3rd Tunisian Chemical Society Conference on Coordination Chemistry

JCC 2019

Organized by

Tunisian Chemical Society

ROYAL SOCIETY
OF **CHEMISTRY**
TUNISIA LOCAL SECTION

26-29 September 2019

Laico Hotel, Yasmine Hammamet, Tunisia

Abstracts of Lectures and Communications
List of Participants

Tunisian Chemical Society - Short Program of JCC 2019

Thursday 26 September 2019	
14.00	**Welcoming participants, distribution of documents and check in**
17.00	**Opening Remarks**
17.20 - 18.00	**Plenary Lecture 1 Azzedine BOUSSEKSOU** *LCC-CNRS, Toulouse, France*
18.00	***RSC Welcome Reception***
19.30	***Dinner***
Friday 27 September 2019	
08.30 - 09.10	**Plenary Lecture 2 Christophe MORELL** *ISA-Lyon, Université de Lyon, France*
09.15 - 10.15	**Oral Communications - Session 1 - OC1 > OC4**
10.15 - 11.00	**Coffee break + Poster Session 1 (P 1 - P 24) Alphabetical Order**
11.00 - 11.40	**Plenary Lecture 3 Anne Marie CAMINADE** *LCC-CNRS, Toulouse, France*
11.45 - 12.45	**Oral Communications - Session 2 - OC5 > OC8**
13.00	***Lunch***
15.00 - 15.40	**Plenary Lecture 4 Alessandro CASELLI** *Università degli Studi di Milano and ISTM-CNR-Milano, Italia*
15.45 - 17.00	**Oral Communications - Session 3 - OC9> OC13**
17.00 - 17.45	**Coffee break + Poster Session 2 (P 25 - P 46) Alphabetical Order**
17.50 - 18.30	**Plenary Lecture 5 M. Abdrerrahmane SANHOURY** *University of Tunis El Manar, Tunisia / Nouakchott University El Aasriya, Mauritania*
19.30	***Dinner***
Saturday 28 September 2019 (Morning)	
08.30 - 09.10	**Plenary Lecture 6 Mark CRIMMIN** *Imperial College London, White City, London W12 0BZ, United Kingdom*
09.15 - 09.30	**JEOL Representative Ahmed DHIFAOUI** *JEOL (Europe) - Nuclear Magnetic Resonance Instruments*
09.30 - 10.30	**Oral Communications - Session 4 - OC14 > OC17**
10.30 - 11.15	**Coffee break + Poster Session 3 (P 47 - P 70) Alphabetical Order**
11.20 - 12.00	**Plenary Lecture 7 Remi CHAUVIN** *Université Toulouse-3/Paul Sabatier, Toulouse, France*
12.00 - 13.00	**Oral Communications - Session 5 - OC18 > OC21**
13.00	***Lunch***
14.30 - 15.10	**Plenary Lecture 8 Eric MANOURY** *LCC-CNRS, Toulouse, France*
15.10 - 15.50	**Plenary Lecture 9 Jean Pascal SUTTER** *LCC-CNRS, Toulouse, France*
16.00	*Social Program - Excursion to some touristic places*
19.30	***Dinner***
Sunday 29 September 2019 (Morning)	
09.00 - 09.40	**Plenary Lecture 10 Lahcene OUAHAB** *ISCR - University of Rennes, France*
09.40 - 10.10	**Invited Speaker Thouraya BARHOUMI SLIMI** *ISSTE, Technopark of Borj-Cedria - University of Carthage, Tunisia*
10.15 - 11.15	***Coffee break***
11.15 - 12.00	**Closing Remarks, Poster Awards and JCC 2021 Announcements**
13.00	***Lunch, Check Out and Departure***

FOREWORD

On behalf of the JCC 2019 organizing committee, we are pleased to welcome you in Hammamet for this third Tunisian Chemical Society Conference on Coordiniation Chemistry (JCC 2019) organised by the Tunisian Chemical Society Coordination Chemistry Group in collaboration with the RSC Tunisia Local Section under the auspices of the Tunisian Chemical Society (SCT).

This JCC 2019 third edition, which will see the participation of more than 7 African and European countries in addition to the Tunisian universities with more than 132 participants from various countries. They will discuss themes involving the science of coordination chemistry carefully distributed over 10 plenary lectures, 1 invited speaker, 42 oral communications and 69 poster presentations.

Many thanks for all participants, for all invited speakers and in particular for Toulouse LCC delegates, who firmly accepted to contribute with lectures at the event in order to make it a very successful coordination chemistry meeting.

Prof Med Taieb Ben Dhia
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JCC 2019 Co-Chair

Prof Hatem Ben Romdhane
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Being on time is the main factor for conference's success

Program of the

Third Tunisian Chemical Society Conference on Coordination Chemistry

JCC 2019

Thursday 26 September 2019		
14.30	**Welcoming participants, distribution of documents and check in**	
17.00	**Opening Remarks**	
17.20 - 18.00	**Plenary Lecture 1** **<u>Azzedine BOUSSEKSOU</u>** *LCC-CNRS, Toulouse, France* **Molecular Spin Crossover Phenomenon at the nanoscale: Recent achievements and prospects**	*Chairman:* Med Taieb Ben Dhia
18.00	***Welcome Reception***	
19.30	***Dinner***	

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Friday 27 September 2019 (morning)				
08.30 - 09.10	**Plenary Lecture 2** **Christophe MORELL** *ISA-Lyon, Université de Lyon, France* **New Tools for the study of coordination compounds: Theoretical developments and applications**			*Chairman:* Alessandro Caselli
Oral Communications - Session 1				
	Room A - *Chairman*: Med Abderrahmane Sanhoury		Room B - *Chairman*: Hatem Ben Romdhane	
	Com.	*Communicating*	*Com.*	*Communicating*
09.15 - 09.30	**OC-01A**	**FAJERWERG Katia** *LCC-CNRS, Toulouse, France*	**OC-01B**	**ROBERT Anne** *LCC-CNRS, Toulouse, France*
09.30 - 09.45	**OC-02A**	**BEN AZIZA Meriem** *CRTEn - Borj Cédria*	**OC-02B**	**ELGHNIJI Kais** *FSG - Gafsa*
09.45 - 10.00	**OC-03A**	**BEN OTHMAN Amel** *FSB - Bizerte*	**OC-03B**	**FRAY Marwa** *FST - Tunis*
10.00 - 10.15	**OC-04A**	**BOUBAKRI Lamia** *ISSTE - Borj Cedria*	**OC-04B**	**GHRAIRI Sondes** *FST - Tunis*
10.15 - 11.00	**Coffee break + Poster Session 1 (P 1 - P 24) Alphabetical Order**			
11.00 - 11.40	**Plenary Lecture 3** **Anne Marie CAMINADE** *LCC-CNRS, Toulouse, France* **Coordination chemistry with phosphorus dendrimers and their applications**			*Chairman:* Mark Crimmin
Oral Communications - Session 2				
	Room A - *Chairman*: Latifa Bergaoui		Room B - *Chairman*: Ikram Chehidi	
	Com.	*Communicating*	*Com.*	*Communicating*
11.45 - 12.00	**OC-05A**	**DHIFAOUI Hassen** *FSM - Monastir*	**OC-05B**	**HANACHI Riadh** *FST - Tunis*
12.00 - 12.15	**OC-06A**	**HANNACHI JMAI Anissa** *FSB - Bizerte*	**OC-06B**	**JBALI Wejden** *FST - Tunis*
12.15 - 12.30	**OC-07A**	**JELALI Hamida** *FSG - Gafsa*	**OC-07B**	**LARIBI Fahima** *FST - Tunis*
12.30 - 12.45	**OC-08A**	**BEGAR Abdelhakim** *University of Biskra, Algeria*	**OC-08B**	**MECHI Hanen** *FST - Tunis*
13.00	***Lunch***			

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Friday 27 September 2019 (afternoon)				
15.00 - 15.40	**Plenary Lecture 4** <u>**Alessandro CASELLI**</u> *Università degli Studi di Milano and ISTM-CNR-Milano, Italia* **Transition metal complexes of pyridine-containing macrocycles as catalysts for selective oxidations and CO_2 valorisation reactions**			*Chairman:* Anne-Marie Caminade
Oral Communications - Session 3				
	Room A - *Chairman*: Rym Labidi		Room B - *Chairman*: Farhat Rezgui	
	Com.	*Communicating*	*Com.*	*Communicating*
15.45 - 16.00	**OC-09A**	**AMIENS Catherine** *LCC-CNRS, Toulouse, France*	**OC-09B**	**CESAR Vincent** *LCC-CNRS, Toulouse, France*
16.00 - 16.15	**OC-10A**	**KANZARI MNALLAH Dorra** *FST - Tunis*	**OC-10B**	**LOUATI Myriam** *FST - Tunis*
16.15 - 16.30	**OC-11A**	**AGREN Soumaya** *IPEIM - Monastir*	**OC-11B**	**EBNOU Fatimetou** *Nouakchott University El Aasriya, Mauritania*
16.30 - 16.45	**OC-12A**	**SLIMANI Ichraf** *ISSTE - Borj Cedria*	**OC-12B**	**EBEID Khaled** *Nouakchott University El Aasriya, Mauritania*
16.45 - 17.00	**OC-13A**	**BENBELLAT Noura** *University of Batna1, Algeria*	**OC-13B**	**BOUGHDIRI Mohamed Ali** *IPEIEM - Tunis*
17.00- 17.45	**Coffee break + Poster Session 2 (P 25 - P 46) Alphabetical Order**			
17.50 - 18.30	**Plenary Lecture 5** <u>**Mohamed Abdrerrahmane SANHOURY**</u> *University of Tunis El Manar, FST - Tunis, Tunisia / Nouakchott University El Aasriya, Mauritania* **Synthesis and applications of phosphine chalcogenide metal complexes**			*Chairman:* Thouraya Barhoumi Slimi
19.30	***Dinner***			

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Saturday 28 September 2019 (morning)				
08.30 - 09.10	**Plenary Lecture 6** **Mark CRIMMIN** *Imperial College London, White City, London W12 0BZ, United Kingdom* **Coordination of Zinc and Magnesium Hydrides to Transition Metals: Structures, Bonding and Applications in Catalysis**			*Chairman:* Med Abderrahmane Sanhoury
09.15 - 09.30	**JEOL Representative** **Ahmed DHIFAOUI** *JEOL (Europe) - Nuclear Magnetic Resonance Instruments* **JEOL Presentation**			*Chairman:* Med Abderrahmane Sanhoury
Oral Communications - Session 4				
	Room A - *Chairman*: Med Taieb Ben Dhia		Room B - *Chairman*: Latifa Latrous	
	Com.	*Communicating*	*Com.*	*Communicating*
09.30 - 09.45	**OC-14A**	**LACROIX Pascal** *LCC-CNRS, Toulouse, France*	**OC-14B**	**VOLKMAN Jérôme** *LCC-CNRS, Toulouse, France*
09.45 - 10.00	**OC-15A**	**NASR Khaoula** *FST - Tunis*	**OC-15B**	**ZARROUG Rim** *FSG - Gabès*
10.00 - 10.15	**OC-16A**	**REZGUI Eya** *FST - Tunis*	**OC-16B**	**M'HAIHAM Mohamed** *Nouakchott University El Aasriya, Mauritania*
10.15 - 10.30	**OC-17A**	**MEJRI Alia** *FST - Tunis*	**OC-17B**	**DKHILI Samiha** *FSB - Bizerte*
10.30 - 11.15	***Coffee break*** **+ Poster Session 3 (P 47 - P 70) Alphabetical Order**			
11.20 - 12.00	**Plenary Lecture 7** **Remi CHAUVIN** *Université Toulouse-3/Paul Sabatier, Toulouse, France* **Coordination in chemistry: Selected issues, ventures, results & applications**			*Chairman:* Lahcène Ouahab
Oral Communications - Session 5				
	Room A - *Chairman*: Thouraya Barhoumi Slimi		Room B - *Chairman*: Khaled Essaleh	
	Com.	*Communicating*	*Com.*	*Communicating*
12.00 - 12.15	**OC-18A**	**MEKLID Abdelhek** *Mohamed Kheider University of Biskra, Algeria*	**OC-18B**	**SLIMI Sami** *FSM - Monastir*
12.15 - 12.30	**OC-19A**	**ZEROUAL Samira** *University of Batna1, Algeria*	**OC-19B**	**ZIDANI Chafika** *University of Tlemcen, Algeria*
12.30 - 12.45	**OC-20A**	**EL BRAHMI Nabil** *University of Fès, Morocco*	**OC-20B**	**BOUTAR Marwa** *FSB - Bizerte*
12.45 - 13.00	**OC-21A**	**ES-SOUNNI Bouchra** *Moulay Ismail University, Morocco*	**OC-21B**	**BYUSA Edwin** *University of Rwanda*
13.00	***Lunch***			

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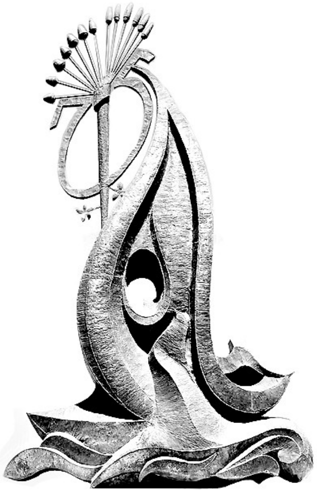
Saturday 28 September 2019 (afternoon)		
14.30 - 15.10	**Plenary Lecture 8** **Eric MANOURY** *LCC-CNRS, Toulouse, France* **Well-Defined Core-shell Functionalized Polymers as Nanoreactors for Biphasic Catalysis**	*Chairman:* Rémi Chauvin
15.10 - 15.50	**Plenary Lecture 9** **Jean Pascal SUTTER** *LCC-CNRS, Toulouse, France* **Pentagonal bipyramid complexes: A journey from magnetic anisotropy to heterometallic molecule-based magnets**	*Chairman:* Christophe Morell
16.00	**Social Program** **Excursion to some touristic places**	
19.30	***Dinner***	

Sunday 29 September 2019 (morning)		
09.00 - 09.40	**Plenary Lecture 10** **Lahcene OUAHAB** *ISCR - University of Rennes, France* **Single Molecule Magnet behaviour and Luminescence in Lanthanides Complexes containing TTFs Ligands**	*Chairman:* Rym Abidi
09.40 - 10.10	**Invited Speaker** **Thouraya BARHOUMI SLIMI** *Higher Institute of Environmental Sciences and Technologies, Borj Cédria, Tunisia* **IYPT 2019 - Lecture: International Year of the Periodic Table**	*Chairman:* Azzedine Bousseksou
10.15 - 11.15	***Coffee break***	
11.15 - 12.00	**Closing Remarks, Poster Awards and JCC 2021 Announcements**	
13.00	***Lunch, Check Out and Departure***	



Speakers' Abstracts

Molecular Spin Crossover Phenomenon at the nanoscale: Recent achievements and prospects

Azzedine Bousseksou, Gabor Molnar,
Lionel Salmon, William Nicolazzi

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[b] *CNRS, LCC, Toulouse (b)*
[c] *CNRS, LCC, Toulouse (c)*
Université Paul Sabatier, LCC, Toulouse (d)

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. [1-4] we are particularly interested in the 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.[1-15]
In this talk, I will discuss recent work in the field of molecule-based spin crossover materials with a special focus on recent achievements and these emerging issues. [16-17]

Key words: Molecular bistability, Spin crossover, Nano-electronic

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[2] Phys. Rev. Lett. 109 (2012) 135702. (2012)
[4] Angew. Chem. Int. Ed. 44 (2005) 4069-4073.
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[16] Phys. Rev. B 96 (2017) 134106.

