helped to conclude that the zeroth order rate constant is neutral towards variation in the reaction parameters such as the concentration of reactants, protons, ionic strength, and dielectric constant. The changes were observed in the second phase. The pseudo-first order rate constant followed as sine-wave pattern upon increasing the concentration of hexacyanoferrate(II) in the reaction mixture. Its value increased upon decreasing the dielectric constant of the medium. An opposite effect on the pseudo-first order rate constant was noticed with increasing ionic strength and the concentration of protons for each reaction. Our results led to propose free ferrocyanide ion and its diprotonated acid as the reactive species, which proceeded the redox reaction(s) with outer-sphere mechanism. These active species were found to control the rate-determining step(s). A common mechanism and the rate law are proposed for the two reactions.

$$Rate = k_1 + k_2\left[Fe^{III}(phen/bpy)_2(CN)_2^{+}\right]\left[Fe^{II}(CN)_6^{4-}\right]_T + \frac{k_3\left[Fe^{III}(phen/bpy)_2(CN)_2^{+}\right]}{K_2\left[H^{+}\right]\left[Fe^{II}(CN)_6^{4-}\right]_T}$$

Key words: Dicyanobis(phen)iron(III), Dicyanobis(bpy)iron(III), Complex Reaxtion, Hexacyanoferrate(II)

Effect of anion type in the performance of ionic liquid/poly(vinylidene fluoride) electromechanical actuators

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Low voltage actuators based on poly(vinylidene fluoride) (PVDF) with 10, 25 and 40% 1-hexyl-3-methylimidazolium chloride ([C6mim][Cl]) and 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([C6mim][NTf2]) are prepared by solvent casting in order to evaluate the effect of anion size in the bending properties. Independently of the ionic liquid type and content, its presence leads to the crystallization of PVDF in the β-phase. The addition of ionic liquid into the polymer matrix decreases significantly its degree of crystallinity and the elastic modulus. It is also confirmed the good miscibility between PVDF and IL, determined by the interaction of the CF2 groups from the PVDF chains with the imidazolium ring in the ionic liquid (IL). The AC conductivity of the composites depends both on the amount of ionic liquid content and anion size. The bending movement of the IL/PVDF composites is correlated to their degree of crystallinity, mechanical properties and ionic conductivity value and the best value of bending response (0.53%) being found for IL/PVDF composite with 40 wt% of [C6mim][Cl] at an applied voltage of 10 V square signal.

Key words: PVDF, Ionic liquid, Actuators, Bending.

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Synthesis and cation biding of a new peripherally functionalized phthalonitrile and their Co metallophthalocyanines .

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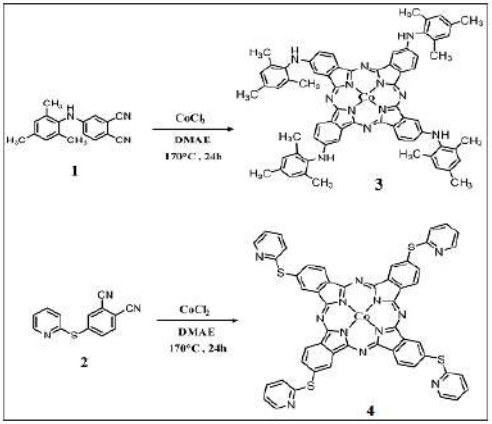
The synthesis of a novel phthalonitrile derivative with pyridine-2-thiol and 2,4,6-trimethylphenylamine substituents functionalized groups **1-2** and its peripherally tetrasubstituted cobalt phthalocyanine **3-4** . The ion binding properties of Co Phthalocyanines compounds **3**,**4** show the formation of stable complex with Co^{2+} in DMSO by means of spectrophotometry absorption and conductivity. The structures of the synthesized compounds have been successfully characterized by the spectroscopic methods (IR, ^{1}H-NMR, ^{13}C-NMR, UV-Vis, mass spectrometry, elemental analysis and NMR 2D).



Title: Chemical structural of ligand used

Keywords: Phthalocyanines, stoichiometry, complexation, ionophores properties.

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Synthesis and chacterization 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 [1,2]. It was generally shown that the coordination through the phosphoryl group or other heteroatoms in the molecule could be responsible of such biological activity [3]. In the present work, we describe the synthesis of phosphonothioamidates [4,5] with tin(IV) tetrachloride and report on the resulting tin complexes with these phosphonothioamidates. The new tin adducts 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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Kinetics study of gas phase reactions of atomic hydrogen with tetramethylsilane, methylsilane and formaldehyde

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One of the best-studied astronomical objects is the carbon-rich evolved star IRC+10216 (also known as CW Leonis) owing to the rich chemistry of its circumstellar shell (CSE). Several molecules have been detected in this environment characterised by high temperatures. Among these species, we can cite formaldehyde and silicon bearing molecules, which are considered as key molecular building blocks in the chemical evolution of the interstellar medium.

We present an ab initio investigation of abstraction reactions by H atom from Si(CH3)4, SiH3CH3 and H2CO molecules. Thermodynamic properties were computed using high-quality ab initio calculations. In order to calculate accurate rate constants, we used a reduced dimensionality quantum scattering and semi-classical methods. The first one is performed treating explicitly the bonds being broken and formed. Analytical potential energy surfaces were developed from a relatively small number of grid points. Semi-classical tunnelling calculations on a ground-state adiabatic minimum energy path (MEP) potential were also performed. The rate constants were computed using the canonical variational transition state method (CVT) with small curvature tunnelling contributions (SCT).

Our results show that the quantum and the CVT/SCT rate constants are in reasonable agreement with the available experiment at high temperatures, but that the last one gives better agreement to experimental results at low temperatures. We also carry out a detailed analysis of the kinetic isotope effects (KIEs) which can bring additional information about the role played by quantum effects on the abstraction reaction of H atoms from Si(CH3)4 and SiH3CH3. Secondary isotope effects contribute only minimally in comparison to the primary effect to a decrease of the rate constants at low temperatures. As expected, all isotopic reaction rates are lower than "non-deuterated" one because tunnelling is more pronounced for the transfer of H atoms over that of D atoms.

Key words: interstellar medium, *ab initio*, potential energy surfaces, rate constants, kinetic isotope effects

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Synthesis, crystal structure, spectroscopic characterization and Hirshfeld surface analysis of iron cyanide complex

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The investigation of novel inorganic-organic hybrid framework assemblies represents an importance of chemical research because of their potential applications, such as magnetic, catalysis and optical [1]. In this work, spectroscopic and structural study of a newly synthesized complex of iron with 1,10-phenanthroline has been discussed. The compound has been determined using single-crystal X-ray diffraction at room temperature. Complex crystallizes in the monoclinic $P2_1/c$ space group. In the crystal structure individual complex is interconnected through strong hydrogen bonds of type O—H…N and N—H…O into 3D layers. The three-dimensional Hirshfeld surface (3D-HS) analysis and the two-dimensional fingerprint plots (2D-FP) reveal that the structure is dominated by H…O, H…N and H…H contacts.

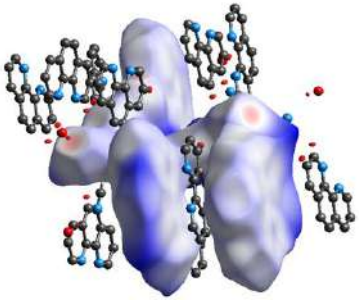

Fig. 3D Hirshfeld surface mapped over d_{norm} for visualizing the molecular interactions of complex

Key words: Iron, crystal structure, IR spectroscopy, Hirshfeld surface analysis

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Characterization of the mill Scale of Hot Rolling Mill IMETAL-EL HADJAR

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The mill scale of hot rolling mill of the steel-making complex of IMETAL-El Hadjar represents 0,1 % of the annual production of the flat products causing significant losses, which can be valued in certain fields of application via appropriate techniques of recycling.

A priori, we studied the thermal properties of mill scale coming from the hot rolling mill. The formation of these scales during hot rolling depends on several metallurgical factors, in particular the temperature in the furnace of reheating, the partial pressure of gases in the various zones of the furnace growing, the residence time inside the furnace, the temperature of strip in the various steps of rolling etc. …

The thermal analysis by DSC and TGA showing exothermic peaks synonym of a dehydrating and oil removal, and endothermic peaks shows a possible recrystallizing of iron oxides in this particular case FeO who is stable beyond a temperature of 570°C.

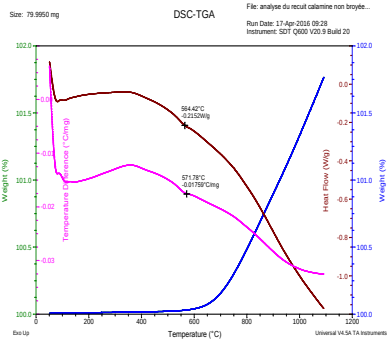

Fig1. Raw scale DSC-TGA Analysis

Keywords: Mill Scale; oxidation; rolling; thermal Properties; DSC-TGA

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New β,β'-aminodiols: Synthesis and reactivity towards phosphoryl chloride

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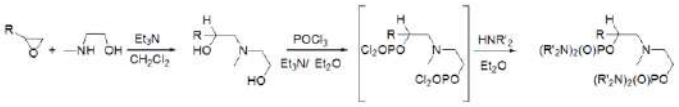
Epoxides are among the most versatile intermediates in organic synthesis because they can be used to diverse stereoselective transformations for the synthesis of highly valuable products including the β-amino alcohols [1]. The latter have received much attention in the pharmaceutical industry, given their importance in the treatment of human diseases [2]. They can also be used as organophosphorus intermediates which have diverse agrochemical uses [3]. In this work, we describe the synthesis of new β,β'-aminodiols through epoxide opening reaction. The reactivity of these diols towards phosphoryl chloride is investigated. All the compounds obtained were characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR and IR spectroscopy. The preliminary results on the preparation of corresponding phosphorochloridates and phosphoramidates from the β,β'-aminodiol precursors will be presented.



(R)= (Me) (a) ; (Bu) (b) ; (CH_2OPh) (c); (-CH_2-)$_4$(d); Ph(e)

Keywords: Epoxides, β,β'-aminodiols, phosphoryl chloride, phosphoroamidate, ^{31}P NMR.

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Synthesis, Crystal Structure And Physico-Chemical Characterization of A New Inorganic Compound: $K_{0.5}Na_4[H_{2.5}SbMo_6O_{24}].18H_2O$

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The antimonopolymolybdate of potassium and sodium by has been isolated by the conventional solution method and characterized by elemental analysis, IR, UV-visible, TG-DTAAN analysis and single-crystal X-ray diffraction. This elaborated compound crystallizes with the unit cell parameters: *a* = 10,783(2) Å, *b* = 14,723(1) Å,*c* = 24,110(1) Å, α = 90(1) °, β = 90(1) °, γ = 90(1)°of the orthorhombic space group Pbcm.

The asymmetric unit is built by Anderson clusters, monovalent Na^+ and K^+ cations as well as water molecules. These folded $[H_{2.5}SbO_6Mo_6O_{24}]^{4.5-}$ clusters are formed of seven octahedra MoO6s sharing edges.

The supramolecular framework of $K_{0.5}Na_4[H_{2.5}SbMo_6O_{24}].18H_2O$ is constructed by assembling hexamolybdoantimonate clusters through sodium and potassium cations via electrostatic interactions. The stability of the crystalline structure is enhanced by a hydrogen bonding network established between the water molecules and the polyanions.

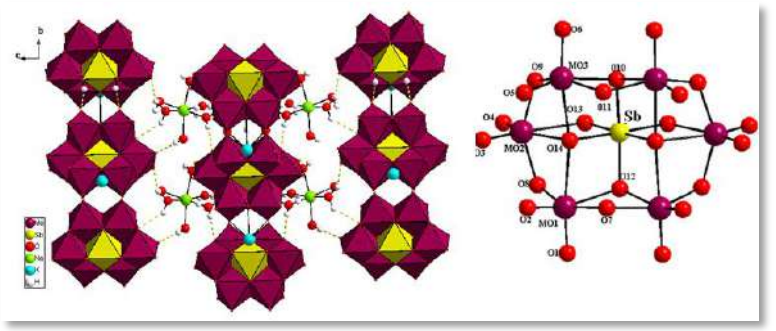

Fig. Projection in tne The Plane (bc) of the atomic arrangement of the compound (1).

HIGHLY ACTIVE PALLADIUM CATALYSTS CONTAINING N-HETEROCYCLIC CARBENE FOR ROOM TEMPERATURE SUZUKI-MIYAURA CROSS-COUPLING OF ARYL BROMIDES WITH ARYLBORONIC ACIDS

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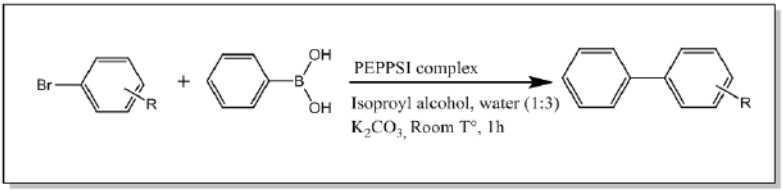
Since the discovery of the Suzuki-Miyaura cross-coupling (SMC) reaction in 1979, it has become the preferred method for preparing biaryls. In addition, the mild conditions and high tolerance for various functional groups have made the SMC reaction an important tool in the synthesis of pharmaceuticals and fine chemicals.[1-3]. In this context we reported in this work, firstly, the synthesis of a new series of Palladium N-heterocyclic carbene complexes. **Scheme 1** Then, the usefulness of these complexes as actif catalysts for Suzuki-Miyaura reaction at room temperature in green solvents. The cross-coupling reactions were highly efficient with low catalysts loadings.



Scheme 1: PEPPSI complex catalysed suzuki-Miyaura reaxtion for synthesis of biaryls

Key words: palladium, N-heterocyclic carbenes, suzuki-miyaura coupling, biaryl, green solvent.

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Synthesis of New Materials for Use As Organic Active Layers Characterization of Z (2, 3-diAryl) Acrylonitrile by Cyclic Voltammetry and Impedance Spectroscopy

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Organic π-conjugated oligomers and polymers constitute an important class of functional materials in organic electronics. They are used as active layers in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs) or in organic solar-cells (OSC). In this latter application, efficient materials usable as p-conducting layer in bulk-heterojunction (BHJ) solar cells in association with fullerene derivatives as n-conducting materials are needed [1, 2] In fact, a material with a bandgap of 1.1 eV is able to absorb 77 % of the solar irradiation, however, semiconducting polymers or oligomers have bandgaps higher than 2 eV and can then harvest only 30 % of the solar photons.

In the last few years, the scientists seek to synthesize organic molecules having gaps similar to those of metals. Recent studies showed that the family of the poly (thienylenevinylene) (PTV) presents a gap electronic Eg lower than that of polythiophen (Pt), 1.8 and 2.1eV respectively. Other work showed that the introduction of an acceptor group into the combined chain has an advantage in the control of this forbidden band. Indeed, the substitution of the electron-withdrawing cyano group in the double connection of the poly (thienylenevinylene) leads to a polymer with a great electronic affinity.

We have synthesized monomers to study a class of soluble low band gap conjugated polymers based on heterocyclic units and cyano vinylenes. We report a sample study of one of this class of material, the poly (Z)(2-phenyl-3-furyl) acrylonitrile.

The poly(Z)(2-phenyl-3-furyl) acrylonitrile film was synthesized electrochemically by anodic way in an electrolytic bath of BU4NBF4 (0,2M)/CH_2Cl_2 with anhydrous conditions and under inert atmosphere. The polymer formed on Pt or ITO electrode, either by cyclic voltammetry or by potentiostatic method, was characterized by spectroscopic methods NMR, IR, UV, fluorescence and differential scanning calorimetry. Its electrochemical impedance study showed the semicircle which is a characteristic of charge-transfer resistance of the electrode/polymer interface at high frequency and at low frequency, the mass transfer process of the redox species.

Key words: Poly Z (2-penyl-3-furyl) acrylonitrile, cyclic voltammetry, impedance spectroscopy, fluorescence

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MODIFICATION D'AMIDON PAR VOIE SECHE- RETENTION DES POLLUANT ORGANIQUE

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Les dérivés de l'amidon jouent un rôle capital dans bon nombre de domaines industriels, ainsi que dans la recherche, notamment en chimie (floculants anioniques [1], résines échangeuses d'ions [2]...). Le développement de nouveaux matériaux à base d'amidon comprend les modifications chimiques d'amidon [3].

Modification chimique a été utilisée pour introduire des nouvelles propriétés d'amidon pour différentes applications.

Le premier objectif de ce travail a donc été d'optimiser la préparation d'un ester d'amidon à partir de grains d'amidon de maïs et d'acide citrique, c'est-à-dire d'obtenir en moins de temps et avec un rendement massique plus élevé des produits d'estérification avec des degrés de substitution importants.

Mots cles: Amidon; Modification; ester.

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METAL-ORGANO-GRAPHITE OXYDE MATRICES AS EFFICIENT SORBENTS FOR HYDROGEN STORAGE

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This study reports the modification of synthetic GO nanoparticles by 3-Aminopropyltriethoxysilane (APTES) grafting and an in-situ dispersion of palladium nanoparticles (PdoNPs). The changes in structural, optical and electrical properties of the resulting Metal-Organo-Graphite oxide (MOG) were investigated. Covalent surface-grafting of (APTES) within GO mesopores was confirmed by Fourier-transformed infrared (FTIR) spectroscopy. Electron microscopy and X-ray diffraction showed that dispersion of fine palladium NPs occurs mainly inside GO mesopores, producing a slight structure expansion. This was accompanied by a significant improvement of the electrical conductivity. Palladium NP incorporation and APTES grafting resulted in a slight decrease in the optical band gap energy in the metal-organo-graphite oxide. Slight shifts towards higher wavelengths are attributed to change in the acceptor capacity level induced by palladium nanoparticles. The capacitance, conductance and relaxation phenomenon of the material were studied by means of impedance spectroscopy measurements at several temperatures. Both PdoNPs incorporation and APTES grafting appear to be, at least partly, responsible for conductance variations. The effects of the surface groups of GO-APTES-Pd and charge transfer were found to be almost proportional to the capacitance. These properties make these materials to be regarded as promising electrode materials for high efficiency energy storage.

Keywords: Graphite Oxyde: 3-Aminopropyltriethoxysilane : palladium nanoparticles.

Poster Communications' List

(alphabetically authors' names)

Name	Ref
H. Abdelgader M.E., B. Mazomenos *Agricultural Research Corporation - Sudan* Response of *Trichogramma oleae* (hymenoptera: trichogrammidae), to host pheromones, frass and scales extracts	**PC01**
A. Abid, F. Charrier El Bouhtoury, S. Gabsi *FSS - Sfax* Characterization of simple and acetylated lignin	**PC02**
I. Abidli, N. Souissi, X.R. Nóvoa *IPEIM - Manar* Corrosion inhibition of steel by prickly pear: Extraction, Characterization and Electrochemical Studies	**PC03**
S. Achour, B. Tangour *FST - Tunis* Theoretical study of a ruthénium complex's reactivity through olefins	**PC04**
H. Agougui, M. Jabli, H. Majdoub, M. Debbabi *FSM - Monastir* Synthesis, characterization of hydroxyapatite-lambda carrageenan and evaluation of its performance for the adsorption of methylene blue from aqueous suspension	**PC05**
J. Ajmi, I. Nagazi, A. Haddad *FSM - Monastir* Synthesis, characterization and crystal structure of ammonium pentamolybdodiseleinte dihydrate $(NH_4)_4[Se_2Mo_5O_{21}].2H_2O$	**PC06**
Z. Aloui, M. Rzaigui, C. Ben Nasr *FSB - Bizerte* Synthesis, crystal structure and characterization of a new organic-inorganic hybrid material: $[C_6H_{16}N_2O]SbCl_5$	**PC07**
F. Al-Sogair, Ahamad F. Aelasyme *College of Basic Education, PAAET - Kuwait* Spectroscopic Characterization of Bimetallic Complexes of Multidentate Ligand	**PC08**
N. Ameur, R. Bachir, S. Bedrane, A. Choukchou-Braham *University of Tlemcen - Algeria* Direct synthesis of adipic acid on Fe-TiO_2 doped materials	**PC09**

Name	Ref
F. Ammari *FSB - Bizerte* A poly (vinyl chloride) functionalized by 4-amino benzo-15-crown-5 and by 2-(aminomethyl)-15-crown-5. Inductively coupled plasma study of the extraction of Li(I) and Cd(II) by modified PVC polymers	**PC10**
F. Ayari, S. Khelifi, M. Trabelsi-Ayadi *FSB - Bizerte* Catalytic and photocatalytic efficiencies of mixed pillared locally bentonite for acid azo dye and real wastewater degradation	**PC11**
F. Ayari, E. Srasra, M. Trabelsi-Ayadi *FSB - Bizerte* Removal of reactive acid dye by TiO_2 and TiO_2 pillared-bentonite effect of various parameters	**PC12**
S. Azouni, M.A. Sanhoury, M.T. Ben Dhia, M.L. Efrit *FST - Tunis* Synthesis and characterisation of new thioamido and phosphono-triazoles	**PC13**
Z. Baccari, M.A. Sanhoury, B. Crousse, T. Barhoumi-Slimi *FST - Tunis* Synthesis, characterization and coordination chemistry of new α-acetoxyphosphonates	**PC14**
N. Barhoumi, S. Ammar, A. Gadri *FSG - Gabès* Degradation/mineralization of the antibiotic tetracycline by the novel heterogeneous electro-Fenton process with solid catalyst chalcopyrite using DSA anode	**PC15**
T. Belaid, K. Bouras, M. Benamor *University of A / Mira de Bejaia - Algeria* Adsorption or phenolic compounds from aqueous solution using $LiNO_3$ loaded mesoporous SBA-15.	**PC16**
O. Ben Ahmed, *FST - Tunis* Zinc complexes of β-chloro-α,β-unsaturated Schiff bases	**PC17**

Name	Ref
M. Ben Jemaa, H. Chebbi, M.F. Zid *FST - Tunis* Crystal structure, DFT study and Hirschfield surface analysis of a new organic perchlorate	**PC18**
E. Ben Khalifa, A. Jelassi, H. Nehdi, R. Chakroun, H. Nouaigui *ISST - Tunis* Application of a Doehlert experimental design for the determination of five chlorinated compounds in air workplace using GC-FID	**PC19**
A. Ben Mansour, M. Bouaziz *ISBS - Sfax* Characterisation of Chemlali olive stones by liquid chromatography-ion trap mass spectrometry	**PC20**
A. Ben Mansour, G. Flamini, M. Bouaziz *ISBS - Sfax* Volatile compounds, tocopherols and squalene content of four olive oil cultivar according to their maturity index using chemometrics	**PC21**
O. Ben Moussa, H. Chebbi, M.F. Zid *FST - Tunis* Theoretical calculations and Hirshfeld surface analysis of cobalt complex based on hydrogenmaleate ligand	**PC22**
S. Ben Moussa, M. Laajimi, M. Gruselle, B. Badraoui *FSM - Monastir* Relation between structural and electrical properties of news fluorobritholite based on lead $Ca_{7-x}Pb_xLa_3(PO_4)_3(SiO_4)_3F_2$ (0 £ x £ 2)	**PC23**
A.H. Benahsene, L. Bendjeddou *University Frères Mentouri - Constantine, Algeria* Synthesis, structural study by XR diffraction on single crystal of a new coordination polymer based on cadmium and 4, 4'-diaminodiphenylsulfone ligand	**PC24**
M.A. Bensegueni, A. Cherouana, S. Dahaoui *URCHEMS - Algeria* *In situ* synthesis, hydrogen bonding network and topological study of two copper complexes	**PC25**

Name	Ref
L. Boubakri, S. Yasar, V. Dorcet, C. Bruneau, I. Özdemir, N. Hamdi *FSB - Bizerte* Sonogashira cross coupling reaction catalyzed by N-Heterocyclic carbenes palladium complexes with triphenylphosphine	**PC26**
K. Bouchemella, B. Anak, M. Bencharif *University of Constantine - Algeria* DFT and TDDFT study of the structure and optical properties of the complexes containing nickel	**PC27**
T. Boudharaa, R. Fezei, A.H. Hamzaoui, A. M'nif *CNRSM - Borj Cédria* Influence of annealing temperature on structure and properties of zinc silicate powders synthesized by sol gel method	**PC28**
A. Boughougal, J.B. Tommasino, G. Pilet, A. Messai, D. Luneau *Abbes Laghrour University - Algeria* New metallo-antibiotic compounds : Synthesis and characterization	**PC29**
A. Boukhris, B. Glorieux, M. Ben Amara *FSM - Monastir* Structure and photoluminescence properties of $Na_2Sr_{0.8}Eu_{0.2}Mg(PO_4)_2$	**PC30**
A. Boukhris, B. Glorieux, M. Ben Amara *FSM - Monastir* Correlation between structure and photoluminescence of divalent europium doped fillowite type phosphate $Na_3SrMg_{11}(PO_4)_2$.	**PC31**
	PC32
M. Boutar, M.H. Noamane, N. Mattoussi, C. Desroches, R. Abidi, D. Luneau *FSB - Bizerte* Synthesis of new complexes of sulfonatocalix [4]arenes: Structure and magnetic properties	**PC33**
N. Braia, M. Merabet-Khelassi, L. Aribi-Zouioueche *University of Badji Mokhtar, Annaba - Algeria* A green way to enantioenriched *(R)*-3-(1-Hydroxyethyl)phenol by lipase-catalyzed alkaline hydrolysis reaction	**PC34**