New tools for the study of coordination compounds: Theoretical developments and applications

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The use of excited states to understand chemical reactivity and selectivity goes back to the 1940's when Walsh[1] attempted to correlate the electronic spectrum of a molecule with its stability. Since then, very scarce theoretical investigations have been undertaken. Among the very rare papers, the one by Pearson[2] entitled electronic spectra and chemical reactivity in which the reactivity of a molecule is related to its maximum absorption wavelength. Since few years ago, only reactivity has been assessed though excited states. In 2005, the Dual Descriptor[3] (DD) has been introduced to describe chemical selectivity from changes in the electron density.

$$f^{(2)}(\vec{r}) = \left(\frac{\partial^2 \rho(\vec{r})}{\partial N^2}\right)_{v(\vec{r})} = \left(\frac{\delta \eta}{\delta v(\vec{r})}\right)_N$$

Recently, new physical bases have been given to the DD [4] by expanding the electron density of a perturbed ground state through excited densities. This expansion had led to the proposal of state specific dual descriptors. The quest for determining which excited state contribute most for a specific perturbation has provided a way to describe electron density polarization using transition densities (unpublished work) closely related to the linear response function[5].

$$\Delta\rho(\vec{r}) \approx 2\sum_{k\neq 0} \frac{\left\langle \psi_0^{(0)} \middle| \delta v(\vec{r}) \middle| \psi_k^{(0)} \right\rangle}{E_0^{(0)} - E_k^{(0)}} \rho_0^k(\vec{r})$$

The main goal of this talk is to present these new theoretical tools as well as their applications [6] especially in coordination chemistry where they have been utilized to provide the very first theoretical scale for the trans effect.

Aknowledgements: The authors would like to acknowledge Aymeric Gotail and Thomas Pigeon (CPE Lyon school of engineers) for their robust implementation of the equations.

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Coordination chemistry with phosphorus dendrimers and their applications

Anne-Marie Caminade

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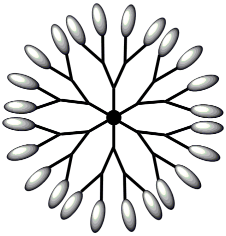

Dendrimers are hyper-branched macromolecules constituted by the association of repetitive branched monomers arranged around a central core [1]. Contrarily to polymers, dendrimers are not synthesized by polymerization reactions, but step-by-step, generally starting from the central core, to afford an increasing number of terminal functions. Each time the number of terminal functions is increased, a new "generation" is obtained (see a second generation in the figure). Several types of dendrimers are known, mainly based on nitrogen as branching points, and have led to different uses. However, dendrimers based on silicon or phosphorus as branching points have also many interesting properties [2].

Phosphorus dendrimers are particularly useful as supports of coordination complexes, to be used as homogeneous catalysts [3]. They are often more efficient than the corresponding monomers, and can be easily recovered [4]. It is also possible to switch (ON/OFF) their catalytic efficiency [5].

Phosphorus dendrimers have also many biological properties [6, 7], which in some cases are due to the presence of metal complexes on the surface. In particular, copper and gold complexes of phosphorus dendrimers have interesting anti-cancer properties toward a panel of cancerous cell lines [8].

Key words: dendrimers, phosphorus, catalysis, oncology

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Transition metal complexes of pyridine-containing macrocycles as catalysts for selective oxidations and CO_2 valorisation reactions

Alessandro Caselli and Nicola Panza

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Iron, the most abundant transition metal on earth, and its complexes are knowing an increasing interest in organic synthesis. The field of iron-catalysed oxidation reactions is of great importance not only in synthetic organic chemistry, but also in biochemistry and industrial applications. In order to design catalysts capable of performing high regio- and/or stereo-selective C-OH, C-H or C=C bond oxidations, it is important the choice of critical components of iron coordination sphere, namely the donor atoms and their geometry. In this lecture, I will provide a perspective on the catalytic applications of iron(III) and zinc(II) metal complexes of tetraaza 12-membered pyridine containing macrocyclic ligands.[1] I will focus on the selective iron(III) catalysed epoxidation or dihydroxylation of alkenes by using hydrogen peroxide as terminal oxidant.[2] Depending on the anion of the iron(III) metal complex employed as catalyst, a completely reversed selectivity was observed (Figure). Our approach towards the selective oxidation of alcohols by using the same catalytic system will also be covered. As for iron, catalytic applications of zinc complexes fall in the scientific community's effort to develop more eco-friendly chemical processes. CO_2 is the principal greenhouse gas, largely recognized as responsible for global warming, but it is also an abundant C_1 source. Limiting CO_2 emissions can only stem the problem but to solve it a circular economy based on carbon dioxide should be pursued and in this respect, research in the last decade has focussed on the design of systems able to promote the functionalisation of CO_2. I will outline our approach towards the synthesis of cyclic carbonates by cycloaddition of CO_2 to epoxides by using zinc(II) complexes.

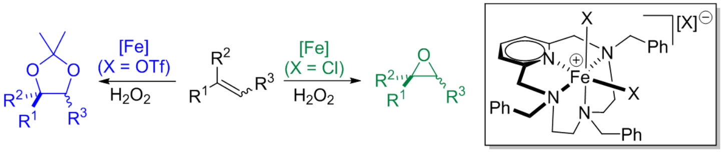

Fig. Controllable iron(III)-catalysed alkene epoxidation or dihydroxylation reactions are performed by judicious choice of anion in [Fe(III)(Pc-L)] catalysts (Pc-L = pyridine-based 12-membered tetraaza-macrocyclic ligands).

Key words: macrocyclic ligands, homogeneous catalysis, iron, zinc, oxidation, CO_2 functionalization.

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Synthesis and applications of phosphine chalcogenide metal complexes

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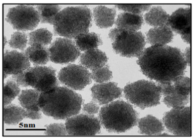
Studies into the coordination chemistry of phosphine chalcogenides R_3PE (E = S, Se or Te) and related compounds have attracted much attention due to their easy preparation, high solubility, and good reactivity toward different metal ions in many organic solvents.[1,2] In addition, there has been a renewed interest in the metal complexes of this class of compounds in view of their increasing use as suitable single-source precursors for the production of binary metal chalcogenide ME thin films (M = Zn, Cd or Hg; E = S, Se or Te) as well as ME quantum dots [3,4]. There is also an increasing interest in photoluminescence studies for both detecting and characterizing heavy metal species, with emphasis on their detection in the environment, especially in systems containing mercury [5]. In this work, the affinity of phosphine chalcogenides to soft metals such as cadmium and mercury is explored for the synthesis of corresponding metal complexes [6]. The characterization and structures of these complexes as well as their use as single source precursors in the preparation of nanomaterials for optical and electronic applications will be presented and discussed.

$$MX_2 + 2\,R_3PE \xrightarrow[\text{2-24 h}]{\text{EtOH}} \left[MX_2(R_3PE)_2\right]^{\cdot}$$

$$\left[MX_2(R_3PE)_n\right]^{\cdot} \xrightarrow[\text{10-150}^0\text{C, 2-12 h}]{\text{ETOH}} ME$$

(M = Zn, Cd or Hg: X = Cl^- or NO_3^-: E = S, Se or Te)



TEM image of ME Nanoparticles

Keywords: Phosphine chalcogenide, metal complex, nanoparticle, NMR spectroscopy.

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[6] See for example: Ebnou, F.; M'Haiham, M.; Ebeid, K.; Carpenter-Warren, C. L.; Slawin, A. M. Z.; Woollins, J. D.; Ben Dhia, M. T.; Sanhoury, M. A. *Polyhedron*. **2019,** *159,* 206–211.

Coordination of zinc and magnesium hydrides to transition metals: Structures, bonding and applications in catalysis.

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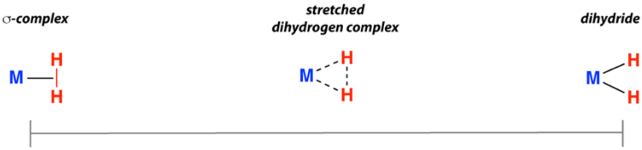
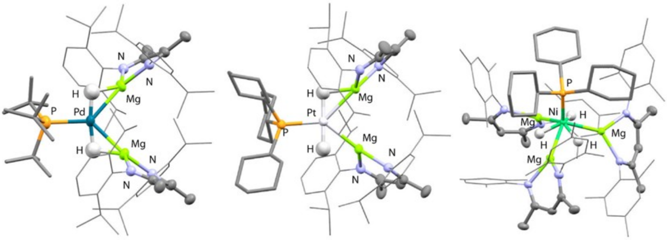
The realisation that H_2 can bind to transition metals was a landmark event in coordination chemistry. Coordination of H_2 to transition metals can be conceptualised within the Dewar-Chatt-Duncanson bonding model and leads to a bonding continuum (Fig. 1).[1]

Fig. 1 Continuum of bonding models for coordinate of H_2 to transition metals



In this lecture, we will explore the coordination of molecular zinc and magnesium hydrides to transition metals.[2-5] We will find that the resulting coordination compounds, while demonstrating high ionic character, aspects of metal–metal bonding and some remarkable structures (Fig. 2), can be described by a similar bonding model to the prototypical dihydrogen analogues. We will see that these types of complexes are catalytically relevant and are implied as intermediates in new transformations that convert C–H bonds to either C–Zn or C–Mg bonds.[6]

Fig. 2: Selected structures of heterometallics



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Coordination *in* chemistry: Selected issues, ventures, results & applications

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Novel appraisals of *electrostatic effects* in coordination chemistry long scrutinized by the Toulouse group, [1] will be disclosed through selected outcomes of ventures on the track of so-called polar "extreme phospho-carbon" ligands.

Beyond the academic concern of the quantification of the dative character of *any* single covalent bond through the *dative covalent energy* (DCE),[2] the coordination ability of P-poor phosphanes with neutral nitro-benzimidazole[3] and α-cationic cyclopropenium[4a] or imidazolium[4b] backbones will be illustrated, in either achiral series (Fig. 1-2)[3-4a] or chiral series (Fig. 3).[4b]

C-rich phosphonium ylides will be envisaged as anti-aromatic intermediates in a selective 3→4 ring expansion process (Fig. 4),[5] or as donor PhosphYl ligands in Pd-catalyzed Heck reactions for the preparation of arylbenzoxazoles.[6]

In closing, the quantification of the donor ability of bidentate ligands,[7a] and critical analysis of metal-triflate anion interactions,[7b] will be briefly addressed.

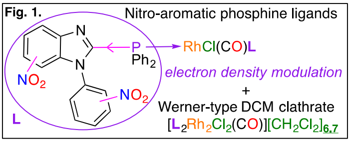

Fig. 1. Nitro-aromatic phosphine ligands

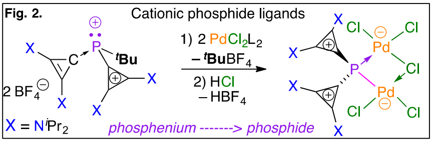

Fig. 2. Cationic phosphide ligands

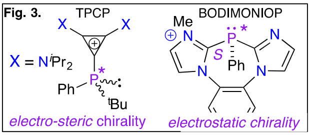

Fig. 3.

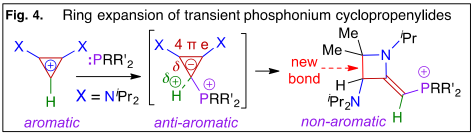

Fig. 4. Ring expansion of transient phosphonium cyclopropenylides

Key words: dative bonding, carbon, phosphorus, transition metals, catalysis

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Well-Defined Core-shell Functionalized Polymers as Nanoreactors for Biphasic Catalysis

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Catalyst recovery and recycling is one very important aspect of the application of catalytic technology, with a strong impact on energy efficiency, industrial economy, and the environment (waste production). We will present a new approach for efficient biphasic catalysis using water to confine the catalyst, based on the catalyst covalent linking to the hydrophobic core of well-defined amphiphilic nanosized core -shell polymers. These polymers (see figure 1) have been efficiently synthesized by RAFT polymerization in aqueous dispersion. The core-shell functionalized polymers were efficiently used in the rhodium-catalyzed hydroformylation of 1-octene under aqueous biphasic conditions The catalyst could be recycled several times by simple decantation with low Rh leaching.[1]

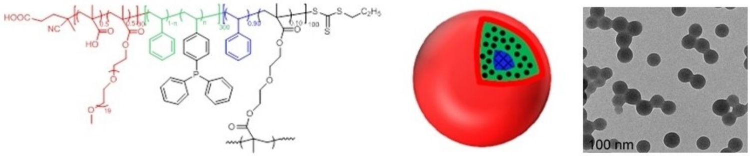

Figure 1 (Left) Structure of 1st generation nanoreactors; (Right) TEM images of nanoreactors

Coordination chemistry and interparticle metal migration studies involving the swollen hydrophobic cores[2] have allowed us to formulate hypotheses on the mass transport mechanisms and of rhodium leaching to the organic phase. The first results in the hydrogenation of alkenes under aqueous biphasic conditions using the same nanoreactors will be also presented.[3]

Keywords: biphasic catalysis, nanoreactors, coordination chemistry, rhodium, hydroformylation, hydrogenation

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PENTAGONAL BIPYRAMID COMPLEXES: A JOURNEY FROM MAGNETIC ANISOTROPY TO HETEROMETALLIC MOLECULE-BASED MAGNETS

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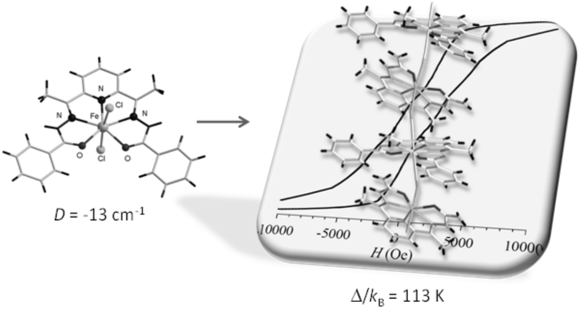
The energy barrier for magnetization reversal of a molecular magnet (i.e. SMM or SCM) is intimately related to the zero-field splitting characteristics (*D*) of its individual building units. However, it is still challenging for chemists to control the actual magnetic anisotropy of the complexes, all the more so when they get involved in the construction of heterometallic magnets.