Name	Ref
N. Braia, M. Merabet-Khelassi, L. Aribi-Zouioueche *University of Badji Mokhtar, Annaba - Algeria* Enzymatic kinetic resolution via transesterification of 1-Indanol and its derivative acetate: Study of some parameters	**PC35**
F. Chahdoura, P. Matthew P. Duffy, J. Crassous, M. Hissler *Laboratoire Hétérochimie Fondamentale et Appliquée* Fluoresence-induite par aggregation : Fluorophores organiques et hybrides	**PC36**
K. Chair, A. Bedoui, N. Bensalah *FSG - Gabès* Treatment of aqueous wastes contaminated with herbicide oxyfluorfen by anodic oxidation on Boron-doped diamond	**PC37**
K. Chair, A. Bedoui, N. Bensalah *FSG - Gabès* Comparative study of electrochemical, photoelectrochemical et sonoelectrochemical treatment of soil-washing effluents polluted with herbicide oxyfluorfen	**PC38**
K. Chakroun, M. Taouai, R. Abidi, M. Benazza *FSB - Bizerte* Synthesis and Fe^{3+}complexation study of new calixarene based ligand	**PC39**
S. Chamali, J. Bouajila, S. Camy, E. Saadaoui, J.S. Condoéret M. Romdhane *ENIG - Gabès* Extraction and modeling of eucalyptus essential oil using supercritical CO_2	**PC40**
S.F. Cherif, K. Essalah, M.F. Zid *IPEIM - Manar* DFT calculations of 3-nitroaniline, 3-nitroanilinium and 3-nitroanilinium chloride	**PC41**
S. Dargouthi, M. Saydou, C. Minot, B. Tangour *IPEIM - Manar* Dihydrogen production on the surface of a TiO_2 nanotube by water splitting	**PC42**

Name	Ref
S. Dbira, N. Bensalah, A. Bedoui *FSG - Gabès* The contribution of mediated oxidation mechanisms in the electrolytic degradation of cyanuric acid using diamond anodes	**PC43**
S. Dbira, N. Bensalah, A. Bedoui *FSG - Gabès* Mechanism and kinetics on the degradation of nicotinic acid in Water by photo-Fenton process	**PC44**
Z.I. Dehimat, S. Yasar, D. Tebbani, I. Özdemir *University of Constantine - Algeria* Suzuki- Miyaura Cross-Coupling reactions catalyzed by new benzyladamantyl substituted N-heterocyclic carbane-Pd(PEPPSI) complexes in water	**PC45**
Z.I. Dehimat, S. Yasar, D. Tebbani, I. Özdemir *University of Constantine - Algeria* Sonogashira coupling reaction catalyzed by sterically bulky NHCPd(II)-PPh_3 complexes	**PC46**
L. Dermeche, M.R. Gerroudj, S. Benadji, T. Mazari, C. Rabia *University Mouloud Mammeri, Tizi-Ouzou - Algeria* Preparation and characterization of Dawson polyoxometallates cesium salt: application to adipic acid synthesis	**PC47**
L. Dermeche, L. Mouheb, R.M. Guerroudj, T. Mazari, S. Benadjiand C. Rabia *University Mouloud Mammeri, Tizi-Ouzou - Algeria* Catalytic application of the Keggin type polyoxometalates namely $Cs_XSn_YH_ZPMo_{12}O_{40}$ to the adipic acid synthesis	**PC48**
Y. Dgachi, F. Chabchoub, J. Marco-Contelles, L. Ismaili *FSS - Sfax* Synthesis and pharmacological evaluation of benzochromenopyrimidinetriones as cholinesterase inhibitors for Alzheimer's disease therapy	**PC49**
Y. Dgachi, F. Chabchoub, J. Marco-Contelles, L. Ismaili *FSS - Sfax* Synthesis and biological evaluation of new Tacrine derivatives as potent antioxidant agents for Alzheimer's disease	**PC50**

Name	Ref
M. Dhifi, S. Thabet, A. Haddad *FSM - Monastir* Synthesis and characterization of a novel paratungstate $Na_{10}[H_2W_{12}O_{42}].26H_2O$	**PC51**
	PC52
P.L. Djonwouo, J. Nenwa, M.M. Bélombé, J. Erwan, B. Fokwa *University of Yaounde - Cameroon* A new dimeric copper(II) material containing oxalate(2-) and oxamide dioxime ligands	**PC53**
S. DKHILI, S. López-Bernabeu, F. Montilla, F. Huerta, S.B. Hentati, E. Morallón *University of Alicante. Spain.* Chemiclal and electrochemical copolymerization of aniline with piperazine on platinum electrodes: Characterization, and application to the detection of dopamine and ascorbic acid	**PC54**
S. DKHILI, M. Labidi, E. Morallon, S. Besbes Hentati *FSB - Bizerte* Effects of pH, concentration and speed on the electrochemical polymerization piperazine	**PC55**
S. Dridi, A. Mechria, M. Msaddek *FSM - Monastir* POLYMERIZATION of methyl acrylate with cationic nickel(IV) difluoride complexe	**PC56**
M. El Glaoui, M. El Glaoui, C. Ben Nasr *FSB - Bizerte* A Hirshfeld surface analysis, crystal structure and spectroscopic properties of new Zn(II) complex with N-aminoethylpiperazine ligand	**PC57**
H. Eloussifi, J. Farjas, P. Roura, M. Dammak *FSS - Sfax* Development of a low fluorine trifluoroacetate route to obtain $YBa_2Cu_3O_7$ films	**PC58**

Name	Ref
N. Ennaceur, R. Henchiri, B. Jalel, M. Cordier, I. Ledoux-Rak, E. Elaloui *University of Gafsa* Synthesis, X-Ray crystal structure and highly non-linear optical properties of inorganic-organic hybrid compound: 1,4-diazbicyclo-octane oxonium tri- nitrates single crystal	**PC59**
K. Essalah, M.A. Sanhoury, M.T. Ben Dhia, M.R. Khaddar *IPEIM - Manar* Theoretical DFT strustural study of beryllium chloride complexes with $(R_2N)_nP(O)F_{3-n}$	**PC60**
G. Ferouani, N. Ameur, C. Ziani-Cherif, R. Bachir ZrO_2 -Supported nano-gold catalyzed one-pot synthesis of 3-methyl-4-arylmethylene-isoxazol-5(4H)-ones compounds	**PC61**
I. Gara Dallali, M. Romdhani Younes, M.M. Chaabouni *FST - Tunis* Diallyl polythioethers in ruthenium complexes and alkene metathesis	**PC62**
Z. Gouid, M.A.K. Sanhoury, M.T. Ben Dhia, R. Linguerri, M. Hochlaf, S. Boughdiri *FST - Tunis* Zinc chloride adducts with phosphine chalcogenides: A DFT study	**PC63**
S. Guiza, S. Guiza Sami, F. Launay, M. Bagane *ENIG - Gabès* Production and characterization of activated carbon from orange peels by chemical activation with sulfuric acid	**PC64**
M. Hachicha, M.A. Sanhoury, M.T. Ben Dhia, M.L. Efrit *FST - Tunis* Synthesis of new functionalized phosphonates molecules as potential ligands for metal complexes	**PC65**
A. Haj Said, T. Jnaoui *CRMNS - Sousse* The Synthesis of a new functional mixed-metal MOFs	**PC66**

Name	Ref
H. Hemissi, S. Abid, M. Nasri, E. Dharhi, E.K. Hlil, M. Rzaigui *FSB - Bizerte* Cyclotetraphosphate-controlled copper(II)-α-amino acid complex: Synthesis, crystal structure, characterization and properties	**PC67**
H. Hemissi, M. Rzaigui *FSB - Bizerte* The first self-assembly of a mixed-ligand coordination compound based on condensed phosphate and cyclam: Single crystal structure, Hirshfeld surface analysis and characterizations	**PC68**
D. Jammazi, M. Rzaigui, S. Akriche *FSB - Bizerte* Synthesis, combined X-Ray and Hirshfeld surface analyses, optical and biological properties of a decavanadate core templates with organic cations	**PC69**
H. Jannadi, M. Mahouachi, R. Abidi, B. Noziere *FSB - Bizerte* Encapsulation and complexation of iminium intermediate in water by calix[4]arene	**PC70**
N. Jebli, K. Van Hecke, C.V. Stevens, S. Touil *FSB - Bizerte* Crystal structures, spectroscopic investigations and physical properties of novel β,β'-keto-bisphosphineoxydes and sulfides	**PC71**
A. Jouili, S. Mansouri, L. El Mir, F. Yakuphanoglu *FSS - Sfax* Studies of surface potential and charge transport in 6,13-bis(triisopropylsilylethynyl) pentacene organic thin film phototransistor	**PC72**
D. Kaddeche, A. Djaidja, A. Barama *USTHB, Algiers - Algeria* Partial oxidation of methane to syngas over co-precipitated Ni/Mg-Al catalysts	**PC73**
A. Khaled, A. Khaled, D. Guibedj, A. Seridi, M. Berredjem, M. Kadri *University 08 May 1945, Guelma - Algeria* Complexes organometallic containing phosphonat moiety experimental and DFT studies	**PC74**

Name	Ref
S. Khelifi, F. Ayari, D. Ben Hassan Chehimi *FSB - Bizerte* Acid reactive dye removal from aqueous solution by natural and low cost materials as solution to water protection and reuse	**PC75**
N. Klai, Y. Touati, C. Bidjou-Haiour *University Badji Mokhtar, El-Hadjar - Annaba, Algeria* Enzymatic synthesis of monolaurate D-xylose in ionic liquids. reusability of CAL B	**PC76**
L. Labiadh, A. Gadri, S. Ammar *FSG - Gabès* Degradation of tyrosol by a novel electro-Fenton process using pyrite as heterogeneous source of iron catalyst	**PC77**
Y-A. Lee, S. Han *Chonbuk National University - Korea* Luminescence On-Off Switching via Reversible Aurophilic Interactions	**PC78**
A. Lehleh, A. Beghidja, C. Beghidja *University Frères Mentouri, Constantine - Algeria* Synthesis, structures and magnetic properties of dimeric copper and trimeric cobalt complexes supported by bridging cinnamate and chelating phenanthroline	**PC79**
M. Mahieddine, A. Yahiaoui *University of Mascara - Algeria* Structuring agent effects on the synthesis of aluminophosphate-type nanocrystals	**PC80**
M. Mahieddine, A. Yahiaoui *University of Mascara - Algeria* Comparison of aluminophosphate catalysts for the preparation of cephalosporin from penicillins	**PC81**
S. Maza, A. Benseguni, A. Cherouana *University of Constantine - Algeria* Synthesis and structural study of a new cadmium and polyazole coordination polymer	**PC82**

Name	Ref
T. Mazari, D. Amitouche, S. Mouanni, S. Benadji, L. Dermeche, C.R. Marchal, C. Rabia *University Mouloud Mammeri, Tizi-Ouzou - Algeria* Zinc-based heteropolysals for a clean synthesis of adipic acid	**PC83**
A. Mejri, K. Alouani *FST - Tunis* Electrochemical and spectroscopic characterization of cadmium(II) complex with bis(tetraethylthiophosphoramidoyl)methylamine	**PC84**
R. Mejri, J.C. Dias, S. Besbes Hentati, C.M. Costa, S. Lanceros Mendez *FSB - Bizerte* Imidazolium-based ionic liquid type dependence of the bending response of polymer actuators	**PC85**
I. Mestiri, M. Ayed, B. Ayed, A. Haddad *FSM - Monastir* Synthesis and characterization of two novel inorganic/organic hybrid materials based on polyoxomolybdate clusters: $(C_5H_5N_5)_2(C_5H_6N_5)_4[(HAsO_4)_2Mo_6O_{18}].11H_2O$ (I) and $Na_2(Himi)_3[SeMo_6O_{21}(CH_3COO)_3].6H_2O$ (II)	**PC86**
I. Mestiri, A, Haddad *FSM - Monastir* Synthesis and structural characterization of a new polyoxovanadate $(C_4H_{10}N)_4.H_2V_{10}O_{28}.2H_2O$	**PC87**
S. Mouanni, D. Amitouche, T. Mazari, A. Boumechhour, S. Benadji, L. Dermeche, C.R. Marchal, C. Rabia *USTHB, Algiers - Algeria* Manganese-cobalt mixed salts for green synthesis of adipic acid	**PC88**
O. Naouali, W. Elgabsi, L. Baklouti, N. Hamdi *FSB - Bizerte* Binding properties of some new azo dyes derived from 4-hydroxycoumarin	**PC89**
M.H. Noamane, S. Ferlay, N. Kyritsakas, R. Abidi, M.W. Hosseini *FSB - Bizerte* Formation of binuclear neutral Copper(II) complexes based on *p-tert*-butyl- calix[4]arene and thiacalix[4]arene in *1,3*-Alternate conformation bearing four catechol at their lower rim	**PC90**

Name	Ref
O. Ouled Ltaief, S. Siffert, S. Fourmentin, M. Benzina *ENIS - Sfax* Removal of VOCs vapors using Faujasite zeolite synthesized from instratified illite-kaolinite Tunisian clay	**PC91**
A. Prishchenko, M.V. Livantsov, O.P. Novikova, L.I. Livantsova, V.S. Petrosyan *M.V. Lomonosov Moscow State University, Moscow, Russia* Diorganotin dihalides complexes with new functionalized mono- and bisphosphonates	**PC92**
A. Prishchenko, M.V. Livantsov, O.P. Novikova, L.I. Livantsova, V.S. Petrosyan *M.V. Lomonosov Moscow State University, Moscow, Russia* New complexes of biogenic metals with mono- and bisorganophosphorus proline derivatives	**PC93**
N. Rahmouni, W. Tahrib, J. Desbriéres, S. Besbes-Hentati *FSB - Bizerte* Synthesis, characterization and antibacterial activity of N-benzimidazole-O-acetyl-chitosan	**PC94**
A. Rayes, F. Mezzadric, G. Calestanic *ENIG - Gabès* Synthesis and crystal structure of a novel inorganic-organic hybrid, [2,2'-(ethylenedioxy)bis(ethylammonium)]$ZnCl_4$	**PC95**
A. Rayes, A. Baâzaoui, F. Mezzadric, G. Calestanic *ENIG - Gabès* Synthesis and crystal structure of a new 2-D chloro-substituted zinc phosphate, $[C_8N_2H_{20}]Zn_2(PO_3(OH))_2Cl_2$, containing (4.8) net layers	**PC96**
H. Romdhana, A. Mejri, F. Ben Hatira, A.H. Hamzaoui *CNSTN - Sidi Thabet* Correlation between EPR and UV absorbed dose response of gamma irradiated bio-polymer (poly glycolic acid)	**PC97**
M. Romdhani Younes, A. Maazaoui, M.A.K. Sanhoury *FST - Tunis* Synthesis and coordination chemistry of 1,5-bis-allyloxy-sulfides	**PC98**

Name	Ref
M. Romdhani Younes, I. Gara Dallali, H.M. Sbihi, M.M. Chaabouni *FST - Tunis* Direct conversion of the β,β'-dihydroxydithioethers into thiols: Synthesis of new tétradentate ligands	**PC99**
F. Saadi, A. Arfaoui, H. Amri *FST - Tunis* An efficient synthesis of polysubstituted vinyl ethers	**PC100**
F. Saidi, Mostafa Kerim Benabadji Ghouti Merad *University Abou Bakr Belkaid, Tlemcen - Algeria* DFT calculations of structural, and mechanical properties of C15, C14 and C36 Laves phases in YCo_2	**PC101**
F.E.E. Salah, A. Abdel Hameed, A. Adam Eisa *University of Gezira - Sudan* Effect of powder preparation of clove, ginger, garad and galangal on the infestation of chick-pea grains caused by cow pea weevil *Callosobruchus maculatus* adults	**PC102**
E. Selmane, Bel Hadj Hmida; N. Salaaoui; J. F. Fauvarque *IPEIM - Manar* Treatment of hard water by electrodialysis	**PC103**
L. Takorabet, H. Khireddine, N. Djelali *University of Bejaia - Algeria* Development of hydroxyapatite, from the natural phosphate of Djebel Onk ore, and its application to the adsorption of the Pb-Cd-Ni ternary mixture in an aqueous medium	**PC104**
A. Talbi, A. Arfaoui, M.A.K. Sanhoury, M.T. Ben Dhia, M.L. Efrit, H. M'rabet *FST - Tunis* Synthesis, characterization and coordination chemistry of α-phosphonomethylbutenolides	**PC105**
K. Talha, L. Belkhiri, A. Boucekkinec *University of Constantine - Algeria* Redox behavior of bis (cyclopentadienyl) complexes of uranium. Study of DFT / zora relativiste	**PC106**

Name	Ref
N. Touj, S. Yaşar, I. Özdemir, N. Hamdi *ISSTE - Borj Cédria* An efficient palladium triphenylphoshine complexes catalysed Sonogashira type cross coupling of aryl halides with terminal alkynes	**PC107**
I. Trabelsi, K. Essid, M.H. Frikha *FSS - Sfax* Synthesis of mixed anhydrides of fatty acids	**PC108**
I. Trabelsi, K. Essid, M.H. Frikha *FSS - Sfax* Mixed carboxylic-fatty anhydride esterification using amberlyst-15 as a Heterogeneous catalyst	**PC109**
M. Yahyaoui, M.A.K. Sanhoury, S. Touil, A. Samarat *FSB - Bizerte* Synthesis and spectroscopic characterization of new tin(IV) complexes with functionalized *gem*-bisphosphonates	**PC110**

Posters Communications' Abstracts

Response of *Trichogramma oleae* (Hymenoptera: Trichogrammidae), to Host Pheromones, Frass and Scales Extracts

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Semiochemicals help natural enemies locate and recognize their hosts. Therefore, knowledge of the nature of these chemicals and their functional roles is important in the design of programmes that use parasitoids as biological control agents. *Trichogramma oleae* has been found to parasitise egg masses of the lepidopterous olive pest. The present study was aiming to developed an IPM for lepidopterous olive pests, based on natural enemies and pheromones. The study investigated the kairomonal effect of *Prays oleae*, and *Palpita unionalis* sex pheromone components, frass and scale extracts. Petri dishes were used for the choice test. A filter paper (PS- Whatman 9 cm) was placed at the bottom of the Petri dish. The filter was separated to quadrants. Egg masses of *Sitotroga* eggs were glued in each quadrant. Testing chemicals were applied to each of the two opposite quadrants at a appropriate rate Pure solvent was applied to each of the two remaining quadrants. Five wasps, 3 days old, were introduced into the centre of the Petri dish. Wasp movements to the treated and control quadrants was observed at regular times interval. The number of black (parasitized) eggs was recorded after 5 days. The results indicate in general a deterrent action of some Pheromones, especially unsaturated aldehydes. Experiments investigating the influence Extracts of scales and Frass indicated,in general, a neutral and or attactive action. However the results showed that the effects were dose and persistence dependent.

Keyword: Semiochemicals, Host Phermones, Frass extract, scale extract *Trichogramma oleae*

Characterization of simple and acetylated lignin

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Lignin is a renewable material obtained in large quantities as a by-product of the olive industry. In this context, this study aims to study lignin as a macromonomer in the rigid synthesis of polyurethane foam after chemical modification. For this purpose, the lignin extracted from spent olive residue by treatment with sulfuric acid according to the method described by Mansour et al. The comparison by characterization of the single and acetylated isolated lignin according to the physico-chemical analyzes ATG, DSC and FTIR shows its value as a biomass capable of being transformed after a chemical modification to polyol.

Key words: Lignin, Olive pomace, polyuréthane, physico-chemical analyzes

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Corrosion inhibition of steel by prickly pear: Extraction, Characterization and Electrochemical Studies

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Aqueous and Methanol extracts of prickly pear was tested as corrosion inhibitor for steel using electrochemical impedance spectroscopy (EIS) in three different medias.
Impedance measurements showed that there are two phenomena in the inhibition process. The obtained results show that this plant extract could serve as an effective inhibitor for corrosion of steel in NaOH (0.1M), NaOH+NaCl (0.1M) and NaOH+NaCl (0.5M) medias. The aqueous extract obtained give inhibition around 63.3% in NaOH (0.1M) and the methanol extract obtained give inhibition around 82.2% in NaOH+NaCl (0.5M). The experimental data obtained from EIS method shows a frequency distribution and therefore a modelling element with frequency dispersion behavior, a constant phase ($CPE_{\alpha,Q}$) has been used. Graphical methods are illustrated by synthetic data to determine the parameter of CPE (α, Q). Chromatographic analysis, on chemical families present in the crude extract, were also carried out to find the main constituents responsible for corrosion inhibition properties of the plant extract.
In another hand, a theoretical study was performed in order to determine active sites in the studied molecules.

Keywords: steel, barrier properties, mechanical properties, EIS, DFT calculations, surface analysis.

THEORETICAL STUDY OF A RUTHÉNIUM COMPLEX'S REACTIVITY THROUGH OLEFINS

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By using a DFT method, we have studied the hydrogenation of olefins catalyzed by a ruthenium II complex, the $RuH_2(\eta^2\text{-}H_2)_2(P(C_6H_{11})_3)_2$. The establishment of an agostic Ru-C bonds followed by the migration of hydrogen atoms from one cyclohexyl of phosphine is the main particularity of this reaction. The transition states associated with the latter migrations were determined. Each transition state is trizonal by involving 3 different areas and 10 active atoms. Energy profiles confirm the simultaneous movement of all these active atoms. Intrinsic reaction coordinate (IRC) calculations allowed following their movements during this reaction. Obtained results highlight the catalytic effect of Ru atoms able, thanks to their versatility, to redistribute their AOs and to to enable the exchange process of the ligands.

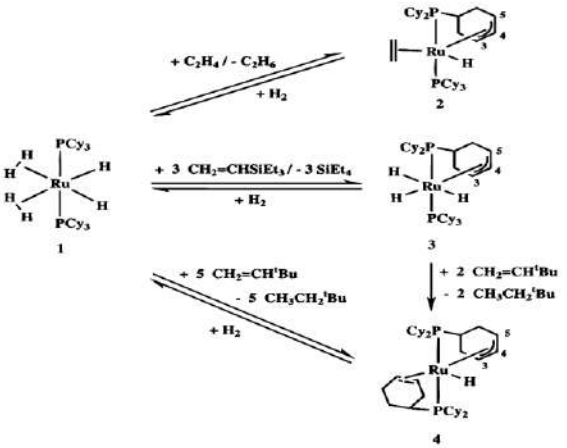

Fig. Different behaviours of functionalized olefins in presence of the catalyst $RuH_2(\eta^2\text{-}H_2)_2(P(C_6H_{11})_3)_2$ complex

Key words: Olefin hydrogenation, agostic bonds, energy profiles.

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Synthesis, Characterization of Hydroxyapatite-Lambda Carrageenan and Evaluation of its Performance for the Adsorption of Methylene Blue from Aqueous Suspension

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Dicalcium phosphate monetite ($CaHPO_4$) synthesized from $CaCl_2$ and Na_2HPO_4, it was characterized by scanning electron microscopy, Fourier transform infrared, and X-ray diffraction. The $CaHPO_4$ was used for the removal of Methylene Blue dye from its aqueous solution. The kinetics, equilibrium, and thermodynamic of the adsorption of the dye onto the $CaHPO_4$ were investigated. The effects of contact time, initial dye concentration, pH as well as temperature on adsorption capacity of $CaHPO_4$ were studied. Experimental data were analyzed using six model equations: Langmuir, Freudlinch, Redlich–Peterson, Temkin and Dubinin–Radushkevich isotherms and it was found that the data fitted well with Langmuir isotherm model. Pseudo-first-order, pseudo-second-order, Elovich, and intra-particular diffusion kinetic models were used to test the experimental data in order to elucidate the kinetic adsorption process and it was found that pseudo-second-order model best fit the data. The calculated thermodynamics parameters ($\Delta G°$, $\Delta H°$ and $\Delta S°$) indicated that the process is spontaneous and endothermic in nature.

Keywords: Monetite, Methylene Blue, Adsorption, Kinetic, Isotherms

Synthesis, characterization and crystal structure of Ammonium Pentamolybdodiseleinte Dihydrate $(NH_4)_4[Se_2Mo_5O_{21}].2H_2O$

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The role of Strandberg-type polyoxoanions as the inorganic building units to construct such extended frameworks has not been so extensively studied **[1-3].**
The crystal of $(NH_4)_4[Se_2Mo_5O_{21}].2H_2O$ has been isolated by conventional solution method and structurally characterized by single-crystal X-ray diffraction methods,IR, UV–vis spectroscopies and thermogravimetric analysis. This compound crystallizes in the orthorhombic system, space group Pbcn with unit a = 15.09271Å, b=13.36338 Å, c= 23.8204 Å and Z = 2. The Strandberg clusters anions $[Se_2Mo_5O_{21}]^{4-}$ in the compound are further inter-linked by water molecules and the ammonium groups $(NH_4)^+$through hydrogen bonds to form a three dimensional supramolecular framework.