We will discuss our approach using heptacoordinated 3d metal with pentagonal bipyramid geometry (Figure). In this environment Fe^{II} and Ni^{II} complexes are characterized by significant Ising-type anisotropy (i.e. D ~-15 cm-1)[1] and may even behave as single-center nanomagnets.[2] Taking advantage of their exchangeable apical positions, heteronuclear compounds were obtained and indeed found to exhibit slow magnetic relaxation.[3] We aimed also at optimizing two other parameters of importance in nanomagnets, namely the co-alignment of the axis of anisotropy and reduced inter-molecular interactions. This resulted in a single chain magnets characterized by energy gaps for the magnetization reversal of up to $\Delta/k_B = 113$ K.[4]



Key words: heptacoordination, molecular magnetism, molecular nano-magnets.

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Single Molecule Magnet behaviour and Luminescence in Lanthanides Complexes containing TTFs Ligands

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Lanthanide-based complexes have greatly contributed to the development of molecular magnetism in the last decade and more particularly in the branch of single molecule magnets (SMMs) [1]. The main reasons are their large magnetic moments associated to their intrinsic large magnetic anisotropy.

We will present an introduction to the molecular building blocks used as well as Lanthanide luminescence and SMMs properties. Then we will focus on TTF (tetrathiafulvalene)-based lanthanide mononuclear and polynuclear complexes showing luminescence through TTF antenna effect, SMM properties and combination of both SMM, luminescence, redox activity, memory effect in diluted frozen solution[3-5] and finaly, the recent finding of Redox- and Hydro- magnetic switches[6].

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RSC Tunisia Local Section Lecture on IYPT 2019

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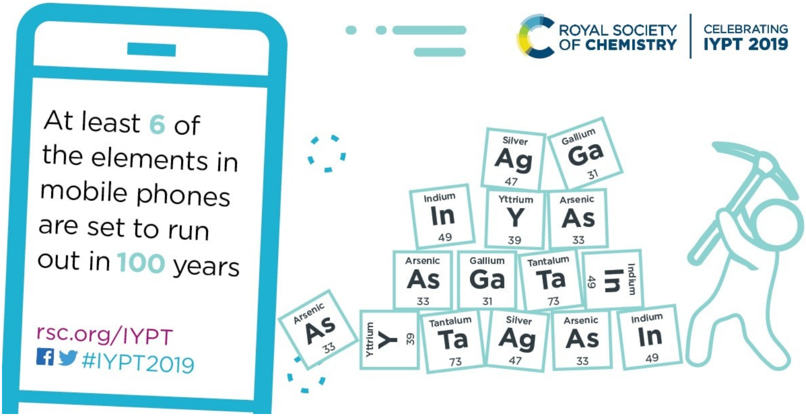
The periodic table of the elements is a great teaching tool and probably the most recognisable thing in chemistry. 2019 has been designated by UNESCO as the International Year of the Periodic Table (IYPT), marking the 150th anniversary of the Mendeleev periodic table, which is an iconic image and a vital tool to all who learn and work in science, at all stages of their learning and careers. In this lecture, IYPT is an opportunity for us to develop new resources and raise awareness, to inspire people of all ages, experience and backgrounds. The lecture will in particular highlight the importance of recycling the elements in danger used in electronic devices such as phones and smart TVs, which contain precious elements, yet the majority of households don't recycle them [1].



References

[1] Royal Society of Chemistry celebrating the IYPT 2019.

Oral Communications' List

(alphabetically authors' name)

Nr.		**Ref**
01	**<u>S. Agren</u>**, M. Chaabene, M. Lahcini, R. Ben Chaâbane, M.H.V Baouab *IPEIM - Monastir* Theoretical and experimental investigations of complexation with $BF_3.Et_2O$ effects on electronic structures, energies and photophysical properties of tetraphenyl (hydroxyl) imidazol	**OC11A**
02	**<u>C. Amiens</u>**, J. De Tovar, N. Thi Quyen, G. Lemercier, E. Rousset, P. Tran Dinh, R. Bofill, P. Lecante, J. García-Antón, K. Philippot, X. Sala *LCC-CNRS, Toulouse, France* Photosensitizer-nanoparticle diads for light driven water oxidation	**OC09A**
03	**<u>A. Begar</u>**, A. Begar, M-S. Chebah, A. Faddal *University of Biskra, Algeria* Zinc extraction from Ghazouat Leach residues	**OC08A**
04	**<u>M. Ben Aziza</u>**, Y. Litaiem, R. Chtourou, S. Ammar *CRTEn - Borj Cédria* The influence of different stabilizers on properties of sol-gel spin coated zinc oxide films: Photoelectrochemical performance	**OC02A**
05	**<u>A. Ben Othman</u>**, F. Ayari, R. Abidi, M. Trabelsi Ayadi *FSB - Bizerte* From calixarenes to hybrid materials	**OC03A**
06	**<u>N. Benbellat</u>**, S. Zeroual, S. Belhouchat, H. Soukehal, A. Gouasmia, S. Golhen, L. Ouahab *University of Batna1, Algeria* Synthesis, X-Ray structure and study of material based on TriMeTTF-CH=CH-py	**OC13A**
07	**<u>L. Boubakri</u>**, K. Dridib, A.S. Al-Ayed, I. Ozdemir, S. Yasard, N. Hamdi *ISSTE - Borj Cedria* Synthesis, characterization and antimicrobial studies of novel Ag(I)-N-heterocyclic carbene complexes	**OC04A**
08	**<u>M.A. Boughdiri</u>**, A. Mejri, B. Tangour *IPEIEM - Tunis* Theoretical study of the stability and reactivity of inclusion complexes inside carbon nanotubes	**OC13B**
09	**<u>M. Boutar</u>**, M.H. Noamane, N. Mattoussi, C. Desroches, R. Abidi, D. Luneau *FSB - Bizerte* Synthesis and coordination chemistry of acid and sulfonate derivatives of calix[4]arene	**OC20B**

Nr.		**Ref**
10	**E. Byusa**, K. Ndihokubwayo, T. Bimenyimana, I. Yutaka *University of Rwanda* Assessment of industrial wastewater effluent into urban ecosystem Kigali, Rwanda	**OC21B**
11	**V. Cesar**, I. Benaissa, K. Azouzi, M. Huynh, M.E. Morantin, Y. Tang, N. Lugan, V. Michelet, Y. Canac, S. Bastin *LCC-CNRS, Toulouse, France* Functionalized imidazo[1,5-*a*]pyridin-3-ylidene (IPy) ligands: Synthesis, coordination chemistry and catalysis	**OC09B**
12	**H. Dhifaoui**, W. Aloui, H. Saidi, A. Bouazizi, T. Boubaker *FSM - Monastir* Investigation of morphological, optical and electrical properties of MEH-PPV: BMN composite films	**OC05A**
13	**S. Dkhili**, S. López-Bernabeu, F. Huerta, F. Montilla, S. Besbes-Hentati, E. Morallón *FSB - Bizerte* A self-doped polyaniline derivative obtained by electrochemical copolymerization of aminoterephthalic acid and aniline	**OC17B**
14	**K. Ebeid**, F. Ebnou, M. M'haiham, C. L. Carpenter-Warren, A.M. Z. Slawin, J.D. Woollins, M.T. Ben Dhia, M.A.K. Sanhoury *Nouakchott University El Aasriya, Mauritania* Synthesis and structural characterization of Hg^{2+}, Cd^{2+} and Zn^{2+} complexes with tripyrrolidinophosphine chalcogenides	**OC12B**
15	**F. Ebnou**, M. M’haiham, K. Sidi, M.T. Ben Dhia, M.A.K. Sanhoury *Nouakchott University El Aasriya, Mauritania* Synthesis and spectroscopic characterization of cobalt(II) and nickel(II) complexes with tripiperidinophosphine chalcogenides	**OC11B**
16	**N. El Brahmi**, S. El Kazzouli *University of Fès, Morocco* New copper (II) and gold (III)-loaded phosphorus dendrimers: Synthesis and biological evaluation	**OC20A**
17	**K. Elghniji**, Y. Moussaoui, R. Ben Salem, E. Elaloui *FSG - Gafsa* Dysprosium doped TiO_2: Understanding the effect of DY^{3+} doping on the stabilization of TiO_2 sol and the sol-gel TiO_2 growth	**OC02B**

Nr.		**Ref**
18	**B. Es-Sounni**, M. Bakhouch, A. Nakkabi, I. Elaaraj, M. El Yazidi, N. El Moualij, M. Fahim *Moulay Ismail University, Morocco* Synthesis of tacrine-cyclam hybrids as promising treatment for Alzheimer's disease	**OC21A**
19	**K. Fajerwerg**, M. Puyo, C. Lepetit, M. Kahn, P. Fau *LCC-CNRS, Toulouse, France* Nanoparticle synthesis through an organometallic approach: From molecule to electrochemistry devices	**OC01A**
20	**M. Fray**, I. Hamzi, A. Thebti, A. Boudabbous, H.I. Ouzari, R. Abidi, T. Barhoumi-Slimi *FST - Tunis* Synthesis, characterisation and biological activities of N-acylhydrazones and their metal complexes	**OC03B**
21	**S. Ghrairi**, B. Crousse, T. Barhoumi-Slimi *FST - Tunis* Synthesis and characterization of new β-aminovinylimine tin(IV) complexes	**OC04B**
22	**R. Hanachi**, R. Ben Said, S. Boughdiri *FST - Tunis* Structural and energetic properties of tautomeric forms of thioamides and pyrazoles	**OC05B**
23	**A. Hannachi Jmai**, W.Smirani Sta, M. Rzaigui *FSB - Bizerte* Synthesis of isomorphous thiocyanate complexes: Metals effect on complexes properties	**OC06A**
24	**W. Jbali**, W. Selmi, L. Jouffret, M.F. Zid *FST - Tunis* Synthesis, crystal structure, vibrational study, optical properties and Hirshfeld surface analysis of $[Ni(C_6H_8N_2)_3]Cl_2 \cdot 2(H_2O)$	**OC06B**
25	**H. Jelali**, T. Dedours, S. Lebrun, E. Deniau, M. Sauthie, N. Hamdi *FSG - Gafsa* Hydro-functionalization of metallo-catalyzed 3-methylene isoindolinones. Application to the synthesis of anti-bacterial molecules	**OC07A**
26	**D. Kanzari Mnallah**, M.L. Efrit, A. Ben Akacha *FST - Tunis* Synthesis, characterization and theoretical analyzes of ligands containing 1,3,2-dioxaphosphorinane	**OC10A**

Nr.		**Ref**
27	**P. Lacroix**, I. Malfant, M. Tassé *LCC-CNRS, Toulouse, France* Nitric oxide Release from Ruthenium-nitrosyl complexes by Two-Photon Absorption	**OC14A**
28	**F. Laribi**, M.A.K Sanhoury, D. Merlet, I. Chehidi *FST - Tunis* Synthesis and characterization of new highly fluorinated *N*-phosphorylated carbamates	**OC07B**
29	**M. Louati**, R. Ksiksi, M.F. Zid *FST - Tunis* Preparation, crystal structure and IR spectroscopie of $(C_7H_{14}N)(C_2H_8N)_4(CH_2N)_2NO_3V_{10}O_{28}.6H_2O$	**OC10B**
30	**H. Mechi**, M.A.K. Sanhoury, E. Manoury, A. Bousseksou, M.T. Ben Dhia *FST - Tunis* Synthesis and coordination chemistry of new bis(fluoroalkyl) and dialkyl ferrocenylphosphonates	**OC08B**
31	**A. Mejri**, B. Tangour, F. Picaud *FST - Tunis* Molecular Dynamic study of drug confinement inside functionalized carbon nanotubes and their release near POPC membrane	**OC17A**
32	**A. Meklid**, Z. Necira, H. Menasra, A. Boutarfaia *Mohamed Kheider University of Biskra, Algeria* Phase formation, microstructure and dielectric properties of PZT–CNS piezoelectric ceramics	**OC18A**
33	**M. M'haiham**, K. Ebeid, F. Ebnou, K. Essalah, M.T. Ben Dhia, C.L. Carpenter-Warren, A.M.Z. Slawin, J.D. Woollins, M.A.K. Sanhoury *Nouakchott University El Aasriya, Mauritania* Zinc(II) and cadmium(II) complexes with tripyrrolidinophosphine oxide: Exprimental and theoretical DFT studies	**OC16B**
34	**K. Nasr**, M.A. Sanhoury, M. Grellier, B. Champagne, M.T. Ben Dhia *FST - Tunis* Tin(IV) complexes with organophosphorus ligands: An experimental and theoretical study	**OC15A**
35	**E. Rezgui**, C. Issaoui, N. Ouerfelli *FST - Tunis* Lithium motion in the crystal structure of $Li_3Fe_3\ (PO_4)_4$, A bond valence sum simulation	**OC16A**