Synthesis, crystal structure and characterization of a new organic-inorganic hybrid material: $[C_6H_{16}N_2O]SbCl_5$

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The present paper undertakes the study of $[C_6H_{16}N_2O]SbCl_5$ which is a new hybrid compound. It is synthesized and characterized by single-crystal X-ray diffraction, thermal analysis, IR and solid state NMR spectroscopy. The centrosymmetric compound crystallizes in the monoclinic space group $P2_1/n$, with the following unit cell parameters: a = 9.8519(2), b = 8.8345(2), c = 17.3087(4) Å, ß = 102.3(1)°, V = 1457.90 (6) $Å^3$ and Z = 4. The atomic arrangement shows an alternation of organic and inorganic entities. The cohesion between these entities is performed via N–H…Cl and O–H…Cl hydrogen bonding to form a three-dimensional network. The ^{13}C CP-MAS NMR spectrum is in agreement with the X-ray structure. Infrared spectrum is recorded in the 4000–400 cm^{-1} frequency region. This study confirms the presence of the organic cation $[C_6H_{16}N_2O]^{2+}$. DFT calculations allow the attribution of the carbon peaks to the different atoms.

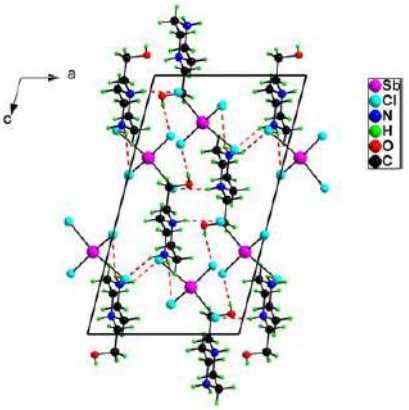

Figure Projection of the structure of $[C_6H_{16}N_2O]SbCl_5$ along the b-axis.

Keywords: X-ray diffraction; Crystal structure; IR spectroscopy; CP-MAS NMR; DFT calculations

Spectroscopic Characterization of Bimetallic Complexes of Multidentate Ligand

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New complexes of (N'1E,N'3E)-N'1,N'3-bis(2-hydroxybenzylidene)-isophthalohydrazide [HBIH] with Cr^{3+}, Mn^{2+}, Fe^{3+}, Co^{2+}, Ni^{2+} and Cu^{2+} will be prepared and spectroscopically will be characterized. The preliminary data suggest the formation of $[Ni_2(HBIH\text{-}2H)\text{-}Cl2].3H_2O$, $[Cu_2(HBIH\text{-}2H)Cl_2]$, $[Co_2(HBIH\text{-}2H)(H_2O)2Cl_2]$, $[Mn_2(HBIH\text{-}_2H)\text{-}Cl_2].2H_2O$, $[Cr_2(HBIH\text{-}4H)Cl_2(H_2O)_4]$, $[Fe_2(HBIH\text{-}4H)Cl_2]C_2H_5OH$. The ligand in these complexes may act as a bi-negative hexa-dentate or tetra-negative hexa-dentate. The magnetic and spectral data will propose the structure of the complexes. The TGA data may confirm the final product of the metal complexes. The molecular modeling of some complexes will be drawn. The mass spectra will depict their molecular ion peaks and the isotopic species of each complex.

Direct synthesis of adipic acid on Fe-TiO_2 doped materials

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Cyclohexene oxidation generates many compounds such as 2-cyclohexenone, 2-cyclohexenol, cyclohexane epoxide,…; how are very interesting intermediaries in the synthesis of several pharmaceutical and chemical products. However, the binary system TiO_2-Fe_2O_3 demonstrated very interested applications (as photo-catalyst) and it was prepared by different technique (impregnation, mechanical milling method and sol gel).

The objective of the present study is the preparation of TiO_2 doped materials by Fe_2O_3 at different mole ratio of Ti/Fe (9, 4 and 2) by sol gel and impregnation method. Their catalytic activities were evaluated on the oxidation of cyclohexene using molecular oxygen as oxidant. These materials where characterized by DR/UV-Vis, IR, BET, ICP and XRD. The characterization techniques were show that Fe particles were well inserted into the framework of the TiO_2 anatase structure, and the mixed oxides exhibited excellence absorption (400-600 nm) in the visible spectral region. The result of the test reaction show that the catalytic activity increases with the iron content on the catalysts. However, we noted an excellent production of adipic acid (98%).

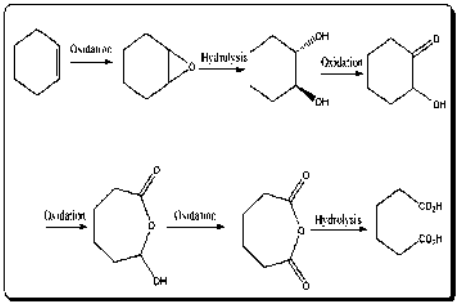

Fig. Reaction pathway for the synthesis of adipic acid

Key words: Oxidation, adipic acid, cyclohexene, iron, titania.

A poly (vinyl chloride) functionalized by 4-amino benzo-15-crown-5 and by 2-(aminomethyl)-15-crown-5. Inductively coupled plasma study of the extraction of Li(I) and Cd(II) by modified PVC polymers.

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The aim of this study was to evaluate the efficiency of for new polymers obtained by functionalization of a commercial poly (vinyl chloride) (Mw = 48000) by grafting 4-amino benzo-15-crown-5 and by 2-(aminomethyl)-15-crown-5 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), differential scanning calorimetry (DSC) 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 Cd^{2+} = 52.34 % which highlight the importance of the substitution of chlorine atoms by amino groups.

Keywords: Poly (vinyl chloride); functionalization; 4-amino benzo-15-crown-5; 2-(aminomethyl)-15-crown-5metal; cations; extraction; inductively coupled plasma- atomic emission spectrometry

Catalytic and photocatalytic efficiencies of mixed pillared locally bentonite for acid azo dye and real wastewater degradation

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Fenton and photochemically assisted Fenton reaction (photo-Fenton) are important because they may be particularly effective for the degradation of harmful organic compounds in the environment using heterogeneous catalysts. The purpose of the present study was to compare the effectiveness of hydroxy FeAl-intercalated bentonites (FeAl-bent) in Fenton and photo-Fenton processes. In particular, different Fe/Al molar ratios were of interest as a means to vary catalytic activity. Intercalation was achieved via an ion-exchange method and Congo red was the test compound for degradation by hydrogen peroxide (H_2O_2) in the dark and under UV-visible light irradiation ($\lambda = 350$ nm) in the presence of FeAl-bent. Also, the degradation of real wastewater was achieved under UV light irradiations. The FeAl-bent materials obtained were characterized by powder X-ray diffraction, N_2 adsorption/desorption, X-ray fluorescence spectroscopy, MET, and ultraviolet-visible spectroscopy. The degradation performance of FeAl-bent was investigated using different experimental parameters, including the Fe/Al molar ratio of the intercalating solution, the catalyst dosage, the H_2O_2 dosage, and the pH. The results of Fenton reaction showed that the catalytic activity of Fe/Al-Mt was enhanced significantly by the extent of hydroxy Al/Fe intercalation. For optimal reaction conditions, 50 % degradation efficiency of Congo red was achieved after 240 min of reaction. However, 100 % degradation was achieved after only 60 min under UV light irradiation. So, this catalyst exhibited the highest degradation ratio both for the mineralization of CR and of real wastewater under UV light. Moreover, the catalyst was stable and could be used repeatedly.

REMOVAL OF REACTIVE ACID DYE BY TiO_2 AND TiO_2 PILLARED-BENTONITE EFFECT OF VARIOUS PARAMETERS

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Many dyes are ubiquitous in the environment, since 15-20% of the word dye production is estimated to be released into the environment. Dyes are not easily biodegradable because of increased complexity of chemical structures and presence of aromatic rings. Recent work has reported the use of TiO_2 in the photocatalytic degradation of textile dye, yet TiO_2 powder used as an aqueous dispersion is very difficult to recover. TiO_2 supported on different minerals or TiO_2 thin films therefore appeared to be a promising way to enlarge application fields and overcome TiO_2 recovery problems, mesoporous materials based on clay minerals have been synthesized

In this investigation pillared bentonite composites were synthesized by dispersion of TiO_2 on the surface of a purified bentonite (bentonite –Na) in order to increase the sorption ability of the purified bentonite. Different materials with various loading in TiO_2 were prepared and characterized by several analytical technique including XRD, BET and SEM analysis. The synthetic procedure allows the formation of a more lamellar-like aggregation for the bentonite-TiO_2 sample relatively to the purified one (bentonite-Na). It was found that the greater pore volume and surface area was reached in the case of the greater percent of TiO_2.

bentonite-TiO_2 samples were calcined at different temperatures (200-800°C) in order to prepare a TiO_2-pillared bentonite samples witch having more mechanical stability. All theses samples (before and after change) were tested as a support to remove a toxic textile dye from aqueous solution (reactive blue II). Experiments were carried out with an aqueous dye concentration of 10^{-4}M at different pH, greater percent of dye removed was observed when used TiO_2-bentonite and TiO_2-pillared bentonite than the purified one. According to UV results, the higher amount of the dye removed was found at acidic rather than at basic pH. Adsorption results followed pseudo-first order kinetics according to the Langmuir-Hinshelwood model. In conclusion, together with their good sedimentation ability the composite materials (TiO_2-bent and TiO_2-pillared bentonite) could be considered as a promising alternative for the removal of organic water contaminants.

SYNTHESIS AND CHARACTERISATION OF NEW THIOAMIDO AND PHOSPHONO-TRIAZOLES

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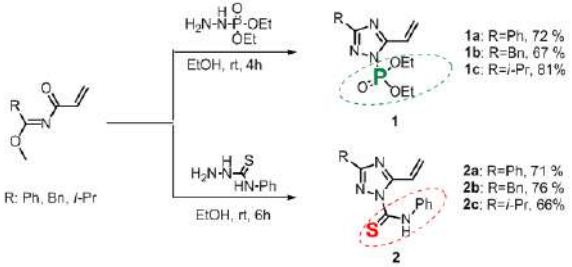
Triazole compounds have attracted considerable interest due to their pharmacological, anticancer, anticonvulsant, antimicrobial, anti-inflammatory, antioxidant, antitubercular and pesticidal properties [1-3]. The presence of the organophosphorus and organosulfur units was found to enhance the biological activity of the triazoles synthesized according to certain results quoted in the literature [4]. The reforming compounds of such units constitute potential ligands for coordination with certain metal cations. In this work, we have proposed to introduce these motifs by reacting suitable reagents on the *N*-acryloyl iminoesters to give new vinyl-1,2,4-triazoles containing thioamide or phosphoramidate groups. These compounds were obtained in good yields and characterized by (^{1}H, ^{13}C and ^{31}P) NMR and IR spectroscopy. The coordination chemistry of theses compounds through the HNC(S) and P(O) groups towards metal ions will be discussed.



Keywords: Triazole derivatives, organophosphorus, organosulfur, ligands.

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Synthesis, characterization and coordination chemistry of new α-acetoxyphosphonates

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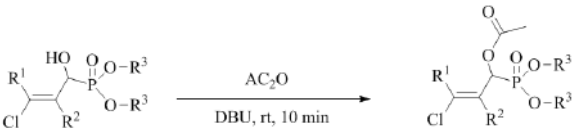
In recent years, the preparation of α-acetoxy and α-hydroxyphosphonates has attracted a great deal of attention due to their potential biological activities with broad applications as enzyme inhibitors or as dinucleotide analogues having antiviral properties [1-3]. In addition, they are useful intermediates in the synthesis of other phosphorus compounds [4]. In this work, we describe a simple and efficient method for the synthesis of α-acetoxyphosphonates through a one-pot reaction of α-hydroxyphosphonates in the presence of acetic anhydride and DBU under solvent-free conditions. This method is easy and rapid for the one-pot synthesis of α-acetoxyphosphonates (**1-12**) in good yields. The compounds were characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR, HRMS and IR spectroscopy. The coordination chemistry of these ***α***-acetoxyphosphonates as new ligands towards tin tetrachloride will be also presented.



1-12
(65-75%)

$R^1 = CH_3$, Ph or tBu
$R^2 = CH_3$, Ph or H
$R^3 = CH_3$, C_2H_5 or C_4H_9

Keywords: β-Chlorovinyl aldehydes, α-hydroxyphosphonates, α-acetoxyphosphonates, NMR spectroscopy.

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Degradation/mineralization of the antibiotic tetracycline by the novel heterogeneous electro-Fenton process with solid catalyst chalcopyrite using DSA anode

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The degradation of solutions of the antibiotic tetracycline (TC) has been studied by a novel electrochemical advanced oxidation process, consisting in electro-Fenton (EF) process using chalcopyrite as heterogeneous catalyst. In fact, chalcopyrite powder was the source of Fe^{2+} and Cu^{2+}ions instead of a soluble catalyst salt used in conventional EF. Experiments were performed in an undivided cell equipped with a DSA anode and a carbon felt cathode, where TC and its oxidation intermediate products were destroyed by hydroxyl radicals ($^{\bullet}OH$) formed both, in the bulk solution from electrochemically induced Fenton's reaction(Fe^{2+} and H_2O_2)and Fenton's-like reaction (Cu^{+} and H_2O_2), and at the anode surface from water oxidation. The effects of operating parameters such as applied current and chalcopyrite concentration.

Keywords: Heterogeneous catalysis; Chalcopyrite; Electro-Fenton; Tetracycline; Wastewater treatment

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Adsorption or phenolic compounds from aqueous solution using $LiNO_3$ loaded mesoporous SBA-15.

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Currently, many industrial processes produce wastewater containing organic refractory compounds. These compounds can be removed by adsorption onto porous solids like activated carbon, clays and mesoporous silicates. Mesoporous silicates offer a number of potential advantages of nanoporous materials (IUPAC classification [1]), as adsorbents including larger pore volume and diameter, high surface area and regular channel type structures. It is also possible to manipulate these properties to suit the adsorbate [2].

The present study consists in synthesizing and using a new mesoporous adsorbents containing silica (SBA-15) in a physicochemical process of adsorption, to treat aqueous solutions containing phenol like organic pollutant. The resulting SBA-15 has been characterised by IR spectra, DRX, MET and textural analysis (BET). The tests of adsorption of phenol on mesoporous $LaNiO_3$/SBA-15 were carried out in system Bach, they showed a remarkable elimination as of the 20 first minutes. The influence of various experimental parameters was studied: time of contacts, pH, mass of adsorbent, stirring velocity and temperature. The experimental results showed that the adsorption of phenol on the mesoporous $30LaNiO_3$/SBA-15 reaches 90% with $pH_{initial}$=4 and with room temperature. The study of the isotherm shows that the model of Freundlich describes well the process of the adsorption of phenol.

Keywords: Phenol, SBA-15, Adsorption, mésoporeux Supports.

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Zinc complexes of β-chloro-α,β-unsaturated Schiff bases

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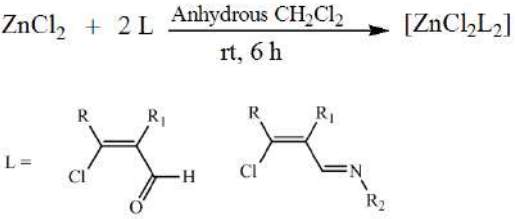
Schiff base ligands play an important role in organic chemistry because of their ease of synthesis by means of condensation reactions[1,2] and their exceptional ability to bind to a wide variety of metal atoms[3].Moreover the great interest of these ligands lies in their broad spectrum of biological activities[4]. Schiff bases have been widely used as ligands because of high stability of the coordination compounds and their good solubility in common solvents [5]. In this work, we describe the synthesis of new zinc complexes of Schiff bases. They were fully characterized by NMR, IR, and UV-Vis spectroscopies. The behavior of the azomethine group towards zinc ions was studied and the magnitude of the metal-ligand interaction was estimated on the basis of the values of the azomethinestretching vibrations in IR spectroscopy and used to classify the Schiff bases according to their Lewis basicity.



Keywords: Schiff bases, aldehyde, zinc complex, spectroscopy.

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Crystal structure, DFT study and Hirschfield surface analysis of a new organic perchlorate

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A new 4-methylanilinium perchlorate, $(C_7H_9N)[ClO_4]$ **(I)**, has been synthesized by slow evaporation at room temperature and characterized by IR, UV-visible and single crystal X-ray diffraction. Compound **(I)** crystallizes in the monoclinic system with the space group $P2_1/c$, Z=4, and unit cell parameters a=9.513(1) Å, b=7.196(5) Å, c=14.297(4) Å, β=90.41(2)°. In the crystal structure, all the amine group H atoms are involved in N-H…O hydrogen bonds with O atoms of ClO_4^- anion. These hydrogen bonds link the anionic units in two-dimensional network parallel to the *bc* plane. The density functional theory (DFT) optimized structure at the B3LYP/6-31G (d,p) level is compared with the experimentally determined molecular structure. The HOMO-LUMO energy gap and other related molecular properties are also calculated. The three-dimensional Hirschfield surface (3D-HS) **[1]** and the two-dimensional fingerprint plots (2D-FP) **[2]** reveal that the structure is dominated by H…O (29.2%) and H…H (26.4%) contacts **(fig.)**.

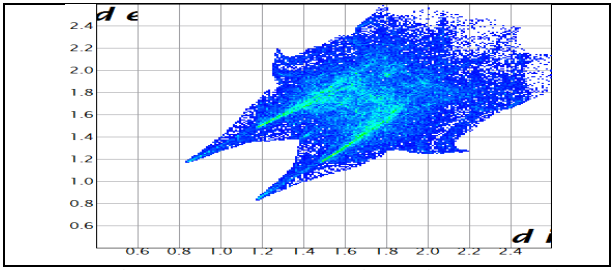

Fig. View of the two-dimensional Hirshfeld surface (2D-FP) of (I).

Key words: Hirschfield surface, 4-methylanilinium perchlorate, crystal structure, fingerprint plots.

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Application of a Doehlert experimental design for the determination of five chlorinated compounds in air workplace using GC-FID

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Environmental monitoring of exposure to chemical pollutants is very important to control the air quality in workplace [1]. Perchloroethylene and trichloroethylene are the most chosen solvents in dry cleaning. These compounds are toxic for human health and are classified as carcinogen by the CIRC [2]. The aim of this work is to optimize the chromatographic conditions in order to get a good resolution and a short analysis time of five chlorinated compounds using the Dohelert experimental design. These compounds are dichloromethane, perchloroethylene, trichloroethylene, chloroform and carbon tetrachloride. Four factors were chosen: the initial temperature, the rate, the final temperature and the residence time. Two responses were determined: Analysis time (Y_1) and Resolution (Y_2).The regression analysis using the ANOVA test showed good fit of the experimental data to the second order polynomial model with a coefficient of determination (R^2) value equal to 0.997 and a model F-Value of 3791,77 and 201,85 for Y_1 and Y_2 respectively.
The optimum conditions of initial temperature (40°C), rate (30°C min^{-1}), final temperature (120°C) and residence time (11 min) were recorded from desirability function. At these conditions, the separation of the five compounds and the internal standard was successfully done in a short analysis time of 13.694 min and a resolution of 1.54.

Key words: Chromatographic separation, Chlorinated compounds, Doehlert experimental design

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Characterisation of Chemlali olive stones by liquid chromatography-ion trap mass spectrometry

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Olea europaea L. (Oleaceae) is abundant in Tunisia with over 50 different known cultivars. Chemlali is the main variety cultivated in central and southern areas of Tunisia, contributing to 80% of the national olive oil production. It is a cultivar well adapted to severe environmental conditions. Aqueous methanol extracts of Chemlali olive stones were analyzed by reverse phase high-performance liquid chromatography (HPLC) with diode array detection and mass spectrometry [LC−MS/MS]. Oleoside, oleoside 11-methyl ester, nuezhenide, oleoside 11-methyloleoside, nuezhenide 11-methyloleoside, oleuropein, and glycosides of tryosol and hydroxytyrosol glycosides were identified in stones of Chemali olives. The antioxidant activity observed for the extract of the olive stones (IC50 = 13.84 µg/mL, TEAC = 0.436 mM) may be due to the high content of phenolic compounds, of which the main compounds are nuezhenide (325.78 mg/100g), methoxy derivative of nuezhenide (132.46 mg/100g), and nuezhenide-11-methyloleoside (82.91 mg/100g). These results suggest the use of olive stones as sources of natural antioxidants.

Keywords: Chemlali olive stones, mass spectrometry, nuezhenide-11-methyl-oleoside, phenolic compounds, antioxidant activity

Volatile compounds, tocopherols and squalene content of four olive oil cultivar according to their maturity index using chemometrics

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This paper evaluates the usefulness of chemical variables such as quality indices, pigments content, fatty acid, phenolic content, tocopherols content, squalene content, oxidative stability, volatile compound and sensorial analysis as a tool to discriminate the olive oils obtained from four varieties (Neb Jmel, Zarrazi, Oueslati and Chemlali). Actually, the influences of maturation index and nature of the cultivar are also discussed. In order to eliminate the geographical and climatic influences, the high total phenolics, tocopherol content and oxidative stability of Neb Jmel and Zarrazi varieties makes their oil superior to other varieties analyzed in this study. Oueslati variety had the highest values of oleic acid, whereas Chemlali was distinguished by its high values of palmitic acid. The levels of the main volatile components decreased during maturation, but were higher in Neb Jmel and Zarrazi olive oils. The major volatile component was the C6 aldehyde fraction, whose content varied greatly between the different studied varieties. Indeed, E-2-hexenal content ranged from 48.1 % in the Zarrazi variety to 27.9 % for Chemlali, the amount of hexanal ranged from 12.9 in Oueslati to 3.7 for Chemlali samples.

Keywords: Tunisian Olive oil, Squalene and tocopherols contents, Maturity index, SPME, Chemometrics.

Theoretical Calculations and Hirshfeld Surface Analysis of Cobalt Complex Based on Hydrogenmaleate Ligand

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The preparation of tertaaquabis(hydrogenmaleate)Cobalt(II), $[Co(C_4H_3O_4)_2(H_2O)_4]$ (I) has been already reported **[1]** and its structure has been characterized by IR, UV-vis and single-crystal X-Ray diffraction techniques. In this work, we interested in theoretical calculations and Hirshfeld surface analysis. The density functional theory (DFT) optimized structure of (I) at the B3LYP/6-311++G(2*d*,2*p*) level was compared with the experimentally determined molecular structure. The HOMO-LUMO energy gap and other related molecular properties are also calculated. Comprehensive experimental and theoretical structural studies on the studied complex are carried out by FT-IR and UV-visible spectroscopies.
The three-dimensional Hirshfeld surface (3D-HS) analysis **[2]** and the two-dimensional fingerprint plots (2D-FP) **[3]** of (I) reveal that the structure is dominated by H…O (54.3%) and H…H (26%) contacts.

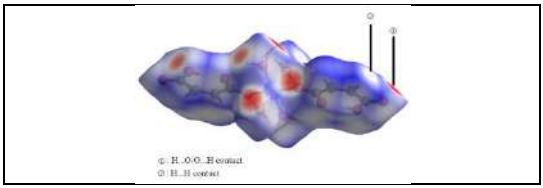

Fig. View of the three-dimensional Hirshfeld surface (3D-HS) of (I). (3D-HS mapped with d_{norm}).

Key words: cobalt (II) complex, theoretical study, DFT, Hirshfeld surface, fingerprint plots.

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Relation between structural and electrical properties of news fluorobritholite based on lead $Ca_{7-x}Pb_xLa_3(PO_4)_3(SiO_4)_3F_2$ $(0 \leq x \leq 2)$

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Fluorobritholites solid solutions, having the general formula $Ca_{7-x}Pb_xLa_3(PO_4)_3(SiO_4)_3F_2$, $(0 \leq x \leq 2)$ were prepared and characterized by X-ray diffraction, infrared spectroscopy and chemical analysis. The structural refinement carried out via the Rietveld method indicated that La^{3+} and Pb^{2+} ions were located into the two sites with a strong preference for metal (2) sites. A progressive shift of the F-ion toward the centre of the triangles formed by the site M(2) metals has been observed when the lead content increased. The electrical conductivity of the fluorobritholite materials was studied as a function of frequency (100 Hz – 10 MHz) by means of the complex impedance spectroscopy. The effect of Pb and La-substitution in fluorobritholite is remarkable on conductivity improvement with increasing Pb content [1]. As results, the carriers that govern the conductivity are the nature of the welcome sites, the dimension of the tunnels and the polarisability of cation [2,3].

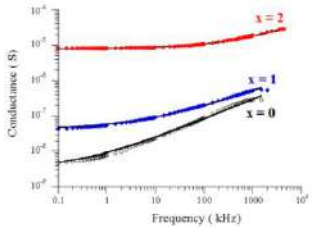

Fig.1. Frequency dependentof Conductance spectra of $Ca_{7-x}Pb_xLa_3(PO_4)_3(SiO_4)_3F_2$, $(0 \leq x \leq 2)$.

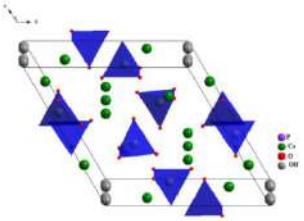

Fig.2. The relaxed primitive unit cell for hydroxyapatite

Keywords: Fluorobritholite, Rare earths, Rietveld refinement, Ionic conductivity.

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SYNTHESIS, STRUCTURAL STUDY BY XR DIFFRACTION ON SINGLE CRYSTAL OF A NEW COORDINATION POLYMER BASED ON CADMIUM AND 4, 4'-DIAMINODIPHENYLSULFONE LIGAND

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Coordination polymers (CPs), have dramatically increased as heterogeneous materials for twenty years. These novel materials have attracted considerable research interest over years as a consequence of their interesting structures, functional properties and potential applications in many scientific areas [1] such as luminescent materials organic and inorganic chemistry, biology, electrochemistry and pharmacology [2-4]. Inspired by the above-mentioned points, we synthesized a new coordination polymers by employing a V-shaped daps ligand reacted with $Cd(NO_3)$. The catena-$[(\mu_4$,-4,4'-sulfonyldianiline)-diaqua trinitrate cadmium (II)$]_n$ crystallises in the monoclinic system, $P2_1/n$ space group with the following cell parameters: a= 10.307(5)Å b= 7.312(5)Å c= 22.971(5)Å with β = 99.376(5)°. Asymmetric Unit of the coordination polymer (Figure.1) consists of one Cd(II) ion, one 4,4' daps ligand two nitrate and one water molecule.