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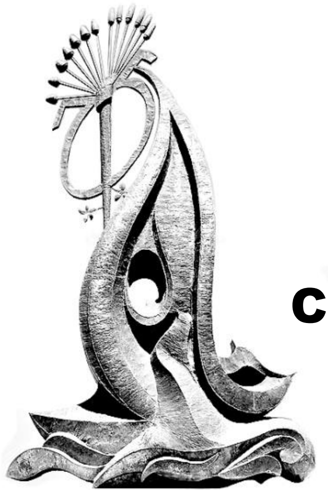
36	**A. Robert**, M. Nguyen, Y. Liu, B. Meunier *LCC-CNRS, Toulouse, France* N4-tetradendate ligands as regulators of copper homeostasis for Alzheimer's disease treatment	**OC1B**
37	**I. Slimani**, I. Özdemir, N. Hamdi *ISSTE - Borj Cedria* Synthesis of N-Heterocyclic carbene-palladium-PEPPSI complexes and their catalytic activity in the direct C–H bond activation	**OC12A**
38	**S. Slimi**, P.Loiko, M. Aguiló, F. Díaz, R.M. Solé, X. Mateos, E. Ben Salem *FSM - Monastir* Europium doped Sodium Bismuth fluorapatite, $Ca_8NaBi(PO_4)_6F_2$, prepared by Pechini process, as a single-component phosphor for white-emitting n-UV convertible phosphor for w-LEDs	**OC18B**
39	**J. Volkman**, M. Darrows, N. Gimeno, M. Gouygou *LCC-CNRS, Toulouse, France* Coordination-driven self-assembly of chiral palladium(II)-based supramolecular coordination complexes	**OC14B**
40	**R. Zarroug**, A. Haj-Abdallah, P. Guionneau, B. Ayed *FSG - Gabès* The new decavanadate compound $(C_5H_{11}N)_4[V_{10}O_{28}]$ 3.25H_2O: Synthesis, characterization and Hirschfield surface analysis	**OC15B**
41	**S. Zeroual**, S. Belhouchat, H. Soukehal, N. Benbellat, H. Chermette *University of Batna1, Algeria* DFT study of organic-inorganic materials based on TTF-derived ligands	**OC19A**
42	**C. Zidani**, B. Benyoucef *University of Tlemcen, Algeria* Analysis of a novel design of conical solar furnace supplied by optical fibers	**OC19B**
43	**H. Chermette**, W. Lamine, L. Merzoud, S. Boughdiri, L. Christ, C. Morell *Université Claude Bernard Lyon 1, Villeurbanne, France* Understanding of Zn-sal(ph)en complexes coordination: Tetrahedral coordination or penta-coordination?	**OCAB**



Oral Communications’ Abstracts

Program of
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27 September 2019

NANOPARTICLE SYNTHESIS THROUGH AN ORGANOMETALLIC APPROACH: FROM MOLECULE TO ELECTROCHEMISTRY DEVICES

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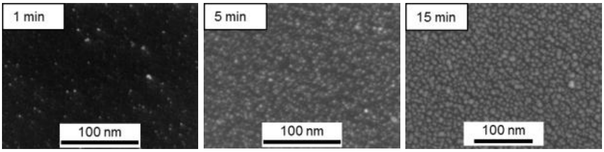
The main objective of the "Nanochemistry, Organization and Sensors" group is to synthesize nanoparticles (NPs) from the organometallic route and use them for the design and development of sensors. This approach is based on various fundamental steps ranging from molecules to devices. In order to investigate the determining factors for the control of the synthesis, the early molecular species formed during the very first steps of the organometallic synthesis, is also studied using a computational molecular approach.

For this purpose, the synthesis of nanoparticles from organometallic precursors is a relevant approach to obtain controlled size, shape and surface chemistry nanomaterials. Indeed, the integration of nanoparticles by this approach requires, beyond the control of their synthesis, a perfect knowledge of their properties (chemical, physicochemical and physical),[1-4] in order to achieve high-performance devices.[5-6] This involves an understanding of the different stages of synthesis and developing new strategies to tune the properties of these nano-objects (in solution or on substrate).

In the present work, We will illustrate this approach through the example of silver nanoparticles (AgNPs) deposited on well defined carbon based surfaces, ultra-flat carbon films formed *via* the pyrolysis of photoresist resins films (PPF) coated on a doped silicon substrate. PPF substrates have been decorated with AgNPs *via* the liquid-phase hydrogenolysis of organometalic silver precursors. AgNPs/PPF composite electrodes have been characterised by SEM, AFM and Raman analyses. These electrodes have been used as working electrode for the detection of 4-nitrophenol, used as a model pollutant



SEM pictures of AgNPs/PPF surfaces with different hydrogenolysis times.

Key words: Organometallic precursors, nanoparticles, surfaces functionalisation, electrochemical sensors, 4-nitrophenol.

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THE INFLUENCE OF DIFFERENT STABILIZERS ON PROPERTIES OF SOL-GEL SPIN COATED ZINC OXIDE FILMS: PHOTOELECTROCHEMICAL PERFORMANCE

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In this study, Zinc oxide thin films have been deposited on FTO substrates by a sol–gel spin coating technique. X-ray diffraction, UV–visible spectrophotometer and photoluminescence spectroscopy have been employed to investigate the effect of different sol stabilizers: monoethanolamine (MEA), diethanolamine (DEA), triethanolamine (TEA) and diethylene glycol (DEG). The XRD analysis shows that the films have hexagonal structure with a preferred growth orientation along the (002) plane indicating that the type is Wurtzite, the average size of crystallites varies from 46,277 to 82,266 nm, Room temperature photoluminescence spectra indicate UV emission at around 377 nm originated from nearby band-edge transitions. Photoelectrochemical performances show that the ZnO films synthesized with diethylene glycol exhibited higher photocurrent.

Key words: Zinc oxide, Thin films, Sol–gel, Spin-coating, Different sol stabilizers, Photoelectrochemical performances

From calixarenes to hybrid materials

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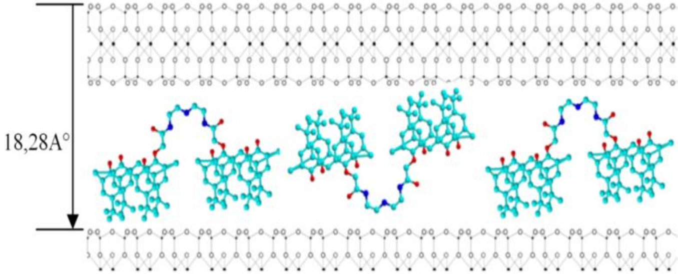
Currently, and faced with the environmental problems caused by pollution of various types, the research work carried out by scientists around the world seems to be increasingly converging towards the protection and enhancement of natural resources. In the particular context of water pollution by chemicals, we thought about the development of new clay-calixarenic hybrid materials. The interest of these hybrids lies in the fact that they have higher performances than the elements taken separately. We considered calixarenes as an organic part and clay as an inorganic part. Indeed, the calixarenes, with their particular architecture, have shown their effectiveness in a multitude of areas, in particular as a platform for the development of nano-composites, in the medical or environmental field. This clay-calixarenic combination was made while trying to respect the environment, by co-grinding in the solid phase.

Following the synthesis of a di-calixarenic derivative, we studied these complexing and extracting properties with respect to metal cations, and then used it to prepare a clay-calixarenic hybrid material.



The confirmation of the intercalation of the calixarenes in the interfoliar space of the clay has been demonstrated by comparison of infrared spectra as well as by X-ray diffraction.

Following a preliminary study of liquid-solid extraction, the retention of two active ingredients has been studied.

It should be noted that in terms of retention capacity, calixarenes are significantly more effective than clay.

On the other hand, the extracting power of the clay is optimized by the incorporation of calixarenic derivatives.

SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL STUDIES OF NOVEL Ag(I)-N-HETEROCYCLIC CARBENE COMPLEXES

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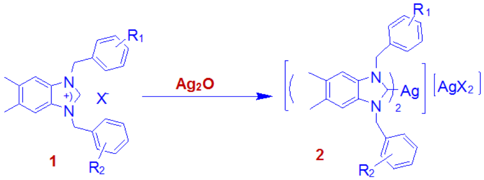
N-Heterocyclic Carbene (NHCs) which are strong σ-donor, low π-acceptor ability, and transition metal carbene complexes obtained by using carbene precursors have had a wide application area in organometallic chemistry[1]. Among various transition metal carbene complexes, silver-N-heterocyclic carbene complexes have played a significant role in the development of NHCs chemistry because of their structural diversity and their widespread successful application as effective carbene transfer reagents in transmetallation reactions. Also, the prominent biological activity of many Ag-NHC complexes as antimicrobial and anticancer agents has been confirmed[2]. Here we report the synthesis of Ag-NHC complexes **2** which obtained from the reaction of 5,6-dimethylbenzimidazolium salts **1** with the addition of silver oxide[3]. The obtained complexes were characterized by ^{1}H and ^{13}C NMR, FT-IR and elemental analysis techniques. In addition, it has been shown higher antimicrobial activity than the free ligand.



Key words: N-Heterocyclic Carbene, Ag-NHC complexes, antimicrobial activity.

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Investigation of morphological, optical and electrical properties of MEH-PPV:BMN composite films

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In the recent decades, π-conjugated small organic molecules have received a much deal of attention as semiconductor materials in optoelectronic applications such as organic light emitting diodes (OLEDs) and organic solar cells (OSCs) **[1.2]**. We aim to incorporate of p-cyano-benzylidenemalononitrile (BMN) molecules in MEH-PPV polymer. We have investigated the effect of BMN concentration on the morphological, optical and electrical properties of conjugated polymer Poly [2-methoxy-5-(2- ethylhexyloxy)-1,4-phenylenevinylene] (MEH-PPV). The surface morphology study via scanning electron microscopy (SEM) of the composite films shows obviously change with the addition of BMN. Introduction of BMN in MEH-PPV leads to a broadening of absorption spectra at the higher wavelengths and a strong quenching of the photoluminescence intensity, suggesting an effective charge transfer between these two organic compounds. The dark I–V characteristics for the ITO/MEH-PPV:BMN/Al structure indicate typical rectifying behavior.

Key words: BMN, composite films, photoluminescence quenching efficiency, I-V characteristics

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SYNTHESIS OF ISOMORPHOUS THIOCYANATE COMPLEXES: METALS EFFECT ON COMPLEXES PROPERTIES

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Many researches focus on metal coordination compounds due to their catalytic[1], fluorescent [2] and magnetic properties. The reaction of 2-methylpiperazine with the thiocyanate ligand and two transition metals leads to the production of two new isomorphous [ML_2SCN_4] where L is the 2-methylpiperazine and [M =Co (1), and Ni (2)], presenting an octahedral configuration. These compounds were characterized by single crystal X-ray crystallography, TG-DTA analysis, as well as infrared and UV-Vis spectroscopy. The magnetic and antibacterial properties are also determined. The studied complexes show the metal center's impact leading to different properties. Indeed the first compound shows high spin orbit coupling, whereas the second one shows a weak antiferromagnetic interaction. The antibacterial activity is enhanced for the nickel compound compared with the cobalt compound and the DTA/TG curves show a phase transition for the nickel compound.

Key words: isomorphous structure, antibacterial activities, magnetic properties.

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Hydro-functionalization of metallo-catalyzed 3-methylene isoindolinones. Application to the synthesis of anti-bacterial molecules.

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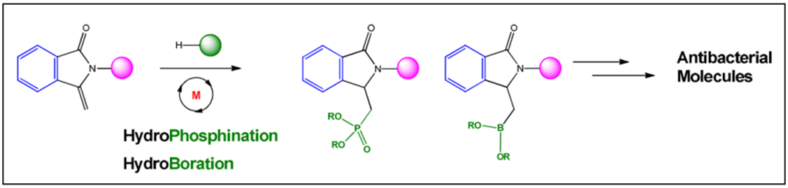
Bacterial resistance to antibiotics is a major public health problem. The emergence and spread of multi-resistant bacteria, associated with the limited number of antibiotics under development, has led to a therapeutic stalemate. The discovery of innovative antibacterial molecules, able to act by new modes of action, has become indispensable. In this context, the modified peptides incorporating a borate analogue of various α- or β-amino acids have demonstrated interesting antibacterial activities.[1]We propose to synthesize various stiffened analogs of b-aminoboric acids based on a copper-catalyzed enamidal hydroboration reaction of 3-methylene isoindolinones.[2]In a second step, the compounds obtained by derivatization of the boronic esters formed will be tested on various bacterial strains to evaluate their activity.



Key words: Hydroboration, Copper-catalyst, Antibacterial Molecules

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ZINC EXTRACTION FROM GHAZOUAT LEACH RESIDUES

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In this paper, it was aimed to select and propose a feasible as well as an applicable method, for the extraction of zinc that is present in the disposed GHAZOUAT leach residues having 17.82 wt. % Zn and 20.82 wt. % Fe. After determination of the components of the residue, acid leaching was performed to reclaim Zn sequentially. Acid leaching experiments were done for Zn extraction by controlling acid concentration, reaction duration and reaction temperature. At the optimum conditions, 240 g/l H_2SO_4 at 90°C for 210 min, 80% of initial iron content was removed.

Key words: sphalerite, Zn, acid leaching, leaching residue, extraction.

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PHOTOSENSITIZER-NANOPARTICLE DIADS FOR LIGHT DRIVEN WATER OXIDATION

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The water oxidation (WO) reaction is a thermodynamically uphill, mechanistically complex and kinetically slow process that limits the production of H_2 from water unless catalytically promoted. Recent literature data underline the interest of a rational design of hybrid photosensitizer-nanoparticle (PS-NP) catalysts from abundant first row metals to cost-efficiently catalyze the WO reaction.[1] The organometallic approach, which affords NPs with high control over the size, composition and surface properties,[2] offers opportunities towards the synthesis of PS-NP diads with covalent bonding between the PS and the NP. Here we report the organometallic synthesis Co and Fe NPs and their controlled oxidation into Co_3O_4 NPs and core-shell Fe/FeOx NPs. Then we present the grafting of polypyridyl-Ru^{II} complexes at the surface of these NPs and first results in light driven WO.

Key words: nanochemistry, coordination chemistry, water splitting

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Synthesis, characterization and theoretical analyzes of ligands containing 1,3,2-dioxaphosphorinane

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1,3,2-Dioxaphosphorinanes derivatives belong to the large family of organophosphorus heterocyclic compounds which continue to receive attention due to their interesting applications in different fields[1].

Our approach towards the synthesis of Oxo, Seleno, Thioxo 2-alkylamino-5-methyl-5-propyl-1,3,2-dioxaphosphorinane **3** is based on two steps sequence. The first step involves the reaction of 2-chloro-5-methyl-5-propyl-1,3,2-dioxaphosphorinane **1** with a set of primary amine. The second step consists in the oxidation of the resulting intermediates **2**. Their characterization is performed by NMR (^{31}P, ^{1} H, ^{13}C), MR-SM, X-ray diffraction. Experimental and theoretical ^{31}P, ^{13}C, ^{1}H NMR chemical shifts were compared [2].

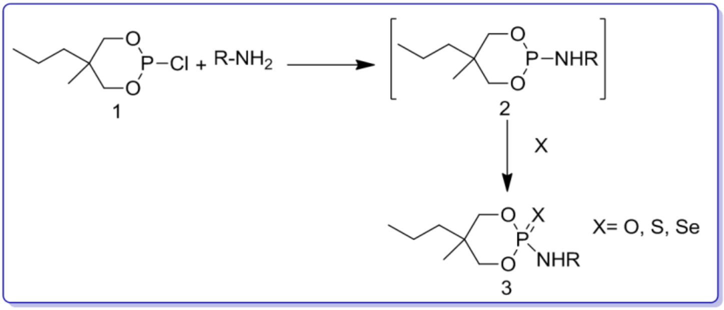

Fig 1. Synthesis of Oxo, Seleno, Thioxo 2-alkylamino-5-methyl-5-propyl-1,3,2-dioxaphosphorinane **3**

Key words: dioxaphosphorinane derivatives, heterocyclic synthesis, ligands

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Theoretical and experimental investigations of complexation with $BF_3.Et_2O$ effects on electronic structures, energies and photophysical properties of tetraphenyl (hydroxyl) imidazol

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Fluorescent Heterocyclic compounds have numerous applications in several life fields [1, 2, 3, 4, 5] such as metal ions detection [6]. We synthesized a tetra substituted hydroxyl phenyl imidazole (HPI) through four component condensation of benzyl, salicylic aldehyde, aniline and ammonium acetate as a source of ammonia and acetic acid as the solvent and its boron difluoride complex (Borate) using BF_3, Et_2O in distilled toluene. Both synthesized compounds chemical structure was resolved using different spectroscopic techniques (Fourier transforms IR, NMR, UV-vis and PL).[7] In addition to experimental analysis, density functional theory (DFT) calculations at the B3LYP/6-311 +G (d, p) level were performed to obtain the optimized geometry and spectroscopic and optical properties. Natural Bonding Orbital (NBO), and nature population analysis (NPA) were performed after optimization of geometry at the same basis set (6-311++ G (d,p)) and all the electronic and quantum chemical parameters (FMOs) of the title compounds were calculated at the CAM-B3LYP-D3 method using 6-311++G (d, p).[8] The HBI Molecule showed good photophysical behavior even after complexation using BF_3, Et_2O due to excited state intramolecular proton transfer (ESIPT) mechanism. The absorption and emission spectra of the model compounds were also simulated and compared to experimental observations in the DMF solvent. Overall, the DFT calculation results supported the structural and spectroscopic experimental data and confirmed the structure modification of frontier molecular orbitals for BF_2 complexes as well as tunable potentials and energy levels.[7]

Key words: DFT calculations, HPI, Borate, FTIR, Fluorescence NBO, HOMO-LUMO analysis, Optical properties

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Synthesis of N -Heterocyclic carbene-palladium-PEPPSI complexes and their catalytic activity in the direct C–H bond activation

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The palladium-catalyzed direct arylation of various heteroaromatics including pyrroles by a C–H bond activation using aryl halides has met great success in recent years, allowing the synthesis of a wide variety of arylated heteroaromatics in only one step [1]. Since these exciting results, the palladium-catalyzed direct arylation of various heteroaromatics with aryl halides has proved to be a powerful method for the synthesis of a wide variety of arylated heterocycles [2]. it's a valubal method for the formation of C(sp^2)–C(sp^2) bonds in contemporary organic synthesis, because of the numerous applications of heteroaromatic compounds as biologically active compounds and functional materials[3].
For this reason, we synthesized a series of new palladium-NHC-PEPPSI complexes. These compounds were characterized by ^{1}H and ^{13}C NMR spectroscopy and IR spectroscopy. We then examined the activity of the PEPPSI-type palladium–NHC complexes in the direct C5-arylation of 2-substituted heteroaromatics derivatives, with various aryl bromides as coupling partners.

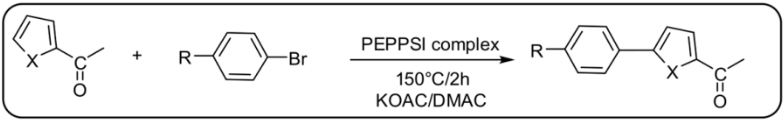

Fig. PEPPSI complex catalysed catalyzed direct C5-arylation

Key words: palladium, N-heterocyclic carbenes, C-H bond activation, arylation.

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SYNTHESIS, X-RAY STRUCTURE AND STUDY OF MATERIAL BASED ON TriMeTTF-CH=CH-py.

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The charge transfer complexes (CTC), radical cation salts (RCS) and hybrid materials based on organic donors such as TTF (tetrathiafulvalene) and its derivatives have been extensively studied.

Ligands based on the pyridine cycle have played a major role in the development of coordination chemistry. Indeed, these nitrogen heterocyclics form stable complexes with transition metals [1, 2]. The uniqueness of the diversity of molecular systems have been achieved major advances in various fields of applications ranging from designing catalysts, materials for optoelectronics, development of derivatives for medical therapeutic [3-5].

In this context, we describe the synthesis and study of organic/ inorganic hybrid material involving a coordination between a paramagnetic transition metal and a TTF aromatic containing a nitrogen bonded via a covalent bridge conjugate; Cu(hfac)2(TriMeTTF-CH=CH-py)1, [hfac = hexafluoro-acethylacetonate]. The complexe crystallizes in the monoclinic system, space group C2/c. The metal lies in a square-pyramidal environment formed by four O atoms and the N atom of the pyridyl.

Key words: Hybrid materials**,** pyridine-unsymmetrical TTF molecules, redox potentials, electrochemical synthesis and chemical synthesis.

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N4-TETRADENDATE LIGANDS AS REGULATORS OF COPPER HOMEOSTASIS FOR ALZHEIMER'S DISEASE TREATMENT

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Alzheimer's disease (AD) is a multi-parameter disease far from the simple concept "one disease, one target-protein, one drug". The dysregulation of metal homeostasis, especially copper, linked to tau pathology, Aβ-aggregation and mitochondrial dysfunction, in the brain of AD patients is at the origin of the oxidative stress responsible for neuron death. Selective chelators able to regulate copper homeostasis are therefore considered as putative anti-Alzheimer drugs.

We designed new tetradentate ligands named "TDMQ" ("TetraDentate MonoQuinolines"), based on a 8-aminoquinoline skeleton, substituted at C2 by a bis-chelating side chain. These ligands are specific for Cu(II) chelation, and not suitable for Cu(I). In fact, due to their coordination properties designed to generate N4-tetradentate square planar Cu(II)-TDMQ complexes, these chelators are able to extract copper ions trapped by amyloids and to transfer them to glutathione which is a natural provider of copper to proteins.

So, *in vitro*, TDMQ are able to retrieve copper from its pathological sink Cu-Aβ, and to reintroduce it into physiological circulation, thus avoiding the oxidative damage that are a hallmark of Cu-Aβ. *In vivo*, these chelators have the capacity to fully reverse the deficit of episodic memory in a reliable non-transgenic mouse model of AD. This clearly confirms that restoration of copper homeostasis is a valuable therapeutic target.

The design of metal chelators as therapeutic agents able to counteract deleterious consequences of metal misregulation in AD brain, must take into account the necessary coordination chemistry background to select the suitable drug-candidates and to enhance the chance of success in clinical trials.

Key words: Alzheimer's disease, Copper homeostasis, Oxidative stress

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DYSPROSIUM DOPED TIO_2: UNDERSTANDING THE EFFECT OF DY^{3+} DOPING ON THE STABILIZATION OF TIO_2 SOL AND THE SOL-GEL TIO_2 GROWTH

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In this work we provide a new investigation on the synthesis of Dy^{3+} doped TiO_2 particles by hydrolysis-condensation at low molar ratio ($[H_2O]/[Ti] = 1.5$), with emphasis on the effect of the Dy^{3+} doping on the growth of TiO_2 anatase particles. Thermogravimetric, differential thermal analysis (TG/DTA) and nuclear magnetic spectroscopy (^1H NMR) show that the presence Dy^{3+} ions slow down the particle growth in water and stabilize the TiO_2 colloidal sol. The effect of Dy^{3+} doping was proved to disprut the mechanism growth of TiO_2 anatase during the heat treatement, leading to amorphization of TiO_2. Scanning electron microscopy (SEM) of the undoped TiO_2 showed non-sintered TiO_2 microspheres. Doping of Dy^{3+} remarkably affects the size and morphology of TiO_2 particles.

Key words: Dy^{3+} doped TiO_2, colloids, microspheres, nucleation, growth, NMR

Synthesis, characterisation and biological activities of N-acylhydrazones and their metal complexes

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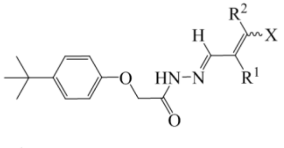
N-Acylhydrazones (NAHs) belong to an important class of biologically active compounds, as anti-inflammatory, anti-cancer and anti-microbial agents [1-3]. Moreover, metal complexes of N-acylhydrazones have been found to have therapeutic activity and this is one practical reason for the continuing interest in these materials [4]. In this work, we describe the synthesis of new metal complexes from the corresponding *β*-chloro-α,β-unsaturated *N*-acylhydrazones. The new adducts were fully characterized by multinuclear NMR, IR, and UV-Vis spectroscopies. The magnitude of the metal-ligand interaction was estimated on the basis of the azomethine valence vibration values and used to classify the NAHs according to their Lewis basicity. Comparative study of biological activity of both ligands and their complexes will be presented.

$$L \quad + \quad MX_2 \quad \xrightarrow[\text{rt, 6h}]{\text{MeOH}} \quad [MX_2L]$$

L:



R^1= H, Et,Me, Pr
R^2=^{t}Bu, Me, Et, Bu, Pr,^{i}Bu

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Synthesis and characterization of new β–aminovinylimine tin(IV) complexes

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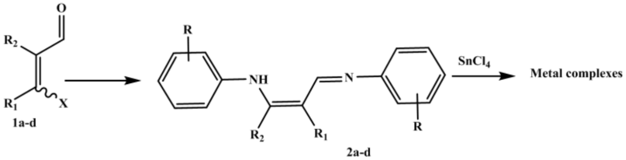
During the last decays, Schiff bases have gained importance in medicinal and pharmaceutical fields due to their broad spectrum of biological activities such as anti-inflammatory [1], analgesic [2], antimicrobial [3], anticonvulsant [4], antitubercular [5], anticancer [6,7], antioxidant [8], anthelmintic [9]. Moreover, they have been used as catalysts, intermediates in organic synthesis, dyes, pigments, polymer stabilizers [10], and corrosion inhibitors [11]. In this work, we report the synthesis and the characterization of new series of β–aminovinylimines and their tin(IV) complexes. The adducts have been characterized in solution using multinuclear (^{1}H,^{13}C and ^{119}Sn) NMR and IR spectroscopy.



Keywords: β-aminovinylimines, tin(IV) complex, characterization, ^{119}Sn NMR.

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Structural and energetic properties of tautomeric forms of thioamides and pyrazoles

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Quantum chemistry is a very powerful tool to study the properties of molecules and their reactions. The recent years, development in quantum chemistry methods, especially that of density functional theory (DFT) methods [1], has made it possible for quantum chemistry calculations to reach accuracies comparable to those obtained in experiments for molecules of moderate sizes. Thioamides and its derivatives are widely used in various chemical applications, they are considered as intermediates in the synthesis of some heterocyclic compounds like thiazoles and amidines. Stable tautomeric forms in a series of phosphonyl thioamides have been studied using DFT methods. The molecules studied in this contribution present a phosphonyl group in β-position of the C–S bond connected to the amine group. The three most stable tautomeric forms with double bonds on either C=N, C=S, or adjacent C=C have been described, and their relative energies together with the transition barriers have been evaluated [2].

The reaction of formation of pyrazole through the action of hydrazine on the thioamide was studied at the DFT level with B3LYP, M05-2x and PBE0 functional using local and global reactivities and by determining the corresponding barriers to each step. Also, we have established a QSAR model based on linear regression to generate a correlation between descriptors and the corresponding activity, to predict the activity of pyrazole derivatives.

Key words: Thioamides, pyrazole, DFT, QSAR.

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Synthesis, crystal structure, vibrational study, optical properties and Hirshfeld surface analysis of $[Ni(C_6H_8N_2)_3]Cl_2{\cdot}2(H_2O)$

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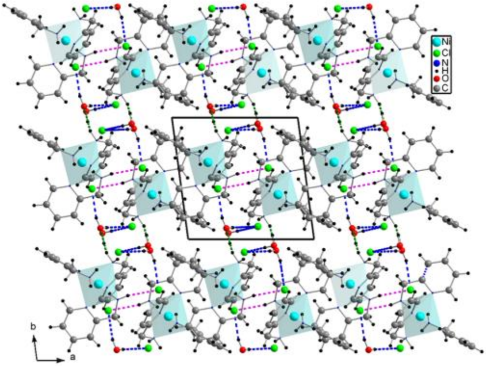
A novel compound dichloro tris (2-aminomethylpyridine) nickel (II) dihydrate, formulated as $[Ni(C_6H_8N_2)_3]Cl_2.2(H_2O)$, was synthesized by the slow evaporation method at ambient temperature. Single-crystal X-ray diffraction analysis indicates that the title compound crystallizes in the triclinic system, P-1 space group with a = 10.222(2) Å, b = 10.757(2) Å, c = 11.441(3) Å, α = 114.30(4) °, β = 99.43(3) °, γ = 93.01(3) °.