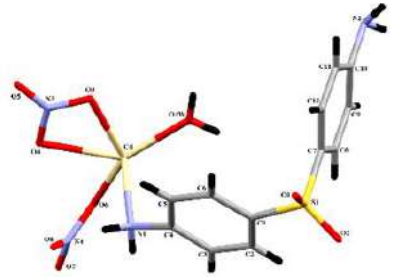

Fig.1: Asymmetric unit of the $C_{12}H_{14}CdN_4O_9S$ polymer

Key words: Coordination polymers, Hydrogen Bounds, Daps ligand.

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In situ synthesis, hydrogen bonding network and topological study of two copper complexes

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Numerous examples have illustrated the ability of the ligands containing the nitrile function to link metal centers forming complexes, and also have the ability to be converted into carboxylic acid or amide functions by a hydrolysis process, thus promoting the formation of complexes based on this type of ligands and the construction of new uni, bi or three-dimensional networks with very varied topologies.
Herein we examine and the report the crystal structure of two complexes ; cis-tetraquabis(pyrazine-2-carboxylato-O,N)strontium(II) and bis(2-imidodicarbonyl-diamide) dinitrato-copper(II), and we study their network and topologies.

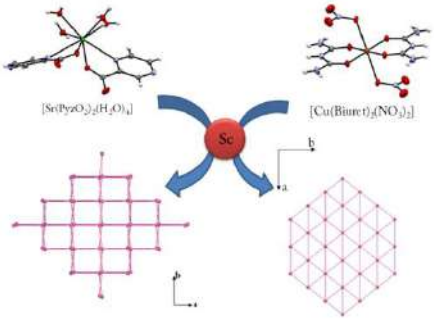

Fig. Simplification of the structures and the net representation

Key words: In-Situ synthesis, Topology, hydrogen bonds

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SONOGASHIRA CROSS COUPLING REACTION CATALYZED BY N-HETEROCYCLIC CARBENES PALLADIUM COMPLEXES WITH TRIPHENYLPHOSPHINE

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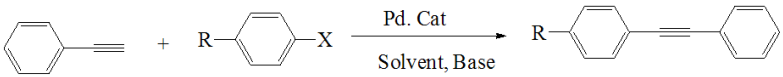
The Sonogashira cross-coupling reaction is one of the most important methods for the construction of some C-C bonds [1]. This cross-coupling reaction is a research field with enormous academic and industrial interest due to extensive use of products in the synthesis of drugs which is used in the treatment of Alzheimer's disease, natural products and biologically active molecules [2]. From environmental and economic points of view, the development of efficient and stable palladium complex catalysts allows to achieve the Sonogashira reaction with low catalyst loadings under copper-free conditions [3]. In this work, we aim to synthesize alkynes derivatives using cross coupling reaction of varying aryl halides with phenylacetylene in the presence of DMF as a solvent and KOtBu as a base. **Scheme1** To demonstrate the general applicability the sonogashira products have been synthesized in good to excellent yields 68 – 100% under mild conditions.



Scheme1: Sonogashira reactions catalyzed by Palladium complexes.

Key words: Palladium complex, triphenylphosphine, phenylacetylene, alkynes derivatives, Sonogashira reactions.

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DFT and TDDFT study of the structure and optical properties of the complexes containing Nickel

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These last years, The chemistry of Nickel (II) complexes has just been updated, thanks to the specific properties of Nickel not only in inorganic chemistry but also in the biochemical, and pharmacological biological fields, Ni (II) forms a large number of complexes of which the most important are tetrahedral octahedral or square planar. The structures of the Ni (II) complexes are generally octahedral in the solid state.
Our research tasks are centered on the study of the complexes containing Nickel in gas and solvent phase,calculations were carried out within the framework of the functional theory of the density DFT independent of time and TD-DFT, It is to calculate the structural properties, energy,absorption spectra by two functional calculuses CAM-B3LYP [1] and LC-M06L [2] and with the base of the type QZVP. Calculations are carried out with the program GAUSSIAN 09.Results obtained reproduced better the experimental results and the comparison between the experimental absorption spectrum and the calculated absorption spectra indicates that the functional that best reproduces the experience is the hybrid functional B3LYP, However, the correction of functional CAMB3LYP and LC-M06L has no influence on our results, Therefore the functionalities used are the parameters that influence the calculation of the gap energetics Regardless of the base used.

Key words: NICKEL (II) COMPLEXES, GAUSSIAN 09, DFT, TD-DFT

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INFLUENCE OF ANNEALING TEMPERATURE ON STRUCTURE AND PROPERTIES OF ZINC SILICATE POWDERS SYNTHESIZED BY SOL GEL METHOD

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Zinc silicate (Zn_2SiO_4) belongs to one of the most important families of inorganic functional materials. With a wide energy band gap (5.5 eV) and excellent chemical stability, it has been used as a luminescent material for lamp and cathode ray tubes and it seen as a promising candidate for divers applications: flat panel displays with unique luminescent properties, X-ray or nuclear medical image receptors, X-ray to light converters coupled to optical detectors, etc. In the present work, we report the synthesis of willemite-Zn_2SiO_4 ceramic powders by sol-gel technique, and study of their structural and optical properties. As revealed by XRD and TGA-DTA analyses, the synthesized Zn_2SiO_4 powders contain two phases, α-Zn_2SiO_4 as the major phase and β-Zn_2SiO_4 as the minor one. FTIR measurements revealed appearance of the symmetric/asymmetric stretching vibrations of SiO_4 and ZnO_4 groups, clearly indicating formation of the Zn_2SiO_4 phase. Photoluminescence analysis emphasized emission bands with anomalous Berthelot-type behavior. Relative photoluminescence intensity was found to increase together with firing temperature. Obtained results point toward an increase in crystallinity as being responsible for the increase in photoluminescence intensity.

Keywords: Synthesis, Sol-gel, Willemite, DRX, Photoluminescence

New metallo-antibiotic compounds : synthesis and characterization

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The development of structurally novel coordination compounds with diverse biological activity, such as antimicrobial, anti-inflammatory, antifungal, antioxidant and anticancer, is a rapidly evolving field of Inorganic Chemistry with potential for direct impact on improving quality of life.[1-2] Metal–drug complexes are of increasing interest in Bioinorganic Chemistry, leveraging the synergistic effect to lead to compounds with improved pharmacological activity.[3-7] The recognition of the role of metal ions in the biological systems and in treatment of various diseases call attention to the benefits of studying the interaction of metal ions with organic drug molecules[8]. In continuation with our previous works, [9] we focus here on the synthesis of a new family of metal-bioligand complexes associating on a single-object an Active Pharmaceutical Ingredient (API): the synergic effect of the antiseptic activity of one metal ion with the bioactivity of one or two type of bioactive molecules (figures 1). Indeed, their additive action should lead to more effective and shorter treatments and strongly minimize the risks for appearance of bacteria mutants.

In this work, the structural on the solid state of these new biomolecules are describes and their chemical-physics properties in solution are studied. Moreover, the synthesis of new trifluorométhylated antimicrobial ligands is describes and characterizes in solution.

Antimicrobial in vitro tests are underway. The first tests show the synergystic effect and very encouraging results. The use of the new bioactive ligands in order to increase the nucleation of the complexes will allow access to a new types of Antimicrobial complexes.

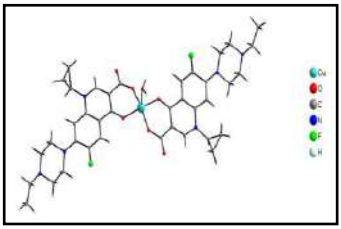

Figure 1*: example of copper antimicrobial complex with bioactive quinolone type ligand*

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Structure and photoluminescence properties of $Na_2Sr_{0.8}Eu_{0.2}Mg(PO_4)_2$

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Alkali and alkaline earth monophosphates are extensively studied for their rich crystal chemistry and their attractive properties. These materials are also of great interest for use in lighting devices because their structures offer important crystallographic possibilities to accommodate luminescent ions. Our interest in these materials concerns the synthesis of new compounds and their structural and optical investigation, in the quest of new potentially interesting materials for light-emitting diode (LEDs). As a part of this ongoing study, we recently synthesized a new compound $Na_2SrMg(PO_4)_2$ as a powdered sample by the Pechini method. Its structural study by X-ray diffraction showed that it crystallizes in the monoclinic system with the space group $P2_1/a$ and the unit cell parameters: a = 9.158(1) Å, b = 5.267(1) Å, c = 13.498 (1) Å and β = 90.01(1)º. Its structure, closely reassembling to that of the well known glaserite type consists of a lamellar anionic framework resulting from the stacking, along the [001] direction of $[MgP_2O_8^{4-}]_\infty$ layers parallel to the (*a*,*b*) plane and consisted by corner-sharing MgO_6 octahedra and PO_4 tetrahedra. Each octahedron is linked to six tetrahedra while each tetrahedron is connected to three octahedra, the fourth oxygen being unshared and points into the Na and Sr sites occupying the interlayer space. An other way to describe this structure is to consider that it is formed by an alternately stacking, along the [210] direction of two kinds of rows propagating along the [001] direction. The first (row A) is consisted by PO_4 tetrahedra and Na atoms while the second (raw B) is formed by Mg and Sr atoms. These rows occur with a sequence of BAAB.

Optical measurements on divalent europium-doped phases showed these materials to be interesting for optical applications.

Correlation between structure and photoluminescence of divalent europium doped fillowite type phosphate $Na_3SrMg_{11}(PO_4)_2$.

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A new phosphate compound, $Na_3SrMg_{11}(PO_4)_9$ was synthesized as single crystals by flux method and as powdered sample by Pechini technique and investigated by X-ray diffraction and photoluminescence spectroscopies. This compound crystallizes in the rhombohedral space group R $\bar{3}$ and its equivalent hexagonal cell has the following parameters: a = 14.941(1) Å, c = 42.478(2) Å and Z = 12. The structure consisted of MgO_x (x=5,6), NaO_x (x=6,7) and $(Na,Sr)O_x$ (x=8,9) polyhedra which are linked either directly through common corners, edges and faces and by means of the PO_4 tetrahedra via common corners and edges, giving rise to a three-dimensional framework, similar to that of the fillowite-like structure. Strontium was partially substitute by divalent europium in order to examine whether this material could be used in optical applications. Optical studies were performed on the $Na_3Sr_{0.98}Eu^{2+}_{0.02}Mg_{11}(PO_4)_9$ compound.

The photoluminescence are consistent with the crystal structural and show various properties as a function of the excitation wavelength.

Synthesis of new complexes of sulfonatocalix [4]arenes: structure and magnetic properties

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P-sulfonatocalix[4]arene (SC4), the smallest analogue in water-soluble calix[4]arenes's family[1], has attract much attention in supramolecular and coordination chemistry particurlarly. P-sulfonato calix(n)arenes are able to complex with variety of organic compounds as well as inorganic ions in water. In our work, we attempt to form mettalic complexes based on p-sulfonatocalix[4]arene[2], therefore, the molecular binding behaviors of p-sulfonatocalix[4]arene were systematically investigated by mono-crystal DRX for crystal structure and by SQUID to evaluate their magnetic properties.

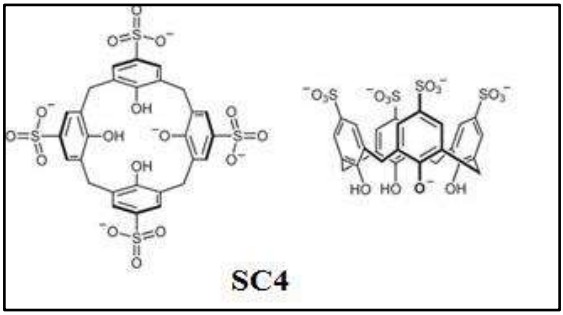

Fig.p-sulfonatocalix[4]arene's structure (SC4)

Key words:p-sulfonatocalix[4]arene, complexes,cristal structure, magnetic properties.

Acknowledgement: we thank the PHC Utique program for the financial support.

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A green way to enantioenriched *(R)*-3-(1-Hydroxyethyl)phenol by lipase-catalyzed alkaline hydrolysis reaction

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Nowadays the preparation of bioactive molecules is become a necessity in different areas such as agrochemicals, cosmetics, drugs and particularly in the pharmaceutical industry considering aspects such as efficiency, regioselectivity, chemoselectivity and enantioselectivity[1]. The kinetic resolution of racemates is increasingly used in synthetic strategies and enzymes used as a routine chiral catalyst for asymmetric synthesis are well documented [2]. Lipases are primarily used for catalyze the hydrolysis and transesterification reaction of a wide range of substrates [3].

Diols are an important intermediates and building blocks for various synthetic applications. We developed a new route for preparing optically active diol 3-(1-Hydroxyethyl)phenol and its derivatives which are an intermediate of ***Rivastigmine***, used for treating Alzheimer disease [4].

We examined the lipasic kinetic resolution by means of hydrolysis assisted by sodium carbonate in organic medium. Our study covered the modulation of several parameters which may interfere on the catalytic process and selectivity such as the amount and the lipase nature, the solvent hydrophobicity and heating.

The obtained results show the efficiency of the unconventional diacetate hydrolysis methodology in terms of reactivity and selectivity. The CAL-B-catalyzed alkaline hydrolysis reaction of shows a selectivity factor of E =200 with conversion c = 40%. The best one are recorded using THF as organic solvent at 40ºC. The enantioenriched (*R*)-diol enantiomer were obtained with high enantiomeric purity (99% ee).

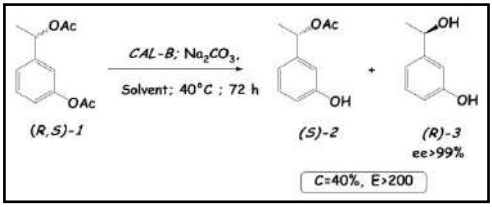

Fig. CAL-B catalyzed alkaline Hydrolysis.

Key words: Enzymatic kinetic resolution, *CAL-B*, Alkalin-enzymatic hydrolysis.

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Enzymatic kinetic resolution via transesterification of 1-Indanol and its derivative acetate: Study of some parameters.

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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 enantioselectivity. For the enzymatic deacetylation of benzylic acetates, we have described, two efficient methods; the first one was performed in biphasic media, and the last one in non aqueous media, and we have that the last one, is the most effective in term of reactivity and enantioselectivity [1].
In the continuity of our investigations focused on the study of the mode of action of lipases in the kinetic resolution are studied such as the transesterification and the alkaline hydrolysis [2].
Herein we describe a comparative study of effect of some crucial parameters interfering significantly on the enzymatic catalytic processes during the transesterification of 1-Indanol and the alkaline hydrolysis of the corresponding acetate. We present the significant effect of the lipase nature, the acetyl donating in two organic solvent having different hydrophobicity during the transesterification and the effect of the solvent during the hydrolysis (Fig. 1).
The obtained results show that the *CAL-B* is the best biocatalyst, promoting both reactions in terms of reactivity and selectivity, with *(R)*-enantioselection. The both reactions transesterification/hydrolysis show a perfect enantiocomplementary applying the optimized conditions.

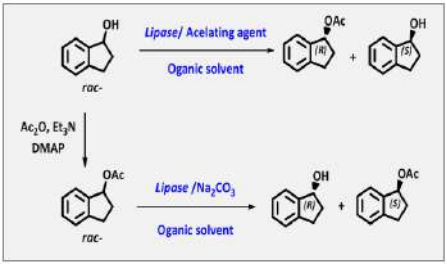

Fig. 1 Transesterification/ Alkaline hydrolysis of 1-Indanol and its corresponding acetate.

Key words: Enzymatic kinetic resolution, transesterification, Alkalin-enzymatic hydrolysis, Indanol

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Fluoresence-induite par aggregation : fluorophores organiques et hybrides

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Certains composés organiques ont une fluorescence exaltée par agrégation. Cette propriété a été mise à profit pour préparer des composés organiques (électro)-luminescents à l'état solide ou des sondes biologiques fluorescentes.[1] Beaucoup de ces composés sont basées sur le squelette polyphénylsilole.
Dans le cadre de ce projet, nous nous sommes intéressés à leurs analogues phosphorés dérivés du pentaphenylphosphole. En effet, contrairement à leur version polycyclique, les dérives pentaphenylphosphole présentent le phénomène de fluorescence induite par agrégation. [2,3]
La réactivité particulière de l'atome de phosphore permet d'envisager diverses approches originales.
En particuliers, nous nous sommes intéressés au greffage de ce type de fluorophores sur des nanoparticules d'oxyde métalliques.

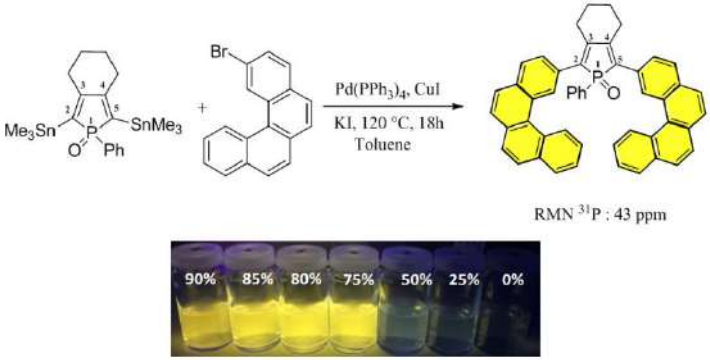

Schéma 1 : Synthèse des chromophores organophosphorés

Mots-clefs: Fluorophores / Agrégation / Matériaux hybrides / Couplage de stille / Hélicène / Absorption / Emission.

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Treatment Of Aqueous Wastes Contaminated With Herbicide Oxyfluorfen By Anodic Oxidation On Boron-Doped Diamond

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In this work, the treatment of effluents polluted with pesticide oxyfluorfen is studied using electrolytic and photoelectric technology. Oxyfluorfen is rapidly and effectively oxidized by the two electrochemical advanced oxidation processes. Applied electric charges below 50 Ah dm^{-3} are required to decrease the concentration of herbicide.

Key words: oxyfluorfen, electrolysis, photo-electrolysis.

Comparative study of electrochemical, photoelectrochemical and sonoelectrochemical treatment of soil-washing effluents polluted with herbicide oxyfluorfen

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In this work, the treatment of soil-washing effluents polluted with herbicide oxyfluorfen is studied using biosorption combined with electrolytic, photoelectric and sonoelectric technology. Results show that oxyfluorfen is very efficiently removed from synthetic soil by soil washing with SDS. The effluent can be treated by biosorption with fresh activated sludge coming and the maximum adsorption capacity of this activated sludge was found to be 18 mg oxyfluorfen g^{-1} biomass. Results show that Oxyfluorfen is rapidly and effectively oxidized by the four electrochemical advanced oxidation processes., electrolysis, photo-electrolysis and sonoelectrolysis can lead to the complete mineralization of the oxyfluorfen.

Key words: oxyfluorfen, SDS, biosorption, electrolysis, photo-electrolysis, sonoelectrolysis

Synthesis and Fe^{3+}complexation study of new calixarene based ligand

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Despite that iron is an essential nutrient that plays an important role in many basic body functions, both iron overload and iron deficiency appear to make people more susceptible to infection.[1] In fact many opportunistic bacteria such as Pseudomonas aerugisnosa 'PA' which develops mainly in immunocompromised individuals use the ferrous iron (Fe^{2+}) as essential nutrient.[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]
Iron serves also in PA biofilm development.[5] Depriving the bacterium from this nutrient can then constitute a new strategy to prevent the biofilm formation. The use of artificial chelators of Fe^{3+} that compete efficiently with pyoverdine I could then induce iron deprivation, biofilm inhibition and consequently bacterial death.
The present work is devoted to the study of a new generation of glycoclusters designed for Fe^{3+} complexation and possible therapeutic strategies.

Key words: calixarene, ligand**,** Pseudomonas aerugisnosa, chelator, ferrous iron.

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Extraction and Modeling of Eucalyptus essential oil using supercritical CO_2

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Nowadays, the increasing environmental concern and the develop of green chemistry stimulates the search for cleaner and less energy-intensive processes to extract the natural products from plants especially the essential oils, with shorten extraction time, reducing energy consumption, lower cost, and preventing pollution.
In the present study, Supercritical carbon dioxide extraction (SC-CO2) of oil from **Eucalyptus** was performed and a comparison was made with conventional hydro distillation (HD). The effects of independent variables, including pressure, temperature, CO2 flow rate, and extraction time, on the yield of oil were investigated. The optimum supercritical carbon dioxide extraction results were obtained at the following experimental conditions: pressure = 90atm, T = 40C, dynamic time 30 min. The composition of the extracts obtained from Eucalyptus using supercritical fluid extraction was compared with the essential oil obtained by hydrodistillation. The composition of the SC-CO2 products was markedly different from the corresponding hydrodistillated oil. Additionally, the inflammatory, antioxidant and anticancer activities of extract were evaluated. The model of Sovava was used to analyse the experimental results of the extraction, the experimental results were successfully fitted.
In conclusion, SC-CO2 is a green, energy saving and environmentally friendly extraction method of essential oil from Eucalyptus.

Key words: Eucalyptus, essential oil, supercritical CO2, hydrodistillation

DFT calculations of 3-nitroaniline, 3-nitroanilinium and 3-nitroanilinium chloride

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The Density Functional Theory (DFT) is a method used in many domains to investigate the structural, magnetic, spectroscopic and electronic properties of molecules [1-2].
In this work, the geometry optimization of 3-nitroaniline, 3-nitroanilinium and 3-nitroanilinium chloride was carried out by DFT/B3LYP calculations with different basis sets using Gaussian 09W program and Gauss View interface [3]. Some electronic parameters (HOMO–LUMO energy gap with graphical representations of the lowering of Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), the global hardness, the electronic chemical potential and the electrophilicity) were calculated.
As well as the 3-nitroanilinium chloride compound is concerned, previous works has studied its X-ray diffraction analysis [4] and a structural comparison with our results is accomplished.

Key words: 3-nitroaniline, 3-nitroanilinium, 3-nitroanilinium chloride, DFT calculations

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Dihydrogen production on the surface of a TiO_2 nanotube by water splitting

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Hydrogen is the ideal fuel for the future because it is clean, energy efficient, and abundant in nature. While various technologies can be used to generate hydrogen, only some of them can be considered environmentally friendly. Recently, water splitting has attracted tremendous attention. In this work, a theoretical study shows that it is possible to produce dihydrogen on the internal surface of a TiO_2 nanotube by water splitting in two essential steps, dissociation of a molecule of water at the first Place, release of a molecule of H_2 and molecule of H_2O_2 in second place. All calculations were performed using the method of Density Functional Theory (DFT) in periodic conditions provided by means of the "VASP 5.2.12" (Vienna Ab Initio Simulation Package) code

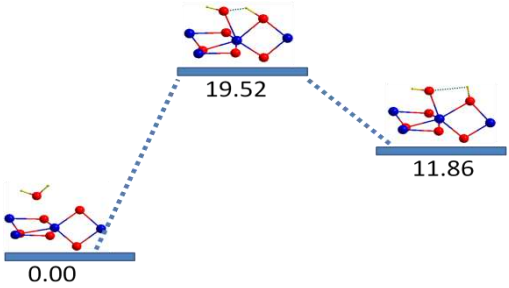

Fig. Energy profile (in kcal/mol) for the dissociation step of water on the (9,0) nanotube.

Key words: TiO_2 nanotube, Water splitting, Hydrogen production, transitory states.

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The contribution of mediated oxidation mechanisms in the electrolytic degradation of cyanuric acid using diamond anodes

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In this work, the contribution of mediated oxidation mechanisms in the electrolytic degradation of cyanuric acid using boron-doped diamond (BDD) anodes was investigated in different electrolytes. A complete mineralization of cyanuric acid was obtained in NaCl; however lower degrees of mineralization of 70% and 40% were obtained in Na_2SO_4 and $NaClO_4$, respectively. This can be explained by the nature of the oxidants electrogenerated in each electrolyte. It is clear that the contribution of active chlorine (Cl_2, HClO, ClO^-) electrogenerated from oxidation of chlorides on BDD is much more important in the electrolytic degradation of cyanuric acid than the persulfate and hydroxyl radicals produced by electro-oxidation of sulfate and water on BDD anodes. This could be explained by the high affinity of active chlorine towards nitrogen compounds. No organic intermediates were detected during the electrolytic degradation of cyanuric acid in any the electrolytes, which can be explained by their immediate depletion by hydroxyl radicals produced on the BDD surface. Nitrates and ammonium were the final products of electrolytic degradation of cyanuric acid on BDD anodes in all electrolytes. In addition, small amounts of chloramines were formed in the chloride medium. Low current density ($\leq$10 mA/cm^2) and neutral medium (pH in the range 6–9) should be used for high efficiency electrolytic degradation and negligible formation of hazardous chlorate and perchlorate.