In the crystal structure, cohesion achieved through the π-π interactions [1] between the two adjacent dimers, thus a three-dimensional network has been formed by the donor-acceptor interactions of the hydrogen bonds N-H ... Cl, O-H ... Cl and N-H…O. The functional groups present in the crystal were studied by FTIR spectroscopy. Investigation of the optical properties of the compound confirmed its semiconducting properties by revealing a direct optical band. The three-dimensional Hirshfeld surface (3D-HS) analysis and the two-dimensional fingerprint plots (2D-FP) reveal that the structure is dominated by the H⋯Cl/Cl⋯H and H/H contacts

Key words: nickel complex, Crystal structure, Vibrational study, Hirshfeld surface analysis



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Synthesis and characterization of new highly fluorinated *N*-phosphorylated carbamates

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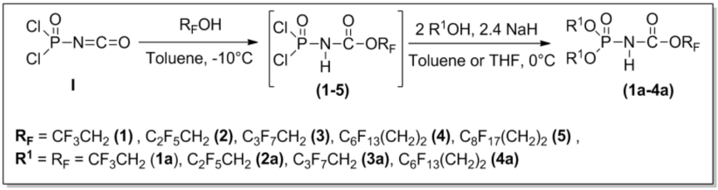
N-phosphorylated carbamates are a class of organophosphorus compounds which have great potential to be used as a pesticides [1], insecticides [2], herbicides [3], flame retardants [4] and antimicrobial agents [5]. They have structural resemblance to acetylcholine, and they possess high affinity for the enzyme cholinesterase [6]. In particular, substituted phosphinylcarbamates gained much interest due to their potential activity against several forms of tumors [7]. In the present work, a one-pot synthesis of new highly fluorinated phosphorylated carbamates (**1a-4a**) was performed from isocyanatophosphonicdichloride (**I**) [8] through the intermediate dichlorophosphinyl carbamates (**1-5**). They have been characterized by multinuclear (^{1}H, ^{13}C, ^{31}P and ^{19} F) NMR and IR spectroscopy. The preliminary coordination chemistry study of these phosphorylated carbamates as potential ligands towards metal cations will be also discussed.



R_F = CF_3CH_2 **(1)**, $C_2F_5CH_2$ **(2)**, $C_3F_7CH_2$ **(3)**, $C_6F_{13}(CH_2)_2$ **(4)**, $C_8F_{17}(CH_2)_2$ **(5)**,
R^1 = R_F = CF_3CH_2 (**1a**), $C_2F_5CH_2$ **(2a)**, $C_3F_7CH_2$ **(3a)**, $C_6F_{13}(CH_2)_2$ **(4a)**

Keywords: Phosphoryl isocyanate, carbamate, fluoroalkyl alcohol, ^{31}P NMR.

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Synthesis and coordination chemistry of new bis(fluoroalkyl) and dialkyl ferrocenylphosphonates

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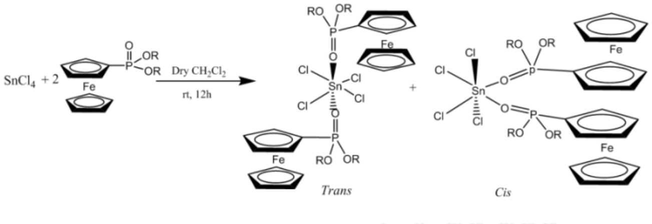
Organophosphorus compounds have attracted considerable attention due to their wide industrial, agricultural, biochemical, and medicinal applications as well as their utility as synthetic intermediates [1-3]. Chemical, physical, and biological properties of such compounds are governed by the substituents around the phosphorous atom. For instance, ferrocenyl-containing compounds are considered as very powerful sensors for metal ions with unique features in metal-catalyzed organic reactions[4,5] as well as potent antimalarial agents[6]. In this context and in continuation of our work on organophosphorus compounds[7], we were inspired to incorporate a ferrocenyl group into different alkyl and fluoroalkyl phosphorus-containing derivatives for the synthesis of new ferrocenylphosphonates. The coordination properties of these compounds as ligands towards tin(IV) chloride were investigated. The bimetallic adducts, thus produced, were characterized by multinuclear (^{1}H, ^{31}P and ^{119}Sn) NMR, IR and UV-Vis spectroscopic techniques. The solution NMR data of these complexes showed the presence of a mixture of *cis* and *trans* isomers. The results are discussed and compared with those obtained for analogous phosphate complexes.



Keywords: Ferrocenylphosphonate, fluoroalkyl, tin(IV) complex, ^{31}P and ^{119}Sn NMR.

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Functionalized imidazo[1,5-*a*]pyridin-3-ylidene (IPy) ligands: Synthesis, coordination chemistry and catalysis.

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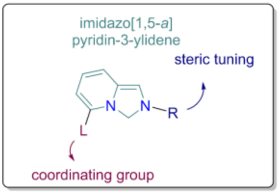
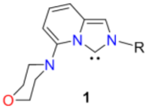
Over the last two decades, N-Heterocyclic Carbenes (NHCs) have gained considerable significance in modern chemistry.[1] We have recently initiated a research program aiming at developing new generations of functionalized NHCs based on the rigid, bicyclic imidazo[1,5-*a*]pyridin-3-ylidene (IPy) framework, a relatively underexplored class of NHCs.[2]

In this communication, we present the chemistry of the three new NHCs **1**, **2** and **3**$^-$, bearing a morpholine, an iminophosphorane and an anionic 'malonate' unit.





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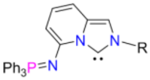

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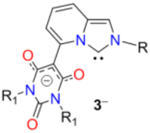

3$^-$

The imidazo[1,5-*a*]pyridinium precursors **1**·HBr, **2**·HOTf and **3**·H were easily obtained on gram scale using a new, highly modular, divergent, and versatile synthetic strategy. Their coordination chemistry towards metallic centers will be then presented, as well as the implementation of the resulting pre-catalysts in homogeneous catalysis.[3,4]

Keywords: carbene, heterocycles, gold, catalysis, organometallic compounds.

Acknowledgment: Support by the CNRS and the ANR (grant ANR-16-CE07-0006-03, GOLDWAR) is gratefully acknowledged.

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PREPARATION, CRYSTAL STRUCTURE AND IR SPECTROSCOPIE OF $(C_7H_{14}N)(C_2H_8N)_4(CH_2N)_2NO_3V_{10}O_{28}.6H_2O$

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Polyoxometalates (POMs) are a kind of inorganic clusters which can be combined with organic ligands and metal ions to form supramolecular compounds. These groups have been extensively studied due to their potential applications in various fields such as catalysis and materials science [1].

A new decavanadate, $(C_7H_{14}N)(C_2H_8N)_4(CH_2N)_2NO_3V_{10}O_{28}.6H_2O$, was synthesized by slow evaporation at room temperature and characterized by single-crystal X-ray diffraction and IR spectroscopie.

The compound crystallizes in the triclinic system, P-1 space group with the cell parameters: a=10.762(3)Å, b=13.273(2)Å, c=18.928(4)Å, α=72.64(2)°, β=81.51(3)°, γ=66.05(2)°, Z=2 and volume V=2357.4(1)Å^3.

The formula unit is composed of: one decavanadate group $V_{10}O_{28}^{6-}$, one organic cation $(C_7H_{14}N)^+$, four organic

cations $(C_2H_8N)^+$, two organic cations $(CH_2N)^+$, one nitrate group and six water molecules (Fig 1).

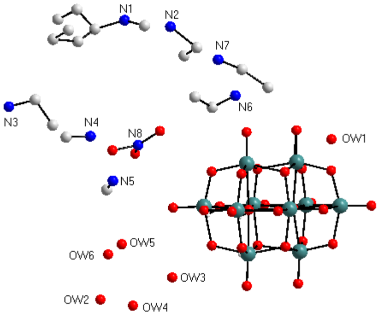

Fig 1. Presentation of unit formula in $(C_7H_{14}N)(C_2H_8N)_4(CH_2N)_2NO_3V_{10}O_{28}.6H_2O$ compound

Key words: Decavanadate, Crystal structure, IR spectroscopie.

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Synthesis and spectroscopic characterization of cobalt(II) and nickel(II) complexes with tripiperidinophosphine chalcogenides

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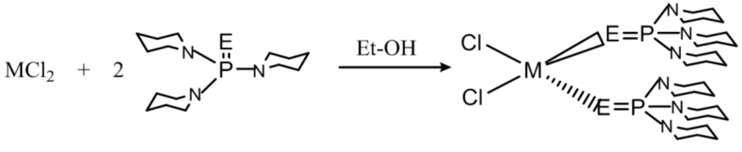
Phosphine chalcogenides of the formula $(R_2N)_3PE$ (E = O, S or Se) are attracting considerable interest owing to their biological activity and selective affinity towards metal ions [1,2]. In particular, transition metal complexes with this type of ligands have been intensively studied in the last years due to their diverse and useful applications [3,4]. In a previous work, we have synthesized a series of Cd^{2+} and Hg^{2+} complexes with tripiperidinophosphine chalcogenides, Pip_3PE (E = O, S or Se)) [5]. In this presentation, we extend the chemistry to transition metalcations and report herein on coordination chemistry of these ligands towards$Co^{2+}$and Ni^{2+}. As a result, complexes of cobalt(II) and nickel(II) chlorides with tripiperidinophosphine chalcogenides were synthesized and fully characterized by UV-Vis, NMR and IR spectroscopic techniques. The results will be compared to those obtained with cadmium(II) and mercury(II) chloride analogs.



M = Co^{2+} or Ni^{2+}; E = S or Se

Keywords: Phosphine chalcogenide, piperidinyl, cobalt and nickel complexes, NMR, UV-Vis.

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SYNTHESIS AND STRUCTURAL CHARACTERIZATION OF Hg^{2+}, Cd^{2+} AND Zn^{2+} COMPLEXES WITH TRIPYRROLIDINOPHOSPHINE CHALCOGENIDES

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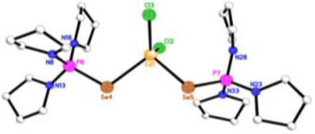
Phosphine chalcogenides of the type R_3PE (E = O, S, Se) are prevalent in the coordination chemistry of both transition and main group metals [1], having found important applications in the fields of bioinorganic chemistry [2] and nanoscience [3], For example, there has been a renewed interest in the metal complexes of this class of compounds in view of their increasing use as suitable single-source precursors for the production of binary metal chalcogenide thin films ME (M = Zn, Cd or Hg;E = S, Se or Te) as well as ME quantum dots [3, 4]. In a previous study, we have reported on mercury, cadmium and zinc complexesù with tripiperidinophine chalcogenides and showed that they exist as dimeric species [5]. Herein, we describe the coordination chemistry of tripyrrolidinophosphine chalcogenides $Pyrr_3PE$ (E = S or Se) towards the same metal cations. The complexes were prepared and characterized by multinuclear (^1H and ^{31}P) NMR, UV-Vis, IR, conductivity and X-Ray analysis. The structures of these complexes were confirmed with X-Ray, NMR and conductivity which reveal that these complexes are tetrahedral adducts containing coordinated chloride atoms and two ligand molecules around the metal center. The results will be discussed and compared to those obtained for their bulkier analogues.



Keywords: Phosphine chalcogenide, pyrrolidinyl group, metal complex, NMR.

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Theoretical study of the stability and reactivity of inclusion complexes inside carbon nanotubes

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Université Tunis El Manar, Unité de recherché Modélisation en Sciences Fondamentales et Didactique, Institut Préparatoire aux Etudes d'Ingénieurs d'El Manar,

The formation of pentacoordinated molecule testifies of sp^3d phosphorus atom hybridization. Phosphorus is known to have biphilic behavior. We will try in this work to respond to issues concerning the nucleophilic and electrophilic steps such as: i) Are- they consecutive or simultaneous? ii) Are they synchronized or independent? iii) Are they regio and/or stereo selective or specific? iv) is-it possible to control the selectivity or specificity by confinement inside carbon nanotubes?

Calculations details

Optimizations of geometries were carried out at the DFT/B3LYP using the Gaussian09 software. We verified that all the saddle points correspond well to the transition states through the tracing of the energy profiles (IRC). Several basis sets with increasing dimension has been tested (6-311G(d,p), (6-311++G(d,p), aug-cc-pVTZ and aug-cc-pV5Z) using different sophistication levels (HF, DFT and CCSD(T)).

Results

1-Potential surface approach: We built the potential surface of the addition of H_2O on the difluorophsphine PF_2H under Cs constraint. Two transition states have been localized leading to the PF_2H_2OH phosphoranes in which the two fluorine atoms occupy axial positions.

2-Thermodynamic approach: We optimized the geometry of the five possible isomers defined by the atoms occupying axial positions: F-F, F-H, F-OH, H-H and H-OH (Fig. 1) They exhibit different stabilities. We success to optimize only three Transition states. IRC calculations lead only to the three latter isomers that exclude the thermodynamic product. The observed region and sterio selectivity have as origin a Quantum/Kinetic/Thermodynamic competitions. The three chemical paths are represented in Figure 2.

3-**Confinement approach**: Depending in the CNT's diameter (Fig.3), a transition state exhibits different behaviors[1] and leads to different products.

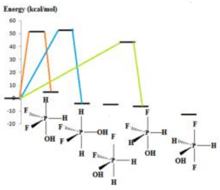

Fig.1: Energetic diagram

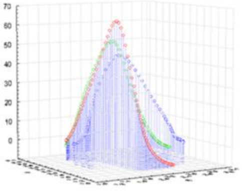

Fig. 2: Reaction paths

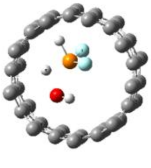

Fig.3: TS@(9,0)

Reference

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Program of
Saturday
28 September 2019

Nitric oxide Release from Ruthenium-nitrosyl complexes by Two-Photon Absorption

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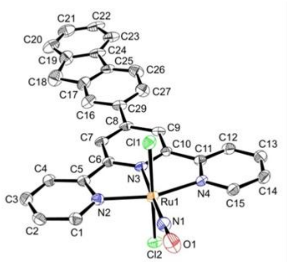
After a short introduction of the biological role of nitric oxide ($NO^{\bullet}$) [1], the photo-release of $NO^{\bullet}$ is presented from irradiation of ruthenium nitrosyl ([RuNO]) complexes, on our reference system shown below [2]:



A special focus is directed towards the released achieved by two-photon absorption (TPA), which allows the experimentalist to work in the therapeutic window (λ = 600 – 1 200 nm). Different [Ru(NO)] species are presented [3,4]. Several strategies are discussed in order to increase the TPA cross-sections at the monometallic and at polymetallic levels with experimental values ranging from 100 to 1 600 GM. The origin of the TPA enhancement is discussed with the computational support of DFT analyses. An example of [Ru(NO)] complexes used as bactericide agent is also provided.