Key words: Electrolytic degradation, Diamond anode, Supporting electrolyte, Mediated oxidation, Cyanuric acid

Mechanism and kinetics on the degradation of nicotinic acid in Water by photo-Fenton process

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Nicotinic acid (NA) is one of the water-soluble B vitamins that is widely used and detected in natural waters. Here, the degradation of nicotinic acid in aqueous solutions by photo-Fenton process ($H_2O_2/Fe^{2+}/UV$) was studied to enhance the biodegradability and the mineralization of this pollutant. The efficiency of three different advanced photo oxidation processes Fenton, UV/H_2O_2 and photo-Fenton were examined. The results demonstrated that, under the same conditions, the degradation of nicotinic acid by photo-Fenton process is more rapid, more effective and powerful than Fenton and UV/H_2O_2 processes. The influence of the experimental parameters such as the initial pH, the hydrogen peroxide concentration, the ferrous iron concentration and the initial concentration of nicotinic acid on kinetics and efficiency of the degradation was investigated. The results show that nicotinic acid was removed mainly by photo-Fenton oxidation. The total organic carbon (TOC) removal reached a maximum of 93.56 % under the optimum conditions ($[H_2O_2]/[Fe^{2+}]$ = 100 for 100 mg/L nicotinic acid, pH = 3 and T = 23 - 25˚C, 300 rpm) at 120 min. It is concluded that the photo-Fenton process is a very interesting technology for the treatment of nicotinic acid wastewater. The kinetic decay of the nicotinic acid was followed by high performance liquid chromatography (HPLC) and obeyed a pseudo-first-order reaction. HPLC analysis of treated solutions revealed that 3-hydroxypyridine, 3-pyridone, maleic acid, oxalic acid and formic acid were the intermediates found. Oxalic acid was the major and most persistent product found. Based on detected intermediates and bibliographic research, a mechanism of uric acid mineralization by anodic oxidation has been proposed. Ionic chromatography analysis confirmed the release of NH_4^+ ions during nicotinic acid treatment.

Key words: Nicotinic acid wastewater, Photo-Fenton Process, Hydroxyl Radicals, Degradation

Suzuki- Miyaura Cross-Coupling Reactions Catalyzed by new benzyladamantyl substituted N-Heterocyclic carbane-Pd(PEPPSI) Complexes in Water

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Suzuki cross coupling reaction is one of the most famous reaction in the field of chemistry. It is a very effective method for making carbon – carbon bonds. This is one of the most useful cross-coupling reactions between aryl or vinyl boronic acid with aryl or vinyl halides and also with different reagents like alkenes. catalyzed by palladium (0) complexes [1][2][3][4]. On the other hand, green chemistry is a rapidly developing new field that provides us a proactive avenue for the sustainable development of future science and technologies. In this study, we have been synthesized a new series of air and moisture-stable N-heterocyclic carbene precursors and their Palladuim (II)-pyridine (PEPPSI) complexes. With the development of a more efficient catalytic system for the cross-coupling of aryl halides in mind, the catalytic performance of the NHC-$PdCl_2$-pyridine complexes for Suzuki cross-coupling under mild conditions in green solvants at room temperature was investigated.

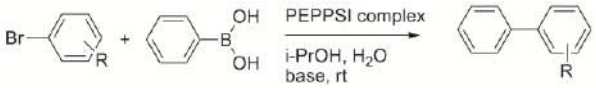

Fig. The Suzuki coupling reaction of aryl bromides with phenylboronic acid catalyzed by Pd-NHC (PEPSSI) complexes

Key words: Suzuki cross-coupling reaction, N-heterocyclic carbene –Pd complexes.

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Sonogashira Coupling Reaction catalyzed by Sterically Bulky NHCPd(II)-PPh_3 complexes

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The sonogashira cross-coupling reaction is well-known as being one of the most important and utilized reactions for the coupling of vinyl or aryl halides with terminal alkynes to form conjugated enynes or aryl alkynes. The reaction has become an essential tool in the synthesis of these compounds, which have applications in natural products chemistry[1], pharmaceuticals[2], polymers[3] and material science[4, 5]. In this study we used new NHC-Pd-PPh_3 complexes and various aryl bromides were coupled with alkynes to afford sonogashira products in DMF at 100°C.

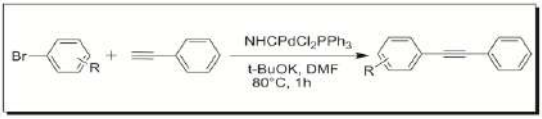

Fig. Sonogashira coupling reaction of phenylacetylene with different aryl halides catalyzed by NHC-Pd-PPh_3 Complexes.

Key words: Sonogashira coupling reaction, NHC-Pd-PPh_3.

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Preparation and characterization of Dawson polyoxometallates cesium salt: application to adipic acid synthesis

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Adipic acid is one of a basic intermediate for the nylon production, however, its industrial production, involves the use of concentrated nitric acid that contributes to atmospheric pollution by release harmful gases. The aim of our work is to develop an ecologic process for adipic acid synthesis using hydrogen peroxide as oxidant and Dawson-type polyoxometalates (POMs) as catalysts.

Dawson polyoxometalate salts, namely $Cs_3SbP_2W_{12}Mo_6O_{62}$ and $Cs_4SnP_2W_{12}Mo_6O_{62}$ were prepared, characterized and tested in the adipic acid synthesis from cyclohexanone at 90°C in the presence of hydrogen peroxide, free solvent. The effects of catalyst amount and heteropolysalts composition were investigated. The highest yield of adipic acid (60.7%) was obtained with $Cs_4SnP_2W_{12}Mo_6O_{62}$ POM, a catalyst mass of 90 mg and a reaction mixture stirring rate of 1000rmp during 20h.

This study demonstrated the efficiency of Dawson type polyoxometalates in the adipic acid synthesis that is a green process where hydrogen peroxide is only reduced to water, compared to industrial process that leads to the N_2O formation, pollutant product.

Key words: polyoxometalates, Dawson, adipic acid, cyclohexanone

Catalytic application of the Keggin type polyoxometalates namely $Cs_XSn_YH_ZPMo_{12}O_{40}$ to the adipic acid synthesis

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Keggin type polyoxometalates have proven their efficiency in the oxidation reactions in both liquid and gas phases. They have also been used as catalysts in organic compounds oxidation due to their composition, redox potential, acidity and solubility. Adipic acid (AA) is used in nylon 6,6 production and food additives. Its industrial production from cyclohexane via cyclohexanone and cyclohexanol, uses nitric acid (50-60%) as oxidant and Cu/V as catalyst. Unfortunately, this method also leads to the nitrogen oxides (NO_2, N_2O, and NO) formation. Among them, N_2O contribute to the atmosphere pollution.

The aim of this study is to substitute the polluting and corrosive nitric acid by hydrogen peroxide, in the presence of Keggin type polyoxometalates as catalyst of $Cs_xSn_yH_zPMo_{12}O_{40}$ formula (noted $HSnPMo_{12}$, $CsSnPMo_{12}$, $Cs_2Sn_{0.5}PMo_{12}$ and $CsSn_{0.5}HPMo_{12}$) according to a green protocol. The prepared polyoxometalates were tested as catalyst in adipic acid synthesis in presence of hydrogen peroxide 30% as oxidant and cyclohexanone as substrate. Thus, this study showed the influence of the chemical composition and redox and acidity properties of POMs on the formation of adipic acid. The catalyst partially substituted with tin and a proton of formula $HSnPMo_{12}$ is the most efficient with a yield of adipic acid equal to 59%.

Key words: heteropolysalt, Keggin, adipic acid, polyoxometalates

Synthesis and pharmacological Evaluation of BenzoChromenoPyrimidinetriones as Cholinesterase inhibitors for Alzheimer's Disease Therapy

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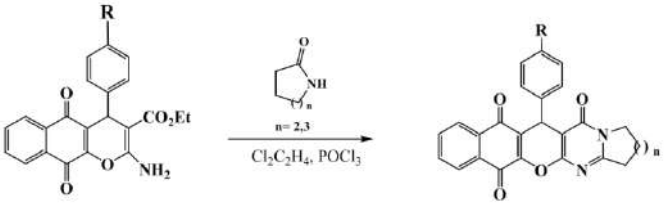
Alzheimer's disease (AD) is an age-related neurodegenerative process characterized by a progressive loss of memory, language skills, disorientation, attention, and depression. Although the etiology of AD is still poorly understood, several factors such as amyloid deposits, protein aggregation, oxidative stress, or low levels of acetylcholine are thought to play significant roles in the pathology of the disease. In spite of the enormous research effort, an efficient strategy for the treatment of AD is still lacking. The cholinergic theory suggests that the selective loss of cholinergic neurons in AD results in a deficit of acetylcholine (ACh) in specific regions of the brain that mediate learning and memory functions. Thus, three acetylcholinesterase (AChE) inhibitors (donepezil, rivastigmine, and galanthamine) have been approved for commercial use, to improve AD symptoms by inhibiting AChE. In the present work we report the straight synthesis and biological assessment of novel racemic BenzoChromenoPyrimidinetriones as Acetylcholinesterase inhibitors properties (Scheme1).



1 a-l **2 a-l**

Scheme1

The biological evaluation of the compound **2** identified compound **-2h-** (R = 3-OCH_3, n=2) displayed a inhibition of acetylcholinesterase *Ee*AChE (**IC_{50} = 0.04 ± 0.01 µM**).

Keywords: Alzheimer's disease; amyloid plaques; BenzoChromenoPyrimidinetriones; cholinesterase inhibitors.

Synthesis and Biological Evaluation of new Tacrine derivatives as Potent Antioxidant Agents for Alzheimer's Disease

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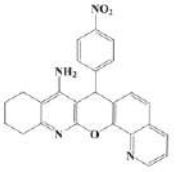
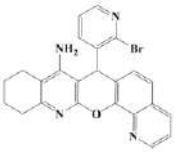
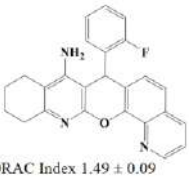
Research in Alzheimer disease has recently demonstrated compelling evidence on the importance of oxidative processes in its pathogenesis. Cellular changes show that oxidative stress is an event that precedes the appearance of the hallmark pathologies of the disease, neurofibrillary tangles, and senile plaques. While it is still unclear what the initial source of the oxidative stress is in Alzheimer disease, it is likely that the process is highly dependent on redox-active transition metals such as iron and copper. Further investigation into the role that oxidative stress mechanisms seem to play in the pathogenesis of Alzheimer disease may lead to novel clinical interventions.
Herein, we assessed the antioxidant activity of racemic compounds **2a-l** using the Oxygen Radical Absorbance Capacity (ORACFL) method. Tacrine and ferulic acid were used as negative and positive reference molecules, respectively. Results are expressed in relation to radical scavenging properties of Trolox yielding the Trolox equivalents (TE) unit. All compounds presented good radical scavenging properties with ORAC values ranging from 1.22 to 2.49 TE. Thus, for compounds of type 2, we hypothesize that the presence of a free (C8)- NH_2 could explain the observed antioxidant effect, due the lability of the N-H bond against any radical oxygenated species.



ORAC Index 2.49 ± 0.19



ORAC Index 2.35 ± 0.26



ORAC Index 1.49 ± 0.09

Keywords: Antioxidant, Acide férulique, ORAC, Tacrine, Alzheimer's Disease.

Synthesis and Characterization of a novel paratungstate $Na_{10}[H_2W_{12}O_{42}].26H_2O$

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The current increasing attention and powerful driving force in the polyoxometalate (POM) chemistry, originated from their fascinating properties in material science, medicine [1], catalysis, etc.

In this context an new paratungstate Na_{10} $[H_2W_{12}O_{42}]\cdot_{26}H_2O$ have been synthesized under mildly acidic conditions. This compound was characterized by single-crystal X-ray diffraction, IR and UV–visible spectroscopies. It crystallizes in the triclinic system space group P-1 with a=11.81367Å, b=12.48593Å, c=22.13615Å, α=86.1723°, β=86.3171°, γ=66.1984°, V=2978.32Å, and Z=1.

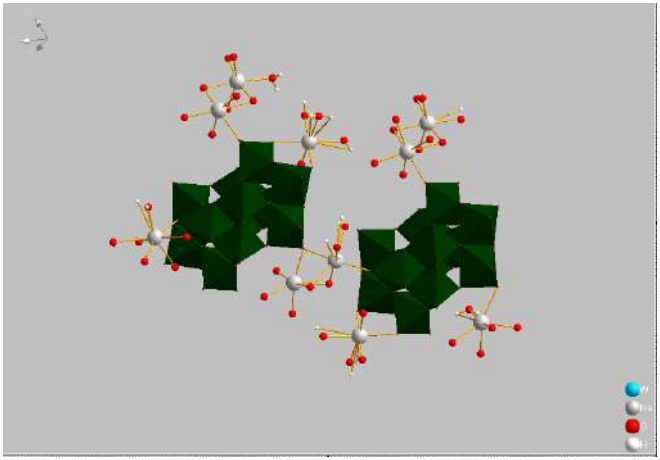

Fig. A view in the direction [111] of the title compound

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

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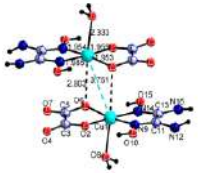
Motivated by the desire to create novel materials that could exhibit currently unavailable properties and enable new applications[1-3], the dimeric copper(II) complex $[Cu(C_2O_4)(H_2oxado)(H_2O)]_2$ (**1**), (where H_2oxado = oxamide dioxime), has been synthesized in water and characterized by elemental and thermal analyses, IR spectroscopy, and single-crystal X-ray diffraction. Complex (**1)** is composed of two neutral $[Cu(C_2O_4)(H_2oxado)(H_2O)]$ entities (Figure 1) connected by Cu–O bonds between oxalate oxygen atoms and copper(II) ions, thereby producing a centrosymmetric dimer, with the Cu(II) centers exhibiting a strongly distorted octahedral coordination. Neighboring dimers are hydrogen-bonded through O–H···O interactions leading overall to a layer structure (Figure 2). Thermal analyses of complex **1** showed two significant weight losses corresponding to the coordinated water molecules, followed by the decomposition of the network. Magnetic susceptibility data revealed very weak antiferromagnetic spin exchange interactions within the dinuclear unit.



Key words: Copper(II) complex, Crystal structure, oxamide dioxime, oxalate.

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Chemical and electrochemical copolymerization of aniline with piperazine on platinum electrodes: Characterization, and Application to the Detection of Dopamine and Ascorbic Acid

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Polyaniline (PANI) ranks among important conducting polymers with highly promising properties for different applications, However, it has been observed that some of its properties still need further improvement, it is electroactive only at low pH and it is insoluble in common solvents in its conductor state [1]. Several authors [2] have studied the synthesis of copolymers of aniline with other molecules such for example aminobenzenesulfonic acids [2]. In this work, the electrochemical polymerization of aniline in presence of piperazine was successfully synthesized from monomers in acidic medium. Several spectroscopic characterization techniques were employed to gain information on the chemical structure and redox behavior of the obtained material. Cyclic voltammetry, XPS and in situ FTIR spectroscopy were combined to study the composition of the copolymer and redox transitions mechanism. The poly(aniline-co-piperazine) was developed and applied for the determination of ascorbic acid and dopamine in perchloric acid solution.

Acknowledgements
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Effects of pH, concentration and speed on the electrochemical polymerization piperazine

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The tripiperazine was successfully electrosynthesized and characterized by cyclic voltametric, chromatography, scanning electron microscopy (SEM), and UV–Visible. By means of the potentiodynamic and the potentiostatic approaches, we highlight a direct ejection of electrons from piperazine. The voltammetric response of this compound was investigated in organic medium (acetonitrile).. In cyclic voltammetry, this trimer undergoes three successive and irreversible oxidation steps that the potentials are notably sensitive to the pH of the electrolyzed solution, the substrate concentration, the nature of the electrolyte and the scan rate. The modified electrode exhibits a biggest oxidation facility than the parent. Figure 1 shows the chemical structure obtained for the tripiperazine. HNMR, XPS and FTIR spectroscopy were combined to study the mechanism of the trimer.

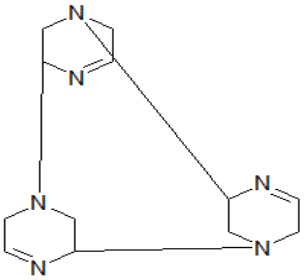

Fig. 1. chemical structure of tripiperazine

Key words: Piperazine, Cyclic Voltammetry, Electrodeposition,tripiperazine. Anodic oxidation, Electrolysis.

POLYMERIZATION OF METHYL ACRYLATE WITH CATIONIC NICKEL(IV) DIFLUORIDE COMPLEXE

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Development a new catalysts with early transition metals has played an important in the fast-growing polyolefins industry [1]. In 1990s Brookhart and his colleagues discovered a new class of catalysts known as late transition metal complexes for ethylene polymerization and copolymerization of ethylene and α-olefins [2].
It was of great importance to test a cationic Nickel(IV) difluoride complexe in polymerisation of methyl acrylate experiments. The polymer was characterised by IR, ^{1}H NMR spectroscopy, then by differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA).

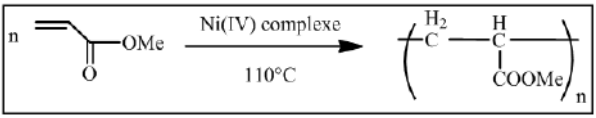

Fig. methyl acrylate polymerization

Key words: polymerization, polyolefin, catalysts

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A Hirshfeld surface analysis, crystal structure and spectroscopic properties of new Zn(II) complex with N-aminoethylpiperazine ligand

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A new organic-inorganic hybrid material, 1-amonioethylpiperazine-1, 4-diium tetrachloridozincate(II) chloride, $(C_6H_{18}N_3)[ZnCl_4]Cl$, has been synthesized and characterized by various physicochemical techniques including UV-visible absorption, Infra-Red (IR), Raman and NMR spectroscopies. The compound crystallizes in the monoclinic system and $P2_1$ space group with $Z = 2$ and the following unit cell dimensions: a = 7.1728 (6), b = 12.4160 (11), c = 8.0278 (7) Å, β = 97.513 (1)°, V = 708.80 (11) Å^3.
In this structure, the Zn^{2+} ion, surrounded by four chlorides, adopts a distorted tetrahedral coordination geometry. The structure of this compound consists of monomeric 1-amonioethylpiperazine-1, 4-diium trications and monomeric $[ZnCl_4]^{2-}$ and Cl^- anions. These entities are interconnected by means of hydrogen bonding contacts [N-H…Cl, C-H…Cl], forming a three-dimensional network. Intermolecular interactions were investigated by Hirshfeld surfaces. More than three quarters of the interaction surface in the crystal packing is constituted by attractive and favored H…Cl hydrogen bonds. The ^{13}C and ^{15}N CP-MAS NMR spectra are discussed and the vibrational absorption bands were identified by infrared and Raman spectroscopy.

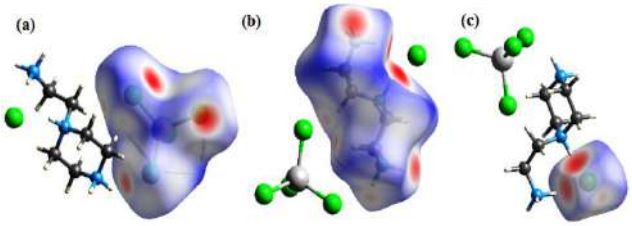

Fig. Hirshfeld surfaces mapped around the cation (a), the $ZnCl_4$ (b) and Cl^- moieties (c) with d_{norm}, the surface is shown as transparent to allow visualization of the orientation of subgroups of the asymmetric unit.

Key words: Zn(II) complex; X-ray diffraction; NMR spectroscopy, Ultraviolet-visible (UV–vis) spectroscopy, Hirshfeld surface analysis, Coordination compound.

Development of a low fluorine trifluoroacetate route to obtain $YBa_2Cu_3O_7$ films

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This communication is devoted to the growth through chemical solution deposition method of superconducting $YBa_2Cu_3O_7$ (YBCO) films. Low fluorine solutions are investigated because they are more ecofriendly when compared to the well-known standard trifluoroacetate (TFA) solutions. Also low fluorine solutions are promising in view to obtain thick films with high critical density currents. Direct thermogravimetric analysis on films and infrared spectroscopy reveals two consecutive thermal decompositions at 265ºC and 310 °C. We will show that using solutions with 20% fluorine, XRD analysis performed directly in films shows YBCO phase. Concerning superconducting properties, we have obtained one film with Tc and Jc (77 K) of 90 K and 4MA cm^{-2}.

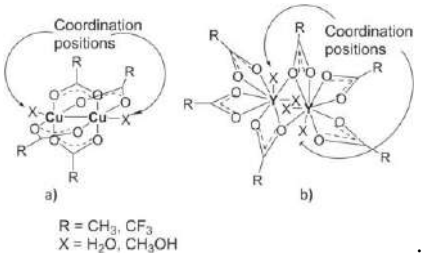

Fig. Representation of the coordination positions for (a) copper and (b) yttrium compounds in solution.

Key words: YBCO films, chemical solution deposition, low-fluorine solutions.

Synthesis, X-Ray crystal structure and highly non-linear optical properties of inorganic-organic hybrid compound: 1,4-Diazbicyclo-octane oxonium tri- nitrates single crystal.

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A new nonlinear optical hybrid crystal 1,4-Diazbicyclo[222]octane oxonium tri-nitrates (DOTN) [1]. The crystal was grown using water as solvent at room temperature and crystal structure was determined by X-Ray diffraction respectively, this title compound was shown to crystallize in non-centrosymmetric trigonal system with space group P31c. The recorded FTIR spectrum has proven the presence of various functional groups in the grown crystal as well as the formation of DOTN. Besides, the thermal stability and melting temperature of the DOTN crystal were identified from the TG/DSC analysis. The suitability of this material for optical application was studied by non-linear optical (NLO) and UV-Visible absorption techniques. Furthermore, the nonlinear optical property was analyzed by Kurtz-Perry powder technique and was 3.4 times than that of KDP (potassium dihydrogen phosphate) single crystals. The first hyperpolarizability of nitrate was determined by Second Harmonic light Scattering.

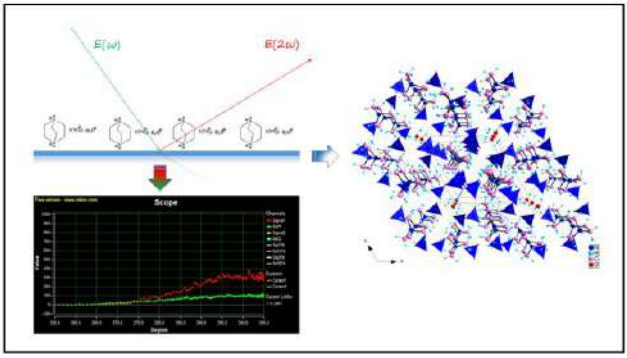

Fig. Graphical Abstract

Key words: Crystal structure, Optical materials, High nonlinearity

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THEORETICAL DFT STRUSTURAL STUDY OF BERYLLIUM CHLORIDE COMPLEXES WITH $(R_2N)_nP(O)F_{3-n}$

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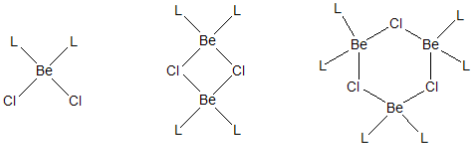
The synthesis and the experimental characterizations in solution by multinuclear NMR (^{31}P, ^{19}F and ^{9}Be) and by IR spectroscopy of the complexes of beryllium chloride with ligands $(R_2N)_2P(O)F(L)$ (R = Me or Et) [1] have shown the existence of several equilibrium species of $BeCl_2L_2$ (**1**), $Be_2Cl_2L_4$ (**2**) and $Be_3Cl_3L_6$ (**3**). The structures of the different adducts observed in solution were assigned by comparing them to the homologous complexes [2]. In this present work, we report on the theoretical structural study of beryllium complexes with fluorophosphoryl ligands of the type $(R_2N)_nP(O)F_{3-n}$ (R = Me or Et; n = 0-3) (**1-3**) by means of DFT/B3LYP/6-31G(d) geometry optimizations.



Key words: Beryllium complexes; phosphoryl ligands; DFT/B3LYP.

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ZrO_2 -SUPPORTED NANO-GOLD CATALYZED ONE-POT SYNTHESIS OF 3-METHYL-4-ARYLMETHYLENE-ISOXAZOL-5(4H)-ONES COMPOUNDS

GHANIYA FEAROUANI, NAWAL AMEUR,
CHEWKI ZIANI-CHERIF, REDOUANE BACHIR

Isoxazolones is an important five-membered heterocycle and synthon for being a core structural unit many biologically and pharmaceutically interesting molecules[1, 2], such as 1,3-oxazin-6-ones, pyrroles, imidazoles, tetrahydro-pyridines and pyridopyrimidines. Additionally, human and anti-fungal activities have also been identified in isoxazolone derivatives. Isoxazol-5(4H)-ones moieties have been used for the design of liquid crystals, merocyanine dyes in optical research, and photochromic compounds.[3],

The synthesis of 4-aryl-3-methylisoxazol-5(4H)-one derivatives was performed using a variety reagents and homogenous catalysts such as pyridine, sodium silicate, sodium benzoate, sodium azide, sodium saccharin sodium citrate, sodium sulfide, sodium ascorbate[4, 5].

In this work we study the activity of supported gold nanoparticles as heterogeneous catalyst for the Isoxazolone production.

So, we prepared Au/ZrO_2 by deposition precipitation with urea (DPU). The prepared catalyst was characterized by different methods: TEM, RD/UV-Vis, ICP and XRD. An important activity was obtained for this reaction and reach 90%.

Key word: Isoxazolones, gold, nanoparticles, zircona.

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Diallyl polythioethers in ruthenium complexes and alkene metathesis

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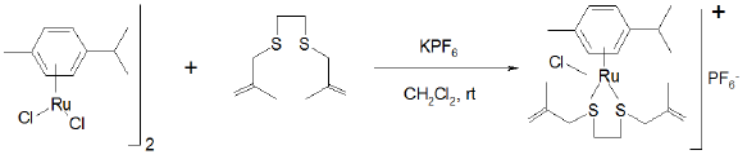
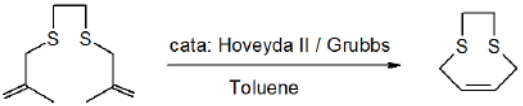
The substituted diallyl polythioethers have remarkable biological activities. For instance, they are excellent X-AND polymerase inhibitors. They have also antiviral and antibiotic properties. On the other hand, compounds having two or more sulfur atoms are particularly interesting for the synthesis of sulfur containing arene-ruthenium complexes that have potential applications in several areas such as homogenous catalysis, precursors of metallic nanoparticles or in the medicinal area[1]. In the present work, we report on the synthesis of new arene-ruthenium complex using a sulfur compound as ligand (Scheme 1).



Scheme 1

In another hand, the preliminary results of reaction of ring closing metathesis performed on these diallyl polythioethers in the presence of Hoveyda II or Grubbs catalysts are rather promising and show the formation of the RCM cyclic product and the formation of a sulfur containing monomer at room temperature (Scheme 2).



Scheme 2

Keywords: Diallayl polythioethers, arene-ruthenium complex, RCM

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Zinc chloride adducts with phosphine chalcogenides: A DFT study

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Zinc chloride adducts of the type $[ZnCl_2(Bu_3P{=}E)_2]$ (E=O, S and Se) have been theoretically studied by means of DFT geometry optimization (B3LYP, M05-2x and PBE0 functionals) and ^{31}P chemical shift calculations. In the complexes, the coordination mode is confirmed by a lengthening of P=E bond compared to that of the free ligands calculated at the same level of theory [1]. This lengthening is consistent with the lower stretching frequency observed in the IR. The binding energies of the complexes were also calculated for better accuracy and simultaneous description of Zn-E covalent coordination interactions. In addition and in order to quantify the nature of intermolecular interactions, the charge transfer zinc complexes, NBO and frontier MO shape analyses were carried out at the M05-2X/6-311++G(d,p) level of theory [2]. The NBO results show that the various kinds of donor–acceptor interactions favor the stability of this type of complexes.

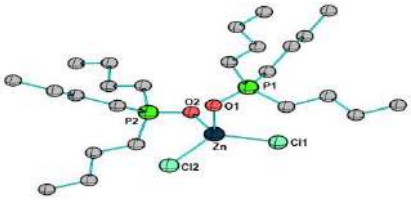

Fig. DFT optimized structures of $[ZnCl_2(Bu_3P{=}O)_2]$

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

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Production and characterization of activated carbon from orange peels by chemical activation with sulfuric acid

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The objective of the present work is the characterization of activated carbons obtained from orange peels that are vegetation wastes of the center of Tunisia. Activated carbons with optimal textural properties were prepared by using H_2SO_4 (50 wt. %) as a chemical activation agent with an imprenation ratioof 4, an impregnation time 2 h, a carbonization temperature of 550°C during 6h. Physicol-chemical properties of the materials were studied by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Nitrogen adsorption-desorption, X-Ray Fluorescence spectroscopy (XRF) and thermogravimetric analyses (TGA).

Key words: Activated carbon, orange peel, chemical activation

SYNTHESIS OF NEW FUNCTIONALIZED PHOSPHONATES MOLECULES AS POTENTIAL LIGANDS FOR METAL COMPLEXES

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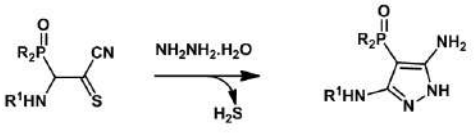
Heterocyclic compounds occur widely in nature and quite few of these are essential to life processes. The literature on hetrocyclic compounds is various with examples of an important number of synthetic methods of naturally occurring systems which are pharmacologically active[1]. Indeed, phosphonated molecules are used for various applications such as synthetic intermediates in organic chemistry and drug designed[2] hybrid materials[3]. In most cases, these systems have good metal coordination properties and coordination with metal through their phosphonate group. To extend the range of heterocyclic compounds synthesized in our laboratory, we report on new family of phosphonate-based ligands which were prepared by reaction between phosphonylated thioamides and hydrazine. The structures of all the newly prepared ligands were confirmed by spectroscopic NMR (^{1}H, ^{13}C and ^{31}P {^{1}H}) and elemental analyses). Furthermore, the preliminary coordination chemistry study towards tin (IV) chloride will be presented.



R	R¹
OMe, OEt	4-ClC$_6$H$_4$, 4-F- C$_6$H$_4$, c-Hex,

Fig: Structures of phosphonate-based ligands

Scheme: Synthesis of 3,5-diamino-4-phosphonopyrazoles

Key words: Heterocyclic compounds, phosphonated aminopyrazole, Ligands.

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The Synthesis of a new Functional Mixed-Metal MOFs

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Metal organic frameworks (MOFs) are among the most studied coordination polymers [1]. They are nanostructured materials resulting from the coordination bonding of metal-oxide units or metal ions with organic linkers. Consequently, they combine high levels of porosity with the functional properties of the metal moiety and/or the organic ligand. Thus, they have potential applications in the areas of sensor elaboration, stimuli-responsive materials design, opto-electronic devices development [1-3]…Furthermore, the recently reported synthesis of Mixed-Metal MOFs [4,5] is expected to endow them with new functionalities and to extend their fields of applications.
In this communication we describe the synthesis of a new Mixed-Metal MOFs with potential spin-crossover character. The prepared material was characterized by XRD, FT-IR spectroscopy and DSC.

Key words: Metal Organic Frameworks, Mixed-Metal MOFs, Smart materials

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Cyclotetraphosphate-controlled copper(II)-α-amino acid complex: Synthesis, crystal structure, characterization and properties

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Transition metal complexes of α-amino acids have been attracted much attention owing to their remarkable physical and chemical properties [1, 2]. In addition, they have interest in supramolecular chemistry and pharmacology because they could serve as model systems to enhance our understanding for the more complicated metalloproteins and biochemical processes as well as drug production [3, 4]. In this context, the design and self-assembly of metal complexes of α-amino acids have attracted several laboratories, including ours. We report here the synthesis and crystal structure of a cyclotetraphosphate-controlled copper(II)-α-amino acid complex formulated as $[Cu(L\text{-}arg)_2(H_2O)]_2(P_4O_{12}).8H_2O$. The spectroscopic properties of the title complex as well as the magnetic measurements are presented. The crystallographic study reveals that the complexation of copper(II) with L-arginine ligand in the presence of the oxo-anion $P_4O_{12}^{4-}$ provides one of rare example of binuclear complex $[Cu(L\text{-}arg)_2(H_2O)]_2^{4+}$ (Fig. 1.a). This latter has a *cis*-configuration wherein the two coppers, Cu(1) and Cu(2), were found in different environments and are linked into *syn–anti* equatorial–apical carboxylate bridge mode (Fig. 1.b). The former complex was found to be stabilized in the solid state through robust H-bonding interactions forming a 3D-supramolecular network which is built up of corrugated 2D-supramolecular layers, $\{[Cu(L\text{-}arg)_2(H_2O)]_2^{4+}\}_\infty$, and 1D-supramolecular anionic chain, $\{[P_4O_{12}(H_2O)_6]^{4-}\}_\infty$. Interestingly, this compound exhibits an antiferromagnetic interactions which are assigned to the *syn–anti* equatorial–apical carboxylate bridge, –Cu1–O_{ap}–C–O_{eq}–Cu2–, connecting the two copper(II)-ions at 6.246(1) Å with total bond length of 7.125 Å.

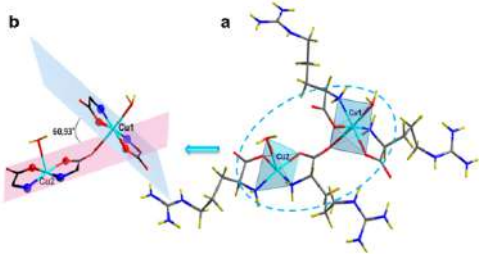

Fig. 1. (a) View showing the binuclear complex $[Cu(L\text{-}arg)_2(H_2O)]_2^{4+}$ and (b) Illustration of the coordination environment around the two Cu(II) metal centers.

Key words: L-Arginine, Copper(II), Cyclotetraphosphate, Binuclear complex, Crystal structure, Magnetism.

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The first self-assembly of a mixed-ligand coordination compound based on condensed phosphate and cyclam: Single crystal structure, Hirshfeld surface analysis and characterizations

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From the system Cu(II)-cyclam-condensed phosphate is isolated the first complex of {(H3O+)2[Cu(II)(μ-P4O12)(cyclam)]}n (1). This complex was characterized by X-ray diffraction (XRD), spectroscopy (diffuse reflectance, UV–Vis and FT-IR) and thermal analysis (DTA/TGA). Solved molecular structure of 1 revealed one rare 1D-anionic polymeric copper(II)-complex, {[Cu(II)(μ-P4O12)(cyclam)]2-}n (Fig. 1.a), involving two distinct ring ligands (cyclam/cyclotetraphosphate), in which a new coordination mode of the $P_4O_{12}^{4-}$ was observed. Counterions (H3O+) ensure the connection between 1D polymers by acting as donor in strong electrostatic H-bonds with P4O12 rings and thus leading to 2D-supromolecular frameworks (Fig. 1.b), arranged in -A-B-A- fashion. We present here Hirshfeld surface (HS) analysis in combination with 2D fingerprint plots to investigate the close intermolecular contacts (Fig. 1.c).

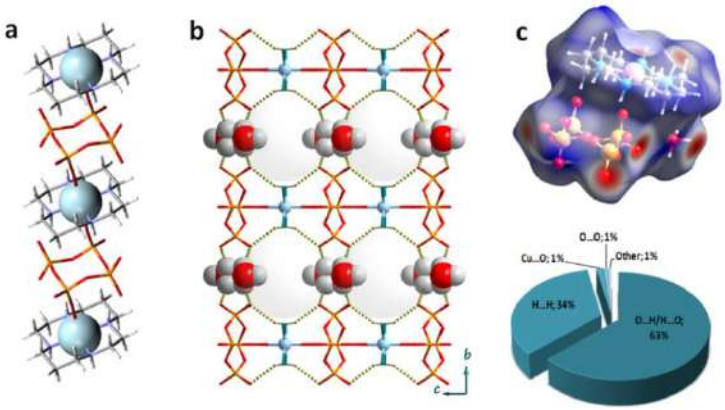

Fig. 1. (a) 1D-coordination polymer of {[Cu(II)(μ-P4O12)(cyclam)]2-}n extending along the c-axis, (b) Projection along a-axis of 2D-supramolecular layer. Carbon and hydrogen of the cyclam ligand are omitted for clarity, (c) HS mapped with dnorm. and the distribution of individual intermolecular interactions on the basis of HS analysis.

Synthesis, Combined X-Ray and Hirshfeld Surface Analyses, Optical and Biological Properties of a Decavanadate Core Templates with Organic cations

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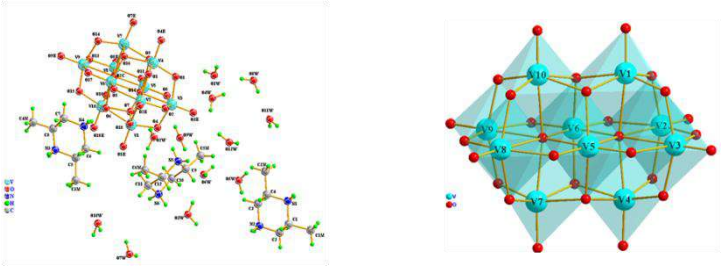
A hybrid decavanadate based material $(C_6H_{16}N_2)_3[V_{10}O_{28}].12H_2O$ (**1**) was obtained by reaction under mild condition at room temperature and characterized by means X-ray diffraction, IR, UV-Vis and fluorescence measurements (**1**) crystallizes in non-centrosymmetrical triclinic P_1 space group with a = 10.4255 (17) Å, b= 10.780 (3) Å, c= 13.6132 (19) Å and α= 101.854 (17)°, β= 100.302 (12)°, γ= 112.662 (18)°. The structural analysis revealed that three diprotonated $[C_6H_{16}N_2]^{2+}$ cations, twelve lattice water molecules and one decavanadate anion are associated through intricate N—H…$O_{decavanadate}$/OW, C—H…$O_{decavanadate}$/OW and OW—H…$O_{decavanadate}$/OW hydrogen bonds leading to the formation of 3D supramolecular network. Furthermore, the spectroscopic and optical properties of the compound have also been investigated showing important gap energy of 3, 72 eV and blue fluorescence. Its bioactivity has also been tested against gram (+) and gram (-) bacteria revealing a promising antibacterial activity.



(a) **(b)**

Fig. (a) Asymmetric unit of the title compound, (b) polyhedral view of the decavanadate cluster showing the VO_6 octahedra

Key words: Decavanadate. Synthesis. Fluorescence. Hirshfeld. Antibacterial activity

Encapsulation and complexation of iminium intermediate in water by calix[4]arene

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The detection and characterization of intermediates in organic reactions is crucial for the understanding of mechanisms and the rational optimization of reaction conditions.
As well as we know, the ability of covalent and self assembled hosts to squester a number of reactive species[1],we sought to use host (calix[4]arene sulphonaté)-guest (iminium intermediate) coordination chemistry as a novel means to encapsulate the intermediate iminium.
The meaning idea is to combine the propionaldehyde and ammonium salts in aqueous solution containing the host at neutral PH ;

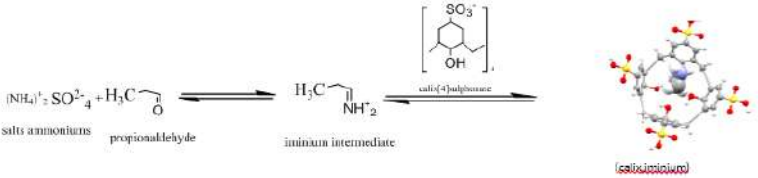

Fig. suggestion of iminium ion encapsulation generated from propionaldehyde and ammoniums salts in water

Key words: encapsulation, coordination chemistry, calix[4]arene, iminium intermediate

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Crystal structures, spectroscopic investigations and physical properties of novel β,β'-keto-bisphosphineoxydes and sulfides

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White light emitting diodes (WLEDs) made from blue or near-ultraviolet (n-UV) LEDs made with phosphors have been attracting much attention for their high luminous efficiency, low energy consumption, good durability and safety [1-3]. This particularity make the study and the exploration of new phosphorus derivatives to get deeper understand to its morphologies and physical properties very interesting and challengeable.
More recently, we have reported on the first synthesis of α,α'-bis(diphenylphosphoryl) and α,α'-bis(diphenylphosphorthioyl)-cycloalkanones [4]. However, satisfying yield and accepted size single-crystals of most of the derivatives prompted us for further investigation.
Herein, multinuclear NMR investigations (IR, UV-Vis., ^{1}H, ^{13}C and ^{31}P), crystal structures and physical properties (PL, EDX, ATG...) of three bisphosphorylated cyclic ketones (2,6-bis(diphenylphosphoryl)cyclohexanone (**1a)**, 2,6-bis(diphenylphosphoryl)-4-methylcyclohexanone (**2a)** and 2,5-bis(diphenylphosphorothioyl)cyclopentanone (**3a**) are reported and discussed.

Keywords: Crystal structure, multinuclear NMR studies, physical properties.

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Studies of surface potential and charge transport in 6,13-bis(triisopropylsilylethynyl) pentacene organic thin film phototransistor

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The effect of white light illumination on the surface potential and charge transport in 6,13-bis(triisopropylsilylethynyl) pentacene (TIPS-pentacene) organic thin film transistor is investigated theoretically. In this work, we present a physical model for OTFTs based on variable range hopping theory (VRH) to demonstrate the Gaussian density of states distribution, the surface potential and the carrier transport in TIPS-pentacene TFT under dark and white light illuminations. Based on the developing model, a variety of applied light intensity and gate voltage dependencies of the surface potential can be well described. The White light illumination effect can remarkably enhance the density of states, the surface potential and effectively the charge carrier transport at high gate voltages.

Key words: Surface potential, VRH theory, TIPS-pentacene, Phototransistor.

PARTIAL OXIDATION OF METHANE TO SYNGAS OVER CO-PRECIPITATED Ni/Mg-Al CATALYSTS

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Ni/Mg-Al catalysts, prepared by Co-precipitation method and characterized by different techniques (DRX, BET, TPR, FTIR), 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) [1, 2]. On the other hand, the addition of copper remarkably improved the catalytic performances of the Ni/Mg-Al solids in POM reaction.

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

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COMPLEXES ORGANOMETALLIC CONTAINING PHOSPHONAT MOIETY EXPERIMENTAL AND DFT STUDIES

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In recent years, there has been a rapid expansion in research and development of novel metal-based drugs to improve clinical effectiveness, reduce general toxicity and broaden the spectrum of activity. However the choice of a suitable ligand is crucial in the design of new bioactive metal complexes and one promising strategy is coordination of the metal moiety to naturally occurring and/or bioactive ligands [1].

The introductions of phosphate moiety in sulfonamides molecules improve bioavailability and biological activities of resulting compounds [2].

The aim of this work is to study the resulting complexes between the ligand and some metallic ions such as Cu^{2+}, Co^{2+}, Zn^{2+} and the Ni^{2+} ions (Fig1).

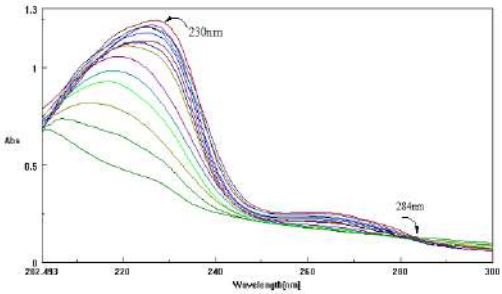

Fig 1: Absorption spectra of 10^{-4} M Cu (II) in methanol solution with a 10^{-3} M solution of Phosphonoethylsulfonamide.

The complexes formation was studied in solution and in solid state. The stability constants, in methanol with ionic strength of 0.1 M KCl and at 25±1°C, and species distribution were calculated using a non-linear least-square fitting program.

In order to gain further insights into the interaction ligand –ion in this system the 1:1 and 1:2 complexes have been optimized by using DFT (B3LYP/ 6-311(d, p) ++) level of theory.

Keyword: sulfonamides, complexes, metal ions, studies in solution, molecular modeling.

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Acid Reactive Dye removal from aqueous solution by natural and low cost materials as solution to water protection and reuse

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Many industries such as paper, food, cosmetics, textiles etc. use dye in order to colour their products. The presence of these dyes in water even at very low concentration is highly visible and undesirable[1]. Colour is the first contaminant to be recognized. The heterogeneous Fenton process offers a good potential to remove colour from wastewater[2] using natural iron-ores as the catalyst. The iron-ore wish is not toxic compound and causes no secondary pollution in the environment[3] was defined and characterized in this study. The structural and textural properties of natural catalysis have been determined by X-ray diffraction, nitrogen adsorption-desorption isotherms, X-ray fluorescence and infrared spectroscopy. Also, adsorption properties were determined to assess dye distribution between solid and aqueous phases and to investigate the effect of contaminant sorption on the catalytic oxidation. The adsorption-desorption isotherms of all samples are a type IV isotherm with a hysteresis loop. The most probable values of samples pore size are about 2 nm indicating they are microporous materials. XRD analysis shows that the same diffraction peaks have appeared in the XRD spectra of the two samples. Some diffraction is related to the presence of goethite, hematite and magnetite iron phases. In order to identify the functional groups of MF and MF01, FT-IR analysis was performed. Various functional groups represented in the IR spectra were the same as that of goethite. Adsorption tests show a high sorption ability of dye on catalyst surface. Regarding their physical and chemical properties, natural iron-ore will be utilized as a heterogeneous catalyst in Fenton process.

Key words: iron-ore, heterogeneous catalyst, adsorptive properties, Fenton process

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ENZYMATIC SYNTHESIS OF MONOLAURATE D-XYLOSE IN IONIC LIQUIDS. REUSABILITY OF CAL B.

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Sugar fatty acid esters are non-ionic surfactants with wide range of commercial applications in particular the cosmetic industry, food and pharmaceutical industries.Their synthesis were performed either by chemical means or enzymatic route. The enzymatic method allows to perform these reactions in the experimental conditions much milder in temperature, pH and solvent. During these last years, ionic liquids have emerged in the field of biocatalysis as an alternative to organic solvents, ionic liquids allow to increase considerably the activity and the enzyme stability in particular the case of acylation reactions[1]. On the other hand, the ease reusability of the biocatalyst which is an important parameter to consider for the reduction of industrial costs.
In this context, we have synthesized the monolaurate D-xylose by enzymatic esterification in the ionic liquids, in the presence of the lipase of *Candida antractica B* (CAL B) immobilized on resin to 60°C during 72h. We reported a study of the parameters that affect the enzymatic activity in the reaction of esterification of D-xylose (solvent, molar ratio Sub/Al, the reuse of the CAL B). Good performance have been recorded in the [Bimim][BF4] as a solvent with a 1:2 molar ratio of the substrate by report to the lauric acid. The CAL-B to presented loss of activity after four cycles**.**

Key words: Sugar ester, esterification**,** lauric acid, lipase**,** ionic liquids.

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Degradation of tyrosol by a novel electro-Fenton process using pyrite as heterogeneous source of iron catalyst

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Tyrosol (TY) is one of the most abundant phenolic components of olive oil mill wastewaters. Here, the degradation of synthetic aqueous solutions of 0.30 mM TY was studied by a novel heterogeneous electro-Fenton (EF) process, so-called EF-pyrite, in which pyrite powder was the source of Fe^{2+} catalyst instead of a soluble iron salt used in classical EF. Experiments were performed with a cell equipped with a boron-doped diamond anode and a carbon-felt cathode, where organics were destroyed by hydroxyl radicals formed at the anode surface from water oxidation and in the bulk from Fenton's reaction between Fe^{2+} and H_2O_2 generated at the cathode. Addition of 1.0 g dm^{-3} pyrite provided an easily adjustable pH to 3.0 and an appropriate Fe^{2+} content to optimize the EF-pyrite treatment. The effect of current on mineralization rate, mineralization current efficiency and specific energy consumption was examined under comparable EF and EF-pyrite conditions. The performance of EF-pyrite was slightly superior due to self-regulation of soluble Fe^{2+} by pyrite. The TY decay in this process followed a pseudo-first-order kinetics. The absolute rate constant for TY hydroxylation was 3.57 10^9 M^{-1} s^{-1}, as determined by the competition kinetics method. Aromatic products like 3,4-dihydroxyphenylethanol, 4-hydroxyphenylacetic acid, 4-hydroxybenzoic acid, 3,4-dihydroxybenzoic acid and catechol, as well as o-benzoquinone, were identified by GC-MS and reversed-phase HPLC. Short-chain aliphatic carboxylic acids like maleic, glycolic, acetic, oxalic and formic were quantified by ion-exclusion HPLC. Oxalic acid was the major and most persistent product found. Based on detected intermediates, a plausible mineralization pathway for TY by EF-pyrite was proposed.

Key words: Electro-Fenton; Heterogeneous catalysis; Hydroxyl radicals; Pyrite; Tyrosol; Water treatment.