Key words: Nitric oxide, Ruthenium nitrosyl, Two-photon absorption, Density functional theory.

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TIN(IV) COMPLEXES WITH ORGANOPHOSPHORUS LIGANDS: AN EXPERIMENTAL AND THEORETICAL STUDY

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Tin compounds have received much attention in inorganic and organometallic chemistry. Studies of these compounds continue to provide fundamental information about the Lewis acid–base model, the reactivity and the Lewis acid catalytic properties of tin(IV) species [1-2]. In particular, tin(IV) chloride and bromide have been reported to be strong Lewis acids, forming adducts with a variety of neutral ligands. In this work, tin(IV) complexes of the type $[SnX_4L_2]$ (X = Cl or Br and L = Tripyrrolidinophosphine oxide) have been synthesized and fully characterized by multinuclear (^{1}H, ^{13}C,^{31}P, and ^{119}Sn) NMR and IR spectroscopy. On the basis of NMR data, we show that the ligands form a mixture of *cis* and *trans* isomers in solution. The complex formation was confirmed by a coordination chemical shift of the ^{31}P NMR signals towards high field compared to those of the free ligands. To support these analysis and NMR interpretation, we have carried out DFT/B3LYP calculations on the *cis* and *trans* isomers of these complexes and their ligand. The results show good agreement between experimental and theoretical data.

Key Words: Tin (IV), Phosphoryl ligands, Tin tetrachloride, ^{119}Sn NMR, DFT/B3LYP

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Lithium motion in the crystal structure of $Li_3Fe_3(PO_4)_4$, A bond valence sum simulation

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$Li_3Fe_3(PO_4)_4$ represents four polymorphs. The monoclinic $P2_1/c$ [1] and $P2_1$ [2] show tunnels along a, b and c axis. However, a monoclinic $P2_1$ polymorph [3] represents cavities along the three directions. The monoclinic $C2/c$ compound [4] represents channels along a and c directions and tunnels along b directions. The Bond Valence Sum model (BVS) is extended to simulate the ionic migration pathways of alkali cations in the crystal bulk of different $Li_3Fe_3(PO_4)_4$ polymorphs. The result thus obtained will be discussed.

Key words: Bond valence sum, Conduction pathways, Crystal structure, Simulation

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[4] http://www.catalysthub.net/materials.php?id=1827764

Molecular Dynamic study of drug confinement inside functionalized carbon nanotubes and their release near POPC membrane

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Carbon nanotubes are still relevant in medicinal research. These hollow structures, have large internal surface area allowing them to introduce other molecules serving to protect the molecules during their transfer to target cells and reducing significantly their side effects. Cisplatin drug molecule (CPT) is widely used in the treatment of various types of cancer, however, it is unstable during its administration, favoring various side effects, even damaging other cells close to those targeted. To remedy even partially the harm caused by CPT they must be confined into carbon cages such as carbon nanotubes[1].
Frequently during their synthesis, the CNTs are cutted and functionalized by oxidation process allowing saturation of CNTs ends carbons with alcohol functions (- OH) for example. Molecular Dynamics study role is to evaluate the influence of CNT's chemical functions (-H, -OH) on the input/output process and the retention time of Cisplatin molecules then the whole system is released near a membrane cell.

Key words: CNT, POPC membrane, encapsulation, drug delivery, Cisplatine

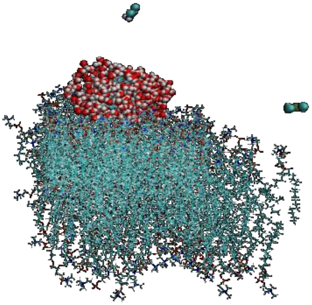

Figure : (NTC + CPT) system near the POPC membrane.

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PHASE FORMATION, MICROSTRUCTURE AND DIELECTRIC PROPERTIES OF PZT–CNS PIEZOELECTRIC CERAMICS

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(0.80- x)Pb $(Cr_{1/5},Ni_{1/5},Sb_{3/5})O_3$-$xPbTiO_3$-$0.20PbZrO_3$ piezoelectric ceramics with x = 0.30, 033,036,0.39 and 0.42 were prepared by the conventional method of thermal synthesis of mixed oxides. Effects of sintering temperature and the influence of Cr, Ni, and Sb contents microstructure, dielectric and piezoelectric properties of a new ceramics material in PZT–CNS systems were investigated. The results of X-ray diffraction (XRD) showed that all the ceramics specimens have a perovskite phase with transforms from tetragonal phase to tetragonal-rhombohedral phase near the morphotropic phase boundary(MPB). The scanning Electron Microscopy (SEM) showed an increase of the mean grain size when the sintering temperature was increased. A sintered density of 92.93% of the theoretical density was obtained for Ti = 42% after sintering at 1180°C. Ceramics sintered at 1180°C with Ti = 42% achieve excellent dielectric properties, which are as follows $\varepsilon_r = 4262.48$, and Tc = 340°C.

Keywords: piezoelectric, dielectric, perovskite, pzt-cns.

DFT STUDY OF ORGANIC-INORGANIC MATERIALS BASED ON TTF-DERIVED LIGANDS

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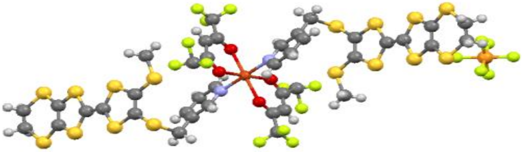
TTF precursors substituted with nitrogen ligands have an important interest in coordination chemistry in order to incorporate, in the same solid, two distinct physical properties such as magnetism and electrical conductivity or superconductivity. The $Co_2(PhCOO)_4(TriMeTTF\text{-}CH{=}CH\text{-}py)_2$ organic material had a significant impact, and opened new perspectives for the synthesis and the study of analogous coordination complexes using other paramagnetic transition metals and other functionalized TTF derivatives [1]. This type of coordination constitutes a new approach for π-d interactions in bifunctional conductors and magnetic molecular materials with multiple properties. The theoretical study has been carried out by the DFT quantum method [2] on the coordination mode of organic/inorganic mononuclear complexes with structures $Cu(hfac)_2(L)$ and $[Cu(hfac)_2(L)_2][PF_6]_2$ based on oxidized copper. The results obtained were in agreement with the experimental data and they explain the complexation reaction.



X-ray crystal structure of $[Cu(hfac)_2(L)_2][PF_6]_2$

Key words: Hybrid materials, pyridine-unsymmetrical TTF molecules, DFT calculations, X-ray structure, radical cation salts.

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NEW COPPER (II) AND GOLD (III)-LOADED PHOSPHORUS DENDRIMERS: SYNTHESIS AND BIOLOGICAL EVALUATION

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Dendrimers are monodisperse nanosized polymeric molecules that are composed of a large number of perfectly branched monomers. The versatile chemical composition of dendrimers strongly offers a variety of applications in different areas such as: chemistry, catalysis, and medicine. Currently, the potential of using dendrimers as nano-carriers for drug delivery is revolutionizing medicine for the efficiency and the reducingof the toxicity of various treatments it has shown [1].

Dendrimers can form either covalent or non-covalent (encapsulation) bonds with bioactive molecules. In the case of covalent bond, drug can be directly attached to dendrimer or via a linker – cleavable or not - and the resulting drug-loaded dendrimer can act as a nano-vehicle for drug transport and controlled release.

We will present the synthesis and characterization of original functionalised phosphorus dendrimers [2] (generations G1 to G3) containing various functional groups on their peripheries such as arene-copper (II) and arene-gold (III). We will also report the studies of the very interesting cytotoxicity activities against different solid and liquid cancer cell lines of these new dendrimers.

Key words: dendrimers, cooper, gold, cancer

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SYNTHESIS OF TACRINE-CYCLAM HYBRIDS AS PROMISING TREATMENT FOR ALZHEIMER'S DISEASE

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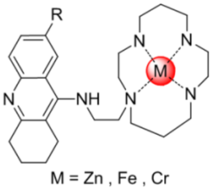
Alzheimer's disease is a progressive neuronal degeneration affecting the elderly leading to memory loss and dementia. The risk of suffering from this disease increases with age: 10% of over 65 years and 50% over 85 years old suffer from this disease. Alzheimer's disease has become a major health problem in developed countries as well as cancers and cardiovascular problems. Tacrine and its derivatives were the first AChEI to be approved for treatment of Alzheimer's disease [1–3].

Moreover, macrocyclic polyamines generate continuous interest because of their biological properties and their importance in coordination chemistry [4].

Cyclam is one of the most used macrocyclic polyamines. It can bind strongly to a wide range of metal ions [5].

Relaying on this diversity of properties, the present work will focus on the synthesis of new cyclam-tacrine hybrids compounds with promising pharmacological bioactivity as well as the study of their coordination behavior with metal ions.



Keywords: Alzheimer, cyclam, tacrine, hybrids, complex, AchEI.

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Coordination-driven self-assembly of chiral palladium(II)-based supramolecular coordination complexes

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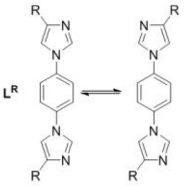
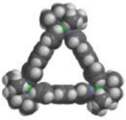
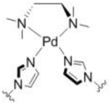
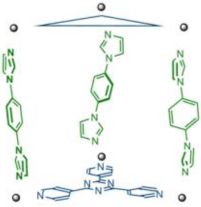
In the present work, chiral supramolecular coordination complexes (SCCs) are described. The self-assembly of ditopic bis(4R-1H-imidazolyl)benzene ligands (**L**$^{\mathbf{R}}$, with R = H or Me) and palladium(II) complexes $[(L_2)Pd(NO_3)_2)]$ afford bi-dimensional SCCs. These SCCs have been fully characterized in solution by NMR spectroscopy and coldspray ionization mass spectrometry. These analyses clearly demonstrate an equilibrium in solution between the triangular and square structures, albeit as minor components. More interestingly, in the case of the triangular structures, the palladium(II) corners exhibit planar chirality and are homochiral [1-2]. The ligands **L**$^{\mathbf{R}}$ have also been utilized in the synthesis of tridimensional SCCs. The full characterization and computational analysis support the inherent chirality of these D_3 symmetric SCCs. Preliminary results of enantio- and diastereopure SCCs will also be presented.









Key words: self-assembly, supramolecular, coordination complexes.

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The new decavanadate compound $(C_5H_{11}N)_4[V_{10}O_{28}]$ 3.25H_2O : Synthesis, characterization and Hirschfield surface analysis

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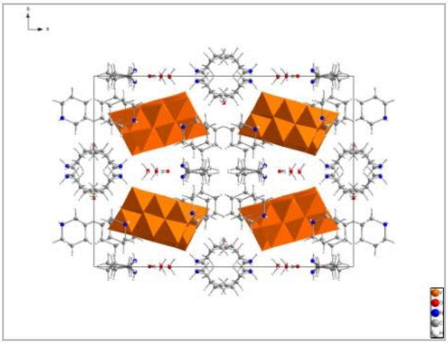
Polyoxometalates(POMs) are a class of molecular - defined inorganic metal oxide clusters formed from early transition metals in their highest oxidation states (V,Nb,Ta, Mo, W) and oxygen, which have been studied in various applications in different fields such as catalysis, energy storage, medicine, magnetism and electro chromic applications to name a few.[1-3]

In order to obtain new materials with novel structures and interesting properties, we report in this work for the first time the synthesis, characterizations, crystal structure and the non-bonding interactions with the help of the Hirshfeld surfaces of the novel decavanadate $(C_5H_{11}N)_4[V_{10}O_{28}]\cdot 3.25H_2O$,crystallized the monoclinic system with the C2/c space group and cellular constants of a = 28.7460 (5) Å, b = 19.2130 (5) Å, c = 18.4853 (4) Å, β = 113.374 (1) ° and Z = 2.

Key words: Synthesis, Characterization, X-ray diffraction, Hirschfield surface



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ZINC(II) AND CADMIUM(II) COMPLEXES WITH TRIPYRROLIDINOPHOSPHINE OXIDE: EXPRIMENTAL AND THEORETICAL DFT STUDIES

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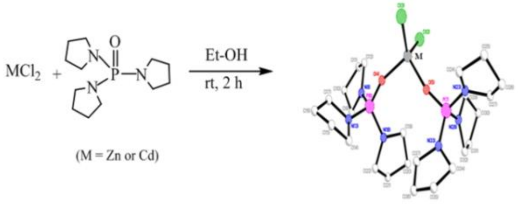
Phosphoramides have been thoroughly reported as potent enzyme inhibitors and can be used in therapies and drug design against bacterial ureases, or as flame retardants [1, 2]. Other important applications include their use as analytical tool to determine the kinetics and activity of other enzyme inhibitors, as appropriate ligands in coordination chemistry or as potent catalysts for a wide variety of chemical reactions in organic synthesis [3]. In this context, we have recently described the synthesis and characterization of tetrahedral metal complexes derived from the tripiperidinophosphine chalcogenides, Pip_3PE (E = S or Se) [4]. In this work, we report on the synthesis of zinc (II) and cadmium (II) complexes with tripyrrolidinophoshine oxide. These complexes were fully characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR, IR spectroscopy, conductimetry and X-ray diffraction analysis. In addition, a DFT/B3LYP theoretical study on the geometry optimization of these complexes has been carried out in order to support and complement the experimental data and to further investigate the nature of the oxygen-metal interaction. The results are compared with those obtained for other chalcogen counterparts.



Keywords: Phosphoramides, cyclic amine, zinc, cadmium, metal complex, NMR, DFT/B3LYP.

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A SELF-DOPED POLYANILINE DERIVATIVE OBTAINED BY ELECTROCHEMICAL COPOLYMERIZATION OF AMINOTEREPHTHALIC ACID AND ANILINE

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The electrochemical copolymerization of aminoterephthalic acid and aniline can be achieved to yield a self-doped material showing electroactivity at physiological pH. The present study focusses on the management of the synthesis conditions to obtain a true copolymerization product and to control the relative amount of both comonomers eventually incorporated to the copolymer chain. Both, in situ FTIR spectroscopy and ex situ XPS techniques proved the successful incorporation of aminoterephthalic acid and, in parallel to other polyaniline parent derivatives, revealed the existence of redox transformations involving leucoemeraldine-emeraldine-pernigraniline transitions. The use of a high inversion potential (1.4V/RHE) during electro-copolymerization resulted in a material enriched in aminoterephthalic acid fraction with respect to aniline, while this last component is favored at lower potentials. The pH behavior of copolymers in combination with in situ FTIR results strongly suggested that a larger content of aminoterephthalic acid (such as that obtained after deposition at 1.4 V) do not ensure an extensive self-doping process because a significant fraction of those carboxylic moieties remain inactive during the redox transformation. Instead, low inversion potentials are preferred to obtain a material with less defects and thoroughly electroactive at physiological pH.