Luminescence On-Off Switching via Reversible Aurophilic Interactions

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The reaction of 2-benzimidazolethiol (BIT) with $Au_2(dppp)(CF_3CO_2)_2$ (dppp = bis(diphenyl-phosphino)propane) in CH_2Cl_2 yields a $Au_2(dppp)(BIT)_2 \cdot 2\ CF_3CO_2H$ (**1a**). The successive addition of a base to **1a** solution produces the acetate-free form of $Au_2(dppp)(BIT)_2$ (**1b**). **1b** shows markedly different structural characteristics from those of **1a**. **1b** actually crystallizes as 1D polymers held together by an intermolecular aurophilic interaction of 3.1586(5) Å, in contrast to intramolecular aurophilic **1a** (3.1312(5) Å).[1] The most interesting feature is the reversible interconversion between inter- and intramolecular aurophilic interactions via the pH condition. A dramatic change of photoluminescence occurs as a function of the exposure time of trifluoroacetic acid and triethylamine in chamber. Exposure of the neutral complex to CF_3CO_2H vapor leads slowly to a loss of luminescence. This process is reversed upon exposure to NEt_3 vapor. The process can be carried out repetitively with no loss of emission intensity. In conclusion, reversible interconversion between inter- and intramolecular Au···Au interactions induces luminescence on/off switching. For the gold(I) photoluminescence system, intermolecular aurophilic interaction is a more significant factor than intramolecular aurophilic interaction.[2]

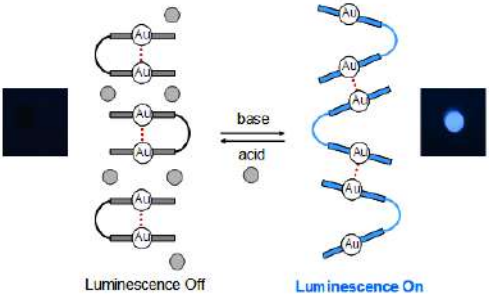

Fig. Luminescence on-off switching system

Key words: Molecular switch, Reversible aurophilicity, Luminescence

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Synthesis, structures and magnetic properties of dimeric copper and trimeric cobalt complexes supported by bridging cinnamate and chelating phenanthroline

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The synthetic and structural chemistry of metal–organic frameworks are fast developing areas of research beaming at the rational design of novel materials for potential applications in fields ranging from catalysis, gas storage, separation, and chromatography.[1]Their physical properties, such as magnetism, proton conduction, dielectricity, and optics are also of major interests. One of the basic rules in the synthesis is the use of multitopic organic ligands to connect metal centers through coordination bonds. We present in this poster, two polynuclear transition-metal complexes,$[Co^{II}_3(cinna)_6(phen)_2]$**(1)**,$[Cu^{II}_2(cinna)_2(phen)_2(NO_3)(H_2O)].NO_3.CH_3OH$ **(2)**, where cinna = trans-cinnamate, PhCH = $CHCO_2^-$ and phen = 1,10-phenanthroline, have been synthesized and characterized by elemental analyses, infrared spectroscopy, single-crystal X-ray diffraction (XRD) and magnetic measurements. **1** contains two independent geometrical isomers of $[Co^{II}_3(cinna)_6(phen)_2]$, where the cobalt atoms form a linear spine bridged by carboxylate from cinnamate radiating perpendicular to it, the 1,10-phenanthroline chelating the ends. **1** behaves as a paramagnet due to the absence of magnetic exchange between the trimers in the absence of chemical bonds between trimers. **2** contains a positively charged dimer of copper ions bridged to two cinnamate in syn–syn mode with two almost parallel phenanthroline molecules chelating the two copper ions, while a water molecule and one $NO3^-$ coordinate their axial positions. The exchange coupling within the doubly- bridged copper atoms is antiferromagnetic (J = -153(1) K). [2]

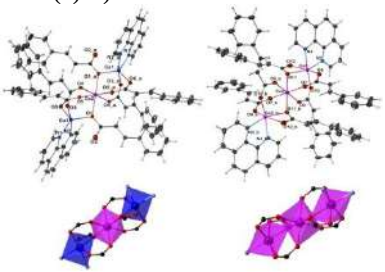

Fig. ORTEP and polyhedral views of $1[Co^{II}_3(cinna)_6(phen)_2]$.

Key words: Trans-cinnamic, 1,10-phenanthroline, Magnetism, Metal complexes.

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STRUCTURING AGENT EFFECTS ON THE SYNTHESIS OF ALUMINOPHOSPHATE-TYPE NANOCRYSTALS

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The aim of this synthesis of crystals of zeolites (1) with a core of different composition to that of its peripheral layer is of great interest to researchers and industrialists, as evidenced by the recent literature. However, this conservation of the crystal structure does not allow the elaboration of a material combining the advantages of two distinct crystal structures. Therefore, the aim of this part of this work was to study the processes of formation of core-shell materials (2) and to define the factors controlling them. After studying the conventional ways of forming such compounds, we will investigate the possibility of using aluminophosphate nuclei in order to obtain a continuous and uniform layer on core crystals. Finally, the materials prepared would be selected according to their structures (porosity), morphologies (nanocrystals), textures (microcomposites) and chemical compositions (isomorphic substitution), to be tested in the formation of active antibiotics against negative and positive germ microbes (Esherichia paris (3), pseudomonas, etc.) such as cephalosporins (4).

Keywords: aluminophosphates, catalysis, penicillin, oxidation. Nanocrystals

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Comparison of Aluminophosphate Catalysts for the Preparation of Cephalosporin from Penicillins

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In this study, aluminophosphate catalysts ALPO4-5 [1], SAPO4 -5, SAPO4 -34, SAPO4 -37, SAPO4 -44, CoAPO4 -5 [2], which were tested in the transformation of Penicillin into cephalosporin.
The transformation of penicillin [3] V potassium into cephalosporin [4] is carried out by various steps: protection of the sulfide function, esterification and finally the final transformation.
Comparison of the biological activities of the products formed with those of penicillins confirms the formation of these antibiotics [5].
We will examine the cristanilite of non-materials by different DRX, FT-IR and NMR methods.

Keywords: aluminophosphates, catalysis, penicillin, oxidation.

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SYNTHESIS AND STRUCTURAL STUDY OF A NEW CADMIUM AND POLYAZOLE COORDINATION POLYMER

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In recent years, the design and synthesis of metal-ligand coordination have been attracted great interest during the past decades because of their potential applications in the fields of gas storage, molecular magnetism and luminescence.[1-3] A lot of works have been devoted to the design of suitable organic ligand to construct new coordination polymers. Among the reported studies, it is an especial attractive area that coordination polymers are build by the organic ligands of polyazol groups because this ligands can adopt a variety of coordination modes.The tetrazole functional group has found a wide range of applications in coordination chemistry as ligands, in me- dicinal chemistry as a metabolically stable surrogate for a carboxylic acid group, and in materials science as high- density energy materials.[4]

The compound : catena[azido 5-(2-pyridyl tetrazolato) aquacadmium(II)], (2-PTZ AZ was obtained through the in-situ hydrothermal reaction.

Figure 1 gives the solid state structure of the polymer, in that the local coordination geometry around the Cd center can be best described as a slightly distorted octahedron, with four plan nitrogen atoms from two 2-PTZ ligands and equatorial water and nitrogen atom of azido.

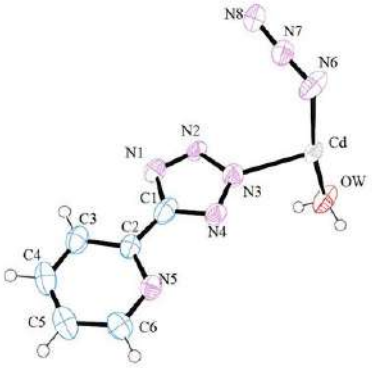

Figure1 : Representation Ortep of the coordination polymer

Key words: coordination complexes, X ray diffraction, Polyazoles

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ZINC-BASED HETEROPOLYSALS FOR A CLEAN SYNTHESIS OF ADIPIC ACID

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This study is of an ecological interest, it consist of a new route to a green synthesis of adipic acid (AA). With a production capacity of> 2Mt /year and as a primary precursor for the manufacture of nylon 6,6, polyurethane plastics, AA is a key intermediate for the industry. It is usually prepared by the oxidation of cyclohexanol and cyclohexanone using nitric acid (50-60%). The major problem of this process is the formation of nitrous oxide N_2O (400,000 t / year), which has a greenhouse effect of 200 times more dangerous than carbon dioxide, it's also a powerful ozone depleting agent.

To work around these disadvantages, our work uses polyoxometallates (POMs), molecular oxides with numerous properties, notable catalysts, which have proved their efficiency in many reactions.

The aims of this present are: first, synthesis by a cationic exchange method of zinc-based heteropolysals with formula of $Zn_xH_{3-2x}PMo_{12}O_{40}$ (x=0-1.5). Next, evaluation of their structural and textural characterization in order to confirm the reliability of the synthesis and the purity of the solids. Finally, the catalytic properties of the salts are examed in the oxidation reaction of cyclohexanone to adipic acid under mild and solvent-free conditions.

Interesting results (57% in AA) were obtained in the presence of this family of salts under moderate operating conditions with H_2O_2 as oxidant. This study can be a successful initiative interesting both ecologically and economical to clean adipic acid production.

Key words: Adipic acid, hydrogen peroxide, POMs, Zn materials, green chemistry, catalysis, environement.

Electrochemical and Spectroscopic characterization of Cadmium(II) complex with Bis(tetraethylthiophosphoramidoyl)methylamine

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The coordination chemistry of the imidodiphosphorus acids of type $\{(XPR_2)(YPR'_2)\}NH$ (X,Y: O,S,Se; R,R' : alkyl, aryl) has become an active area of research due to their selective complexation properties towards 'hard/soft' metal cations [1]. In contrast, a little attention has been paid to the coordination chemistry of the neutral ligands of the type $RN\{P(E)R'_2\}_2$ and few examples of their complexes have been described in literature [2]. In this work, we present a new complex Cd(II) with neutral bidentate ligand, bis(tetraethylthiophosphoramidoyl)methylamine, $MeN[P(S)(NEt_2)_2]_2$. The electrochemical and spectroscopic studies reveal that the bis(tetraethylthiophosphoramidoyl)-methylamine is able to bind the cation Cd^{2+} and indicate the 1:2 metal-ligand stoichiometry of the formed complex. A great anodic potential shift in the oxidation peak of the ligand was observed during the cadmium chelation process confirming the high stability and the strong interaction between Cd (II) and sulfur atoms presented in the ligand.

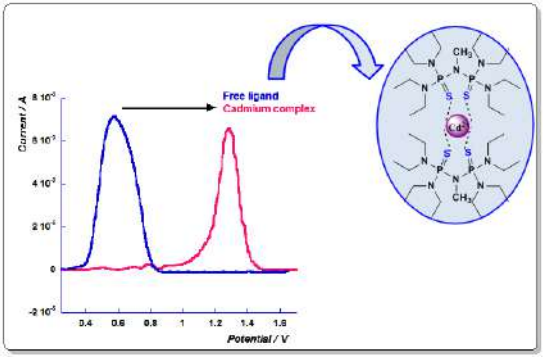

Fig. Potentiometric response of the cadmium(II) chelation process

Key words: Cadmium complex, neutral bidentate ligand, NMR spectroscopy, voltammetry technique

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Imidazolium-based ionic liquid type dependence of the bending response of polymer actuators

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Actuators based on polymer blends of poly(vinylidene fluoride) (PVDF) with 40% of different ionic liquids (IL) are prepared by solvent casting. [C2mim][Cl], [C6mim][Cl], [C10mim][Cl], [C2mim][NTf2], [C6mim][NTf2] and [C10mim][NTf2] were selected in order to evaluate the effect of anion and cation sizes in the bending properties. The microstructure, mechanical and electrical properties of the blend depend on the IL type, which in turn leads to a different bending response. In particular, the mechanical properties are independent on the IL type but the AC conductivity of the composites depend more on the anion type than on the size of the alkyl chain connected to the imidazolium based cation. Thus, the bending response of the IL/PVDF composites is correlated with the anion and cation sizes and a maximum bending response of 0.3% is achieved for a 10 V square signal in the IL/PVDF composite with 40 wt% content of [C2mim][NTf2].

Key words: PVDF, Ionic liquid, Actuator, Electrical conductivity, Bending

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Synthesis and characterization of two novel inorganic/organic hybrid materials based on polyoxomolybdate clusters: $(C_5H_5N_5)_2(C_5H_6N_5)_4[(HAsO_4)_2Mo_6O_{18}].11H_2O$ (I) and $Na_2(Himi)_3[SeMo_6O_{21}(CH_3COO)_3].6H_2O$ (II)

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Polyoxometalates (POMs) have been a center of research interest for a long time, as they exhibit a great variety of structures and rich diversity of remarkable properties [1]. In the past decades, an important advance in polyoxometalate chemistry is the polyoxometalates-based organic-inorganic hybrid materials [2].
Two new organic-inorganic hybrid compound, $(C_5H_5N_5)_2(C_5H_6N_5)_4[(HasO_4)_2Mo_6O_{18}].11H_2O$ (I) and $Na_2(Himi)_3[SeMo_6O_{21}(CH_3COO)_3].6H_2O$ (II) were synthesized and structurally characterized by scanning electron microscopy (SEM), elemental analyses, FTIR, UV spectroscopy, thermal stability analysis, XRD and single crystal X-ray diffraction. Crystal data: (I) triclinic system, space group P-1, a = 11,217 (9) Å, b = 11,637 (8) Å, c =14,919 (8) Å, α = 70,90 (5), β=70,83 (2), γ = 62,00(1) and Z = 1; (II) triclinic system, space group P-1, a =10.6740(1) Å, b =10.6740(1) Å, c = 20.0570(1) Å, α=76.285(1), β=82.198(2), γ= 87.075(1) and Z = 1.

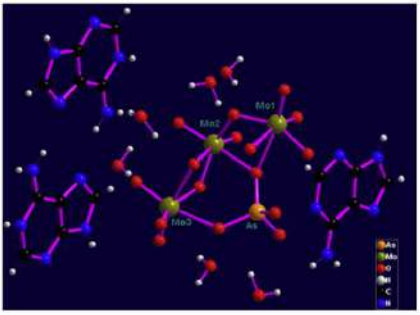

Fig. 1. The asymmetric unit of $(C_5H_5N_5)_2(C_5H_6N_5)_4[(HAsO_4)_2Mo_6O_{18}].11H_2O$

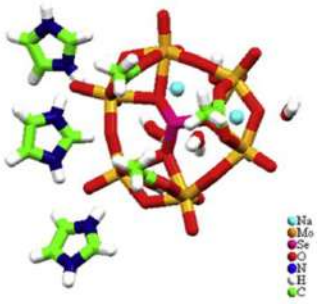

Fig. 2. The asymmetric unit of $Na_2(Himi)_3[SeMo_6O_{21}(CH_3COO)_3].6H_2O$

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Synthesis and structural characterization of a new polyoxovanadate $(C_4H_{10}N)_4.H_2V_{10}O_{28}.2H_2O$

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A new organic-inorganic compound based on decavanadate clusters $(C_4H_{10}N)_4.H_2V_{10}O_{28}.2H_2O$ have been isolated by conventional solution method and structurally characterized by single-crystal X-Ray diffraction method, scanning electron microscopy (SEM), IR spectra thermogravimetric analysis (TGA) and cyclic voltammetry measurements. This compound crystallized in the triclinic (P-1) symmetry a=11.792(6) Å, b=13.335(6) Å, c=14.117(6) Å, α=78.366(4), β=65.815(4), γ=84.725(4) and is based on dihydrogen-decavanadate(V), $[H_2V_{10}O_{28}]^{4-}$ and pyrrolidinium cation.

Single-crystal X-ray reveals that the asymmetric unit is constructed from one hydrogenodecavanadate polyanion $(H_2V_{10}O_{28})^{4-}$, four cations pyrrolidinium $(C_4H_{10}N)^{+}$ and two water molecules.

The decavanadate polyoxoanion display a cage likes structure, composed of ten $\{VO_6\}$ octahedral by edge and corner sharing. Each two $\{VO_6\}$ units from above and below share the equatorial oxygens at the apexes of the octahedral in the rectangle. Similarly, the other 6 vanadium atoms in equatorial plane also form the $\{VO_6\}$ units sharing the oxygen atoms form above and below this equatorial plane.

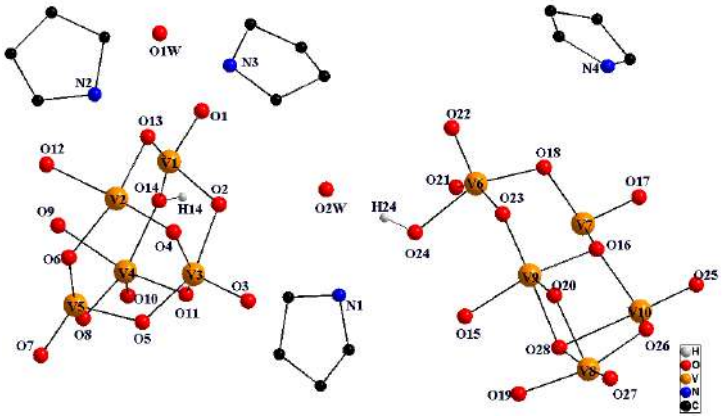

Fig. The asymmetric unit of $(C_4H_{10}N)_4.H_2V_{10}O_{28}.2H_2O$

MANGANESE-COBALT MIXED SALTS FOR GREEN SYNTHESIS OF ADIPIC ACID

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In the context of sustainable chemistry, alternative oxidizing systems more ecological such as hydrogen peroxide (H_2O_2) have appeared to replace conventional oxidizing systems little respectful of the environment. The latter is the preferred oxidant of industrialists. Indeed, in addition to being relatively non-toxic, easy to manipulate, its decomposition leads only to water as a by-product. On the other hand, its use as a substituent for nitric acid in the process of adipic acid production via cyclohexanone oxidation also requires an acidic medium. This acidity constitutes another source of pollution, as it is generally caused by organic or mineral acids, which have negative consequences on the environment due to corrosion and toxicity phenomenons.

The use of Keggin type polyoxometallates (POMs) as catalyst is a potential way for dealing with these disadvantages [1-3]. Indeed, they are of bifunctional nature (acid and redox). Thus, the acidity and the oxidizing properties necessary for the substrate oxidation could come only from the POM.

This study is an attempt to substitute nitric acid in the conventional (industrial) process for the production of adipic acid (AA) by a combination of Keggin mixed salts $H_{3-2(x+y)}\ Mn_xCo_yPMo_{12}O_{40}$ with $x + y = 3/2$ denoted $Mn_xCo_yPMo_{12}$, which are clean, non-toxic and non-corrosive catalysts, easy to prepare and oxygenated water as oxidant via the oxidation of cyclohexanone in free solvent. The effect of some operating conditions and the POM composition on AA yield were examined.

Promising results were obtained in the presence of the $Mn_{0.25}Co_{0.75}PMo_{12}$ catalyst system (61%) under very mild favorable economical and ecologically operating conditions.

Key words: Keggin-type mixed salts, Oxidation, Hydrogen peroxide, Cyclohexanone, Adipic acid.

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Binding properties of Some New Azo Dyes Derived from 4-Hydroxycoumarin

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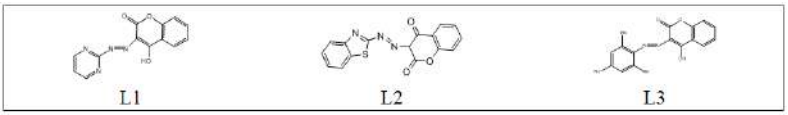
Azo compounds are a class of chemical compounds that are continuously receiving attention in scientific research[1]. Nowadays, synthetic azo compounds are widely used in different application fields, such as medicines, cosmetics, food, paints, plastics, shipbuilding, automobile industry, cable manufacture, etc [2]

In this work, we present our contribution to the study of the complexation and extraction of some transition metal cations have been followed by UV-visible spectrophotometry absorption. The conductivity studies have been used in order to confirm complex's stoichiometries.



Title: Chemical structural of ligand used

Key words: Synthesis; conductivity; binding properties; complexation; extraction

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Formation of binuclear neutral Copper(II) complexes based on *p-tert*-butyl- calix[4]arene and thiacalix[4]arene in *1,3*-Alternate conformation bearing four catechol at their lower rim

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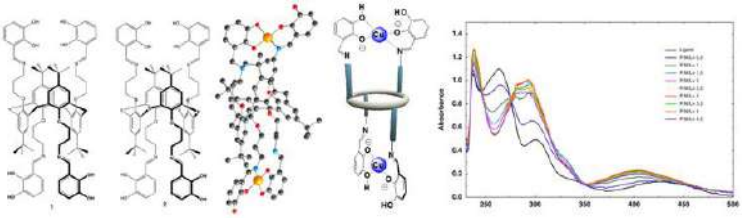
Binding of metal cations by calixarene derivatives in solution as well as in the solid state has been widely studied.[1] In particular, derivatives bearing mainly at the lower rim peripheral coordinating sites such as nitrile,[2] carboxylate,[3] or pyridyl units[4] have been used to generate a variety of 1-, 2- and 3-D coordination networks in the presence of Ag^{+} or Hg^{2+} cations for example. In this contribution, we report the synthesis, characterization in solution and in the solid state of ligands **1** and **2** (CA and TCA successively) backbones in *1,3*-Alternate conformation bearing four imino-catechol units. The solid-state behaviour of both ligands **1** and **2** towards binding of Copper(II) was investigated. Furthermore, we describe the propensity of ligands **1** and **2** to bind transition metals M (M = Zn, Cu, Ni and Co) in the oxidation state II, in solution, affording binuclear complexes.



Key words: calix[4]arene, thiacalix[4]arene, iminocatechol, copper(II).

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Removal of VOCs vapors using Faujasite zeolite synthesized from instratified Illite-Kaolinite Tunisian clay

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In last decades, air pollution problem have become more and more frequent and dangerous. BTEX represent one of the most important categories of air pollutants due to their toxic and carcinogenic properties. Atmospheric emissions of these volatile organic compounds (VOCs) from industrial plants and motor vehicle can cause serious environmental problems. They are toxic and carcinogenic to human health. There are many processes to resolve this problem: adsorption, condensation, absorption... The most commonly used process is adsorption for which adsorbents are of high specific surface areas and possibility to be used in many cycles as needed. Pore size, pore distribution and surface area are the major factors in the adsorption process. Zeolites are a class of porous materials which meet these requirements thanks to their high specific surface areas, stability even after many adsorption cycles, they are easily recovered and they exhibit capacities which enormously exceed that of commonly used adsorbents. The present study reports the preparation and characterization of Faujasite type zeolites from Tunisian clay material. The aim of the study was to determine the feasibility of using these materials in adsorption process of BTEX vapors from waste gas streams. The results of characterization showed that the raw clay was activated completely after fusion with NaOH and a pure phase and highly crystalline faujasite zeolite was obtained after 24 h of crystallization at 60°C with high specific surface area (360 m^2/g)in contrast with the raw clay material (50 $m^{2/}$g). The obtained results showed also that the synthesized zeolite exhibits effective adsorption for VOCs vapors, with adsorption capacities in the order xylene > toluene> benzene in a single component system and the adsorption capacity in the case of p-xylene reached 9 mg/g. The equilibrium data have been fitted using Freundlich and Langmuir equation model.

Key words: BTEX, adsorption, zeolite, clay.

Diorganotin dihalides complexes with new functionalized mono- and bisphosphonates

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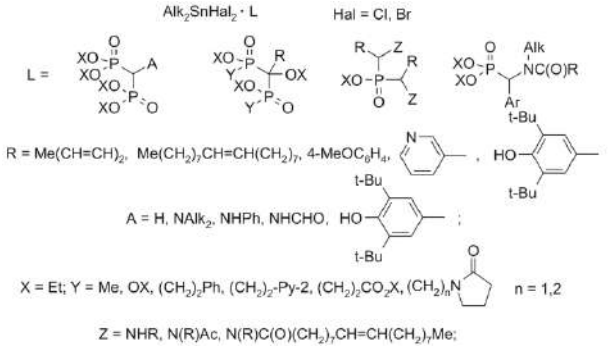
Functionalized organophosphorus acids and their derivatives with heterocyclic and unsaturated fragments are of great interest as effective chelating ligands, perspective bioactive substances, and well-known organophosphorus biomimetics of hydroxy (amino) acids or natural pyrophosphates[1]. The series of diorganotin dihalides complexes with new functionalized mono- and bisphosphonates are synthesized by us and characterized *via* NMR spectroscopy and X-ray structural analysis. We have developed the convenient methods of synthesis of new functionalized mono- and bisorganophosphorus acids and their derivatives using as starting compounds the trimethylsilyl esters of several trivalent phosphorus acids and functionalized alkenes, aldehydes, and carboxylic acids. The obtained complexes are presented below.



The complicated complexes of diorganotin dihalides with functionalized mono- and bisphosphonates possess antitumour and antioxidant activities with multifactor mode of action[2,3]. This work was supported by the Russian Foundation for Basic Research, grants 15-03-00002 and 17-03-00169.

Key words: diorganotin dihalides, mono- and bisphosphonates, complexes

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New Complexes of Biogenic Metals with Mono- and Bisorganophosphorus Proline Derivatives

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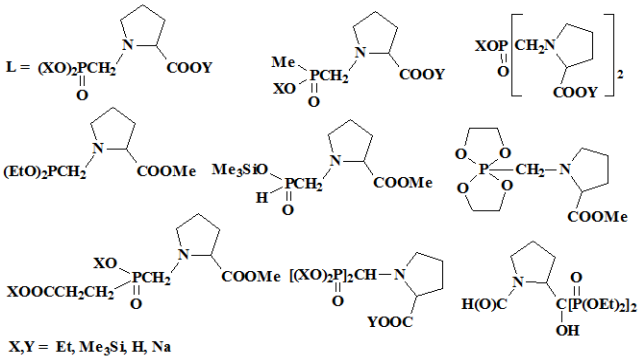
The functionalized organophosphorus derivatives of aminocarboxylic acids and their corresponding peptides are the perspective organophosphorus biomimetics of natural phosphates and hydroxy or amino acids. These compounds with nonhydrolysable P-C bonds interfere with various enzymatic processes and possess the antibacterial, antiviral, antitumor and enzyme inhibitory properties. Several organophosphorus containing peptides with proline moieties have attached attention in the capacity of the competitive inhibitors of human immunodeficiency virus protease [1]. Previously the series of diorganotin dihalides complexes with new functionalized mono- and bisphosphonates are synthesized by us and characterized via NMR spectroscopy and X-ray structural analysis [2,3]. We have synthesized the new complexes of biogenic metals with mono- and bisorganophosphorus proline derivatives with P-C-N moieties.



This work was supported by RFBR (grants 15-03-00002 and 17-03-00169).

Key words: organophosphorus proline derivatives, biogenic metals, complexes

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Synthesis, characterization and antibacterial activity of N-benzimidazole-O-acetyl-chitosan

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A novel chitosan derivative, N-benzimidazole-O-acetyl-chitosan (BZMACH) was prepared in acid acetic solution from imidate N-benzimidazole and shrimp-shell chitosan. The chemical structure and physical properties of BZMACH were characterized by FTIR, 1H NMR, DSC, TGA and XRD techniques. Besides, an enhancement of the antibacterial activity of chitosan against *Salmonella typhimurium* and *Pseudomoenas aeruginosa* bacteria has been also observed with this modification.

Key words: Chitosan, N-Benzimidazole-O-acetyl-chitosan, Characterization, antibacterial activity.

Synthesis and crystal structure of a novel inorganic-organic hybrid, [2,2'-(ethylenedioxy)bis(ethylammonium)]$ZnCl_4$

Ali Rayes,[a] Francesco Mezzadric[b] and Gianluca Calestanic[b]

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We report in this work the preparation, structural study and spectroscopic characterization of a novel organic-inorganic hybrid compound, 2,2'-(ethylenedioxy)bis(ethylammonium) tetrachloridozincate, $[C_6H_{18}N_2O_2]ZnCl_4$. This compound crystallizes in the triclinic system with the space group P-1 (No. 2), with cell parameters a = 7.147 (2) Å, b = 8.191(3) Å, c = 13.113(4) Å, α = 76.880 (4)°, β = 78.271(5)°, γ = 85.377(5)°, Z = 2 and V = 731.5 (4) $Å^3$. The structure contains isolated and perfectly packed $ZnCl_4$ tetrahedrons, which is stabilized via electrostatic and hydrogen-bonding interactions with the 2,2'-(ethylenedioxy)bis(ethylammonium) cations.

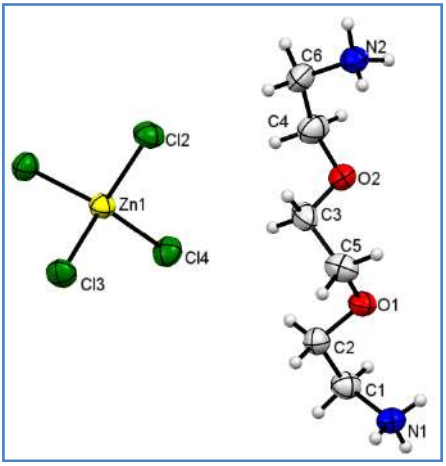

Fig. The asymmetric unit of $[C_6H_{18}N_2O_2]ZnCl_4$ showing the atom numbering scheme.

Key words: metal halides; Crystal structure; chemical preparation; intermolecular interactions.

Synthesis and crystal structure of a new 2-D chloro-substituted zinc phosphate, $[C_8N_2H_{20}]Zn_2(PO_3(OH))_2Cl_2$, containing (4.8) net layers.

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A new layered chloro-substituted zinc-phosphate, $[C_8H_{20}N_2]Zn_2(PO_3(OH))_2Cl_2$, has been synthesized in acidic conditions at room temperature in the presence of 1,3-cyclohexanebis(methylamine). The structure of this compound is determined by single-crystal X-ray diffraction at 293 K. Crystal data: monoclinic, $P2_1/c$ (No. 14), a = 8.7209(11) Å, b = 9.5504(12) Å, c = 21.866(3) Å, β = 99.986(2)°, V = 1793.6(4) $Å^3$, Z = 4, R = 0.0303 and Rw = 0.0766. The structure consists of vertex linked ZnO_3Cl and $PO_3(OH)$ tetrahedra assembled into corrugated porous layers $[Zn_2(PO_3(OH))_2Cl_2]_\infty$ with (4.8^2) topology. The organic cations are confined between anionic layers to maximize the electrostatic interactions and are linked to the inorganic framework via N-H···O and N-H···Cl hydrogen bonds. The (4.8^2) porous layers are found in a number of zeolite structures and related zinc phosphates phases. This compound has also been chraracterized by infrared spectroscopy, solid state MAS-NMR and thermal analysis.

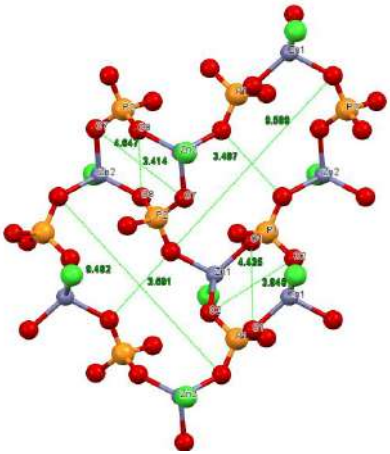

Fig. Topological connectivity of a $[Zn_2(HPO_4)_2Cl_2]_2\sim$ layer in $[C_8H_{20}N_2]Zn_2(PO_3(OH))_2Cl_2$, showing the presence of 4-rings and 8-rings.

Key words: Zincophosphate; open framework structure; Crystal structure; Zinc phosphate; Organic template, Chloride-substitution.

Communication's Title: Correlation between EPR and UV absorbed dose response of gamma irradiated bio-polymer (Poly Glycolic Acid)

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Gamma-irradiation of solid bio-polymer Poly Glycolic Acid (PGA) induces stable electron paramagnetic resonance (EPR) detectable free radicals. Upon dissolving in water solution, irradiated PGA develops an UV measurable absorption spectrum. Mutually the EPR intensity of gamma-irradiated solid PGA and its UV solution absorbance linearly depend on the radiation absorbed dose in the dose range of 0.1-10 kGy. Combination of EPR and UV spectral data is possible to use for independent Solid State/EPR calibration and for the control and monitoring of radiation processing application purpose.

Key words: *Dosimetry; Poly Glycolic Acid (PGA); Electron Spin Resonance (ESR); UV spectral.*

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Synthesis and coordination chemistry of 1,5-bis-allyloxy-sulfides

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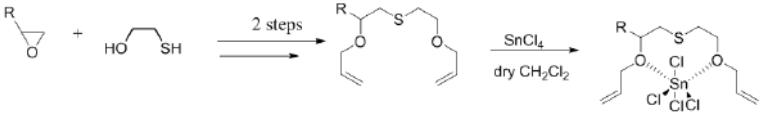
Allyl ethers are important starting materials for a wide range of organic reactions [1]. The reactivity of alkenes allows them to be used in many areas such as coordination chemistry, pharmaceuticals, agrochemicals and polymers [2]. The most commonly used method is Williamson synthesis for the preparation of allyl ethers. Herein, we report on the synthesis of novel substituted 1,5-bis(allyloxy)sulfides obtained from the products of opening of epoxides by the mercaptoethanol [3]. The study of coordination chemistry of these sulfides as new ligands to wards tin tetrachloride was carried out. The ^{1}H and ^{13}C NMR data show that both oxygen atoms of these molecules are coordinated to the tin center in a bidentate fashion. The stability and solution behavior of these tin(IV) complexes will be presented and discussed.



R= Me (a) ; Et (b) ; $(CH_2)_4$ (c) ; (CH_2OPh,H) (d); Ph (e)

Keywords: Epoxide, mercaptoethanol, allylchloride tin complex, NMR spectroscopy.

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Direct conversion of the β,β'-dihydroxydithioethers into thiols: Synthesis of new tétradentate ligands

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The growing interest in the synthesis of thioetherdithiols is due to their use in polymer synthesis [1], biochemistry [2], extraction of metal ions and in medical and environmental applications. The existence of sulphur atoms in their structures makes these compounds very useful as selective ligands towards soft metal cations [3]. On the other hand, when these compounds contain functional groups, they are usual as precursors in the synthesis of cyclic sulphur-containing compounds [4]. In this work, we present a simple method for the preparation of a new series of alkyl and functional substituted symmetric thioetherdithiols. Colloidal solutions of gold nanoparticles (AuNPs) with their ligands were prepared and showed a good stability from tight binding offered by the thiol group on the Au surfaces.

Keywords: hydroxythioethers, thiols, gold nanoparticles (AuNPs), ligands

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An Efficient Synthesis of PolySubstituted Vinyl Ethers

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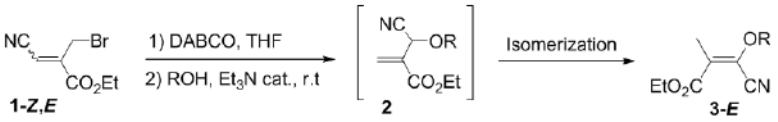
Allyl bromides [1,2] are considered as interesting intermediates in several synthetic fields including the preparation of pyrrolin-2-ones derivatives [2], 4-methoxycarbonyl-2(5*H*)-furanones [3] and 3,4-disubstituted pyrrolidin-2-ones [4]. As part of our continuing study on the electrophilic reactivity of ethyl 2-(bromomethyl)-3-cyanoacrylate **1** towards alcohol as nucleophile, we describe in this communication, an efficient approach for the synthesis of vinyl ethers **3** through successive *O*-alkylation-isomerization reaction. The strategy proceeds by the direct substitution of a bromine atom with the 1,4-diazabicyclo[2.2.2]octane, providing a quaternary ammonium salt. The latter can be dislodged via S_N2' reaction using oxygen nucleophiles such as aliphatic and aromatic alcohols in the presence of triethylamine as catalyst at room temperature, to produce the intermediate functionalized allyl ethers **2** which undergo a spontaneous isomerization to provide stereoselectively the polysubstituted vinyl ethers **3** in 55-82% yield.



Keywords: Ethyl 2-(bromomethyl)-3-cyanoacrylate, alcohols, isomerization, vinyl ethers.

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DFT calculations of structural, and mechanical properties of C15, C14 and C36 Laves phases in YCo_2

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First principles calculations have been carried out to investigate the structural stability, and mechanical properties of YCo2 with well defined C15, C14 and C36 Laves phases structures.
Density functional theory is considered within framework of both pseudo-potentials and plane waves basis using VASP (Vienna ab initio Software Package). Formation heat has been computed and showed that YCo2 with C15 (Cubic) Laves phases have the strongest alloying ability and structural stability.
Electronic density of states (DOSs) and mechanical properties were calculated, discussed, and analyzed in terms of structure stability.

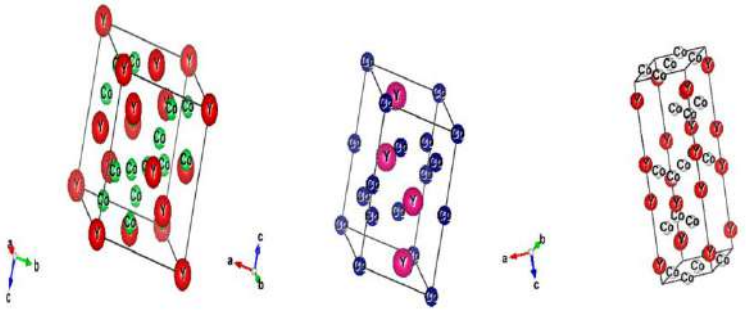

Fig. Crystal structures of C15 (a), C14 (b) and C36 (c) AB_2 type Laves phases

Keywords: Laves phases, mechanical properties, DFT, ab initio.

Effect of powder preparation of Clove, Ginger, Garad and Galangal on the infestation of Chick-pea grains caused by Cow pea weevil *Callosobruchus maculatus* adults

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Chick-pea,*Cicer arietinum* L.(Fabaceae) is the most important legumes crop in Sudan. Cow pea weevil, *Callosobruchus maculatus* (Coleoptera: bruchidae) is the major store pest of chick-pea grains. This study was conducted to investigate the efficacy of flower buds powder of clove, *Syzygium aromaticum* Cl, rhizomes powder of ginger, *Zingiber officinale* Rose, galangal, *Alpinia officinarum* Hance, and fruits powder of garad, *Acacia nilotica*, on the level of infestation of cowpea weevil adult. The experiments were carried out in the laboratory to rear cowpea weevil adults on chick-pea grains treated with?/ powder of the above natural products. Ten cowpea weevil adults were introduced to each treatment. Chick-pea grains were treated with powder of clove, ginger, galangal, garad,and untreated chick-pea grains as control, replicated five times and arranged in a completely randomized design. Parameters studied were weight loss, adult mortality, seed damage and seed germination; weight loss and adult mortality were determined weekly, seed damage and seed germination were assessed at the end of the experiment.The results indicated that these natural products significantly ($p<0.05$) reduced the percentage of damage of cowpea weevil adult on chick-pea grains which were 8.40%, 19.60%, 32.00%, 33.20% and 66.00%recorded in clove,ginger, galangal, garad, and the control, respectively. percentages of weight loss were 1.81%, 3.31%, 4.03%, 4.35% and 5.31% recorded in clove, ginger, galangal, garad, and the control respectively. Percentages of adult mortality were 93.33%, 61.99%, 54.66%, 41.40%,and 30.06% recorded in clove, ginger, galangal,garad and the control respectively. Percentages of seed germination were 83.20%, 74.00%, 68.00%, 64,40% and 41.60% recorded in clove, ginger, galangal, garad, and the control respectively. Apparently clove powder was the most effective one followed by ginger, galangal and garad compared to the control. It is concluded that clove powder is the most effective in reducing cow pea weevil adult infestation on chick-pea grains, and there for recommended for chick-pea grains protection against cowpea weevil in grain stores.

Treatment of hard water by electrodialysis

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For long periods, water has been regarded as natural source free and inexhaustible. However there distribution on Earth is uneven, also, the drinking water needs are increasing in recent years. To cope with this shortage, we have descovered the appearance of several processes of analysis as membranes and electrmembranes processes. The purpose of this study is to treat hard water by electrodialysis [1]. This technique involves the use of ion exchange membranes which are efficient during electrochemical treatment. Two types of solutions have undergone electrochemical treatment: synthetic and natural water. Electrodialysis with our membranes gives good results, with calcium test solutions becoming depleted in the synthetic solution and in the real one. Indeed, the cationic membrane presents a good selectivity for the transfer of calcium and magnsium ions, which are responsable to the hardness of water, from synthetic and real water respectively. The softening water has been obtained for two solutions.We now intend to use big cells with continuous solution flows in the aim to confirm its suitability for large industrial applications.

Key words: Electrodialysis, Calcium and magnesium, ion exchange membranes, selectivity.

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Development of hydroxyapatite, from the natural phosphate of Djebel Onk ore, and its application to the adsorption of the Pb-Cd-Ni ternary mixture in an aqueous medium

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The mining industry, which is based on the extraction and processing of different ores, greatly influences the pace and effectiveness of the development of the national economy. Among these ores, we can cite the phosphate [1].
Natural phosphate being a raw material and an abundant source in nature which is used mainly in the manufacture of fertilizers, phosphoric acids ... etc. The composition of the latter changes from one deposit to another and usually incorporates a wide variety of mineral compounds. Phosphate in particular of apatitic type is studied as a method of depollution of liquid effluents, polluted by trace elements [2].
The study of natural and synthetic apatites made it possible to evaluate their adsorption capacities in order to eliminate heavy metals and organic substances and to use them as a coating material for metallic prostheses to improve their function and protect them Against corrosion [3-6]. The objective of our work is to prepare powders of hydroxyapatites by different precursors (natural or chemical) and their application for the study of the adsorption of the ternary mixture Pb-Cd-Ni in aqueous solution. We have prepared our hydroxyapatites by the precipitation method, the natural precursor used is the black phosphate of Djebel Onk (Tebessa), the chemical precursor used is the pair [$Ca(OH)_2$, $NH_4H_2PO_4$]. The powders prepared were characterized by DRX, FTIR and BET. The results obtained are identical to those reported in the literature. The DRX spectra show a majority phase of the hydroxyapatite, and the specific surface area is of the order of 95 m^2 / g.
The main objective of this study is to evaluate the adsorptive power of hydroxyapatite, with respect to the metal cations Pb, Cd and Ni; As well as the different parameters influencing it. The results show rapid kinetics of adsorption for the three metals with high removal rates (99%, 87% and 26% for Pb, Cd and Ni respectively); The optimum value of pH being 4, that of the concentration of adsorbent is 5 g / l.

Key words: Adsorption, heavy metals, lead, cadmium, nickel, hydroxyapatite.

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Synthesis, characterization and coordination chemistry of α-phosphonomethylbutenolides

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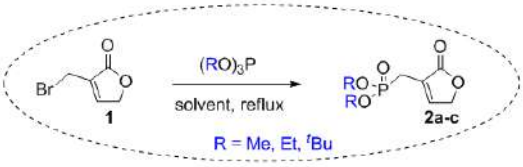
Substituted butenolides has attracted much attention due to their presence in many natural products [1] with a broad spectrum of biological activities [2]. In this communication, we describe an efficient synthesis of α-phosphonomethylbutenolide **2** from the coupling reaction of trialkylphosphites with lactone bromide **1** via the Michaelis Arbusov reaction. In order to test the coordination chemistry of allylphosphonates **2**, we have initially carried out its reactivity towards tin tetrachloride in anhydrous dichloromethane at room temperature to produce α-phosphonomethylbutenolides tin complexes as mixtures of *cis* and *trans* isomers in good yield. These new tin(IV) adducts were characterized by multinuclear (^{1}H, ^{31}P and ^{119}Sn) NMR and IR spectroscopy. The effects of R groups on the magnitude of the P=O-tin interaction as well as comparison with closely related complexes [3,4] will be discussed.



Keywords: Lactone bromide, α-phosphonomethylbutenolide, tin complex, NMR spectroscopy.

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REDOX BEHAVIOR OF BIS (CYCLOPENTADIENYL) COMPLEXES OF URANIUM. STUDY OF DFT / ZORA RELATIVISTE.

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In this work, we are interested in the quantochemical study of a family of tris (cyclopentadienyl) complexes of uranium Cp * 3UL (X) associated with functionalized X and / or donor ligands. The RX structure of some of them is known, have not been theoretically studied until now. We will study in particular molecular geometries, the relationship between electronic structure and redox behavior and the nature of the Metal-ligand interactions involved. We will analyze the possible correlations between the values of the calculated quantum quantities (AE, net metal charge, HOMO / LUMO and linkage indices) with the half-wave redox potential variations (-E1 / 2) experimentally measured. In the framework of the predictive aspect of the DFT method, we will analyze the redox properties of some unknown or not yet isolated species.

Key words:v Uranium complexes, Redox potential, Electron affinity, DFT / ZORA, solvent effect, COSMO, spin-orbit.

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AN EFFICIENT PALLADIUM TRIPHENYLPHOSHINE COMPLEXES CATALYSED SONOGASHIRA TYPE CROSS COUPLING OF ARYL HALIDES WITH TERMINAL ALKYNES

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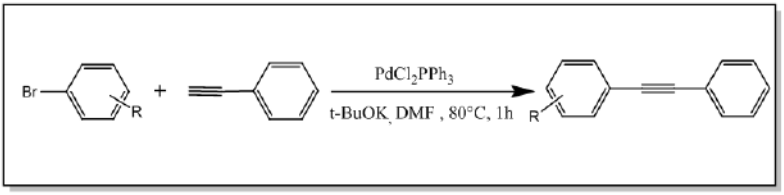
The so-called Sonogashira cross-coupling palladiumcatalysed reaction between aryl halides and alkynes is among the most widely used methodology in organic synthesis [1]. In recent years, the efficiency of several palladium catalysts for this reaction has been described [2]. The reaction of heteroaryl halides has attracted less attention than the coupling with aryl halides, and suffers generally from high catalysts loadings. A few ligands have been successfully employed for the reaction with these substrates [3-4]. Here, we wish to describe our results involving the use of a new series of Palladium triphenylphosphine to catalyze the coupling of aryl halides with terminal alkynes with high efficiency under Sonogashira reaction conditions in absence of co-catalyst. **Scheme 1**



Scheme 1: PdCl2PPh3catalysed sonogashira reaction

Key words: palladium triphenylphosphine complexes, sonogashira cross-coupling, aryl halide, alkyne.

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SYNTHESIS OF MIXED ANHYDRIDES OF FATTY ACIDS

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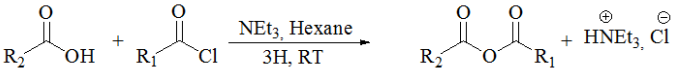
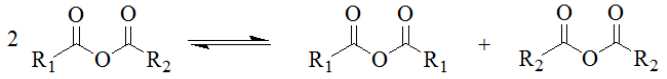
Carboxylic anhydrides in organic chemistry are acylating agents appreciated for their high reactivity compared to carboxylic acids. They are also important classes of chemicals that have been used extensively as synthetic intermediates in the preparation of a variety of fine or special chemicals such as amides, esters, peptides, drugs, etc. Mixed anhydrides obtained from two different carboxylic acids are molecules finding an increasing interest in the chemical industry due to their high reactivity due to the difference in the pK values of the two moieties of the asymmetric molecules. Many useful methods have been reported in the literature for the synthesis of carboxylic acid anhydrides. The preferred method is the reaction between the carboxylic acid and acid chloride.

Unsymmetric anhydrides, characterized by the general formula $R_1CO\text{-}O\text{-}COR_2$, can be easily prepared by the reaction of the fatty acid (R_1) with the acid chloride (R_2) in organic solvent and in the presence of triethylamine as catalyst (acid acceptor) as it is indicated in scheme 1 [1].



Scheme 1. Synthesis of mixed carboxylic acid anhydride.

The main difficulty in the synthesis of the mixed anhydride is its instability when formed and it disproportionation into correspondent symmetrical anhydrides. The stability of mixed anhydrides ($R_1CO\text{-}O\text{-}COR_2$) is generally related to the nature of R_1 and R_2 groups. When the sizes of the two alkyl or aryl carboxylic acids are decidedly different, the mixed anhydrides tend to decompose easily. A chemical equilibrium established between the three types of anhydrides which form a mixture in the crude as it is indicated in scheme 2 [2].



Scheme 2. Disproportionation reaction between two mixed anhydrides.

Key words: fatty acid, mixed anhydride, symmetrical anhydride.

References

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MIXED CARBOXYLIC-FATTY ANHYDRIDE ESTERIFICATION USING AMBERLYST-15 AS A HETEROGENEOUS CATALYST

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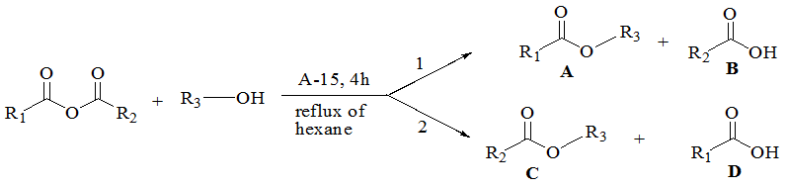
The esterification of fatty acid with alcohol under an acid catalyst is a reversible reaction limited by the low equilibrium conversion and slow reaction rate. To perform high-yielding esterification with equimolar reactions of carboxylic acids and alcohols under mild conditions, the coupling reactions between activated derivatives of carboxylic acids (carboxylic acid chlorides or anhydrides) and alcohols have been often employed.

The esterification by solid acid catalysts, which have the advantages of being easily recovered and reused as well as being compatible with environmental considerations, has also been studied. Ion-exchange resins such as Amberlyst-15 are convenient catalysts for etherification, esterification and transesterification reactions. These resins are composed of copolymers of divinylbenzene (DVB), styrene and sulfonic acid groups [being the active site (Brønsted acidity)].

The fatty ester was performed by the esterification reaction of alcohol with mixed carboxylic-fatty anhydride ($R_1CO\text{-}O\text{-}COR_2$) in organic solvent in the presence resin Amberlyst-15 as heterogeneous acid catalyst [1]. The reaction of the mixed anhydride with an alcohol leads to a complex mixture comprising the two esters and two correspondent acids as shown in Scheme 1 [1].



Scheme 2. Esterification reaction of a mixed anhydride with an alcohol.

Keywords: fatty acid, mixed anhydride, heterogeneous acid catalyst, resin Amberlyst-15, esterification.

References

[1] Trabelsi, I.; Essid, K.; Frikha, M.H. Synthesis of mixed anhydrides of fatty acids: Stability and Reactivity. Ind. Crop. Prod. 2017? 97, 552-557.

Synthesis and spectroscopic characterization of new tin(IV) complexes with functionalized *gem*-bisphosphonates

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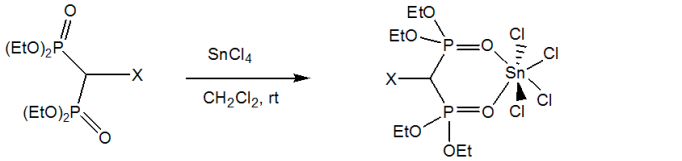
The ability of the strong Lewis acid tin tetrachloride to form 1:2 adducts with a variety of neutral ligands is well known [1-5]. For instance, phosphoramides show strong affinity to this Lewis acid and produce hexacoordinate, 2:1, *cis*- or trans-complexes. These complexes have been characterized in solution and in the solid state [6]. On the other hand, diphosphorylated compounds are attracting considerable attention owing to their various useful properties ranging from pharmacological activities to their heavy metal chelating ability [7]. The coordination chemistry of these molecules could represent another venue towards a further understanding of their chemistry. In this work, we report on the synthesis and characterization of $SnCl_4$ complexes with functionalized *gem*-bisphophonates. These new diphosphoryl tin(IV) adducts (**1-3**) were fully characterized by multinuclear (^{1}H, ^{13}C, ^{31}P and ^{119}Sn) NMR and IR spectroscopy. The NMR data show that the title bisphophonate ligands are coordinated to the tin center through both phosphoryl groups in a bidentate fashion, giving *cis* octahedral complexes (**1-3**). The solution behavior of these new tin complexes in the presence of excess ligand is also investigated using variable temperature NMR spectroscopy.



X: =CH_2 (**1**), CH_2CN (**2**) or CH_2NHCH_2Ph (**3**)

(72-80%)

Key words: Lewis acid, tin tetrachloride, *gem*-bisphosphonates, tin complexes, NMR spectroscopy.

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