Keywords: polyaniline; self-doped conducting polymer; in situ FTIR; electrochemical copolymerization; XPS

Europium doped Sodium Bismuth fluorapatite, $Ca_8NaBi(PO_4)_6F_2$, prepared by Pechini process, as a single-component phosphor for white-emitting n-UV convertible phosphor for w-LEDs

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White LEDs (white light-emitting diode) are regarded as the most ideal solid-state lighting source for the next generation due to several superior properties, such as high brightness, long lifetime, energy saving and environment friendliness [1].As we known, the w-LEDs that based on the combination of a blue LED and yellow phosphor have low color rendering index, and those based on the combination of the n-UV chip with blue, green, and red phosphors together produces emission reabsorption and poor efficiency [2]. As an important family of trivalent rare earth ions, Europium (Eu^{3+}) is used to act as a potential candidate to absorb n-UV light and emit a srong emission in the red regions, corresponding to $^5D_0 \rightarrow {}^7F_2$ transition (615nm) [3]. In order to obtain a high-quality solid-state light source, phosphors used in LEDs should contain the following basic characteristics Excitation spectrum, matching well with the pumping LED chips, shows a large absorption intensity of n-UV (360-420 nm) or blue light (420-480 nm). (2) Emission spectrum, combination with the emission of LED chips and phosphors, produces a pure white emission with a specific CRI or Ra and corresponding color temperature (CCT). (3) Efficient luminescence with high quantum efficiency (QE). (4) Good physical, chemical and thermal stability under application conditions, e.g., high stability against moisture, oxygen, and heating [4]. Apatite-type alkaline-earth halophosphates with the general formula of $M_{10}(PO_4)_6F_2$ (M = Ca, Sr, Ba, Na, Bi) as host of luminescence materials have been widely investigated because of the flexibility of host lattice, good thermal stability, cheap raw materials, and simple synthesis conditions [5].

In this work, we report for the first time, on the phosphore $Eu:Ca_8NaBi(PO_4)_6F_2$ prepared by the modified Pechini method, Well crystallized microparticles of size around 200 nm with rod morphologies, structural and vibrational spectroscopic charcterization (FTIR and RAMAN spectroscopy) as well as optical proprieties, the photoluminescence excitation (PLE) and emission (PL) spectra, the concentration dependence of the emission intensity, decay curves and Commission International de I'Eclairage (CIE) of the phosphors are investigated,It has been revealed that the emission spectra from all the synthesized samples contain a set of spectral lines due to the 4f – 4f transitions of Eu^{3+} ions, which predominantly occupy the A_1 sites of C_3 symmetry in the apatite structure. The calculated color coordinates lie in the red region. Therefore, phosphors $Eu:Ca_8NaBi(PO_4)_6F_2$ may be good candidates for red components in near-UV white LEDs.

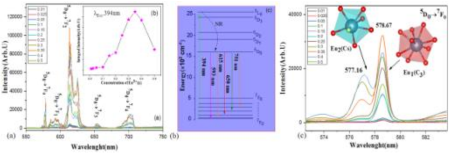

Fig.(a) RT-PL (λex = 394 nm) spectra of the phosphor $xEu:Ca_8NaBi(PO_4)_6F_2$ (x = 0.01→x=0.5), Inset is the dependence of the PL intensities on the content of Eu^{3+}(x).**(b)** Simplified energy level diagram, excitation and visible emission schemes for Eu^{3+} doped $Ca_8NaBi(PO_4)_6F_2$.**(c)** The non-degenerate $^5D_0 \rightarrow {}^7F_0$ emission line with Eu^{3+} different environments in the matrix $Ca_8NaBi(PO_4)_6F_2$.

Key words: Europium, red components in near-UV, Sodium Bismuth fluoroapatite, Pechini Process, Microrods particles, Luminescence, CIE, w-LEDs.

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Analysis of a novel design of conical solar furnace supplied by optical fibers

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Optical fibers can add interesting possibilities in solar concentrator systems. The aims of this study are to optimize the coupling of a paraboloidal dish, which concentrates direct solar irradiance with dual axes tracking component, and the optical fiber, which transmits concentrated solar energy.

We present review previous studies on the transmission of concentrated solar energy via optical fibers (TCSEvOF), and provide a mathematical model for coupling paraboloidal dish and the optical fiber.

This paper reports on theoretical realization of a recently proposed solar optical fiber mini dish light concentrator connected to a conical solar furnace. The prototype dish is 21.8 cm in diameter. We present the daily power obtained at the output of the optical fiber, the power supply is estimated to be 25 W at the end. Then we show that the energy transported is diffused until the enclosure then disperse inside it, the receiver absorbs this energy. Temperatures higher than 800°K may be reached while maintaining very good efficiency.

Key words: solar energy; optical fiber; paraboloidal dish; conical solar furnace

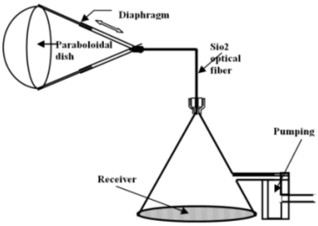

Figure. The coupling between the concentrator, the optical fiber and the solar furnace proposed

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Synthesis and coordination chemistry of acid and sulfonate derivatives of calix[4]arene

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The work presented concerns the synthesis of calix[4]arenes functionalized with sulfonate and carboxylate groups and the study of their coordination chemistry with 3d and 4f transition metals respectively for calixarenes based on carboxylate and sulfonate groups. One of the major concerns of this work concerns the understanding of supramolecular assemblages in these systems.

With the dimethoxycarboxylate calix[4]arene (AC2), we obtained two isostructural complexes with Zn and Mn, in which two AC2 are coordinated with two metal centers to form a coordination polymer, a study of their gas adsorption properties, as well as the analysis of the thermal and magnetic properties of the complexes were performed. In addition, the coordination chemistry of sulfonated calix[4]arenes with four lanthanides (Dy, Eu, Yb and Gd) was studied. Thus, we synthetized four isostructural complexes that form chains in zigzag which the lanthanide ions play the role of an assembler of the calixarenes by the coordination of the sulfonate groups with water molecules.

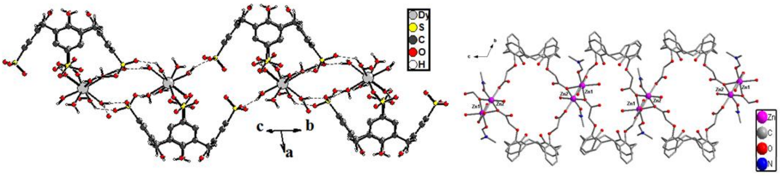

Fig. calix[4]arene's complexes

Key words: acid calix[4]arene, sulfonated calix[4]arene, synthesis, coordination chemistry

Assessment of industrial wastewater effluent into urban ecosystem Kigali, Rwanda

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Rwanda is developing its industrial sector for economic development; however, those industries are regularly generating wastes, either solid, liquid, or gas which can in one way or another harm the living species. For the purpose of this study, an assessment of industrial wastewater effluents into urban wetland ecosystem was done and the City of Kigali was considered. The objectives of the study were to establish the pollutants in the effluent of key point sources of Kigali and then assess the effluent discharge management methods and treatments regimes, if any, of three key identified pollution point sources. Therefore, the effluents from some industries were analysed through laboratory experiments and then compare the results to the national standards maximum limits required for effluents to be discharged to the environment. It was found that the urban wetland is polluted by the presence of a higher concentration of TSS, COD, Faecal Coliforms, Cd, Cu, CN, Ni and Phenol in all the tree sampling sites. Furthermore, TDS, Fe, Cr (VI), and Hg (in higher quantity) were found at UTEXRWA, As was found at both UTEXRWA and RUGANWA, while both BOD and Pb were found at UTEXRWA and KABUYE sugar works. However, the pH value was found to be higher at UTEXRWA and lower at Kabuye. The problem of unplanned settlement leads to having many human activities near those effluents point. Both animal and plant communities are highly affected by the polluted effluents, so we are here to recommend all concerned industries to treat their effluents to protect the biodiversity and reuse them for saving costs in order to regulate water and improve the industry's public image. The government should ensure that the fixed standards are respected by monitoring wastewater discharges. The principle of intergeneration equity should guide all of us, as environmental protection is concerned. This is the wise use of the environment, natural resources for present and future generations.

Keywords: industrial wastewater, urban ecosystem, UTEXRWA, RUGANWA, KABUYE sugar works, Kigali Rwanda

UNDERSTANDING OF Zn-sal(ph)en COMPLEXES COORDINATION: TETRAHEDRAL COORDINATION OR PENTA-COORDINATION?

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The Lewis acidic character within a series of Zn-Sal(ph)en complexes is reviewed and revisited. Thus, both usual dual descriptor (DD) and state specific dual descriptor (SSDD) have been applied to understand the nature of the bridging diamine linker in the Schiff base ligand controls this feature mainly responsible of the coordination geometry of these complexes. The application of the usual dual descriptor (DD) to a prototypical complex, namely $ZnCl_4^{2-}$, exhibits significant weaknesses to retrieve the electrophile part on the metal cation of sal(ph)en complexes. The inclusion of the densities of the electronic excited states by the so-called state specific dual descriptor (SSDD) allows us to recover successfully the appropriate reactivity of these chosen complexes with different diamine bridges in flexible to semi-rigid then to rigid ranges

Key words: Zn-sal(ph)en complex; conceptual DFT; dual descriptor (DD); state specific dual descriptor (SSDD); electronic relaxation.

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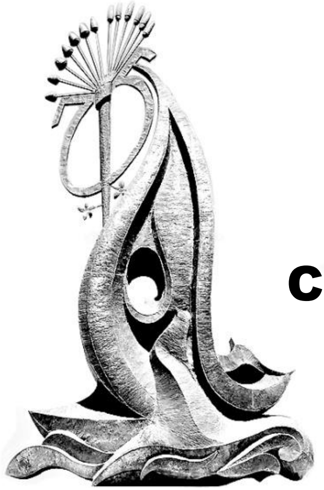

Posters Communications’ Abstracts

Structural Property Study of a new PCaMN-PZT ceramic material

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This project aims to improve the electrical properties of ceramics. These properties are generally improved by the addition of one or more cations which will replace the Pb^{2+} in site A and / or couple (Zr^{4+} / Ti^{4+}) in site B of the perovskite structure **[1]**.
Substitutions in the crystal lattice called doping **[2]**. In fact any change by doping by means of metal oxides or substitution of elements, moves the morphotropic border to the right or to the left **[1]**. Various methods are used to locate the corresponding compositions at the phase morphotropic boundary of PZT ceramics and these derivatives (addition of dopants) **[3]**. Among these methods used for the investigation:

- X-ray diffraction analysis (X-ray spectra analyzes).
- the analysis by study of physical properties (measurement of dielectric, piezoelectric and electromechanical properties).

We are interested in the study of the ternary PZT-CMMN abridge system
As ubstitution in the site To which was carried out in order to improve its physical properties. The samples selected for this study were prepared by the method of synthesis in a solid way. A thermal treatment was applied to these compositions at different temperatures: 1100 ° C, 1150 ° C, 1180 ° C, 1200 ° C and 1230 ° C. density) and therefore the product is better physical quality.

Key words: Perovskite / PZT / DRX / PZT-CMMN / MEB / Sintering.

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DFT Studies on the Reaction Mechanism of butene Isomerization Catalyzed by Ruthenium Hydride: Stepwise or concerted mechanism?

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The isomerization reaction mechanism of butene catalysed by the ruthenium model complex $RuH(CO)(Cl)(PMe_3)_2$ has been studied theoretically by two different mechanisms, a stepwise mechanism and a Concerted mechanism .The stepwise reaction mechanism shows that the first proton transfer is common for both Z and E regenerates the two products 4Z and 4E. Although 4Z is lower in energy than 4E, the transformation between them is likely to occur and that both isomers are taken into account in the calculations of the reaction pathway.
The most important difference between the two pathways is the β-H proton elimination step. The results show that the 5E formation is favorable both kinetically (lower barrier) and thermodynamically (more stable compound) this which indicate that the reaction will preferentially generate the product 5E. The step barriers stepwise H-migration pathway is compared with the H-migration concert. The calculated elementary stepwise mechanism are 15.1 and 8.8 $kcal.mol^{-1}$, in contrast to 32.1 $kcal.mol^{-1}$ found in the concerted mechanism.
This fact implies that the isomerization reaction may proceed according to the stepwise rather than concerted mechanism.

Key words: Butene, Double bond isomerization, mechanism, DFT.

Mechanistic insights of peptide bond formation In the presence of polar and non polar solvents

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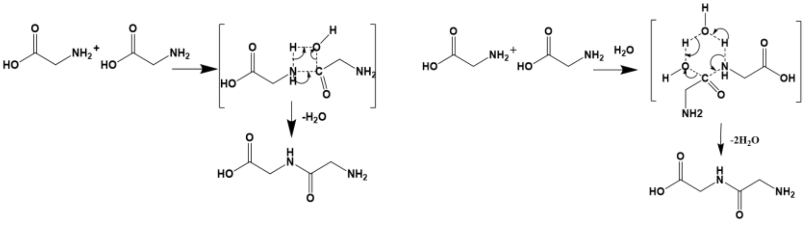
Peptide bond formation is a crucial chemical process that dominates most biological mechanisms and is claimed to be a governing factor in the origin of life. Dipeptides made from glycine are studied computationally via Density Functional Theory (DFT) using two different basis sets. This reaction was investigated from both a thermodynamic and kinetic point of view. The effect of explicit solvation via the introduction of discreet solvent molecules was investigated. Water, methanol, and cyclohexane were all employed as solvent media in addition to gas to investigate their effects on the mechanism of peptide bond formation. This computational investigation revealed that methanol is slightly better than water to leverage peptide bond formation both kinetically and thermodynamically, while cyclohexane, a non-polar and non-protic solvent, is the least effective after gas as a medium of solvation. Energetic results in the gas environment are very close to those obtained in polar and protic solvents, suggesting that peptide bonds can be formed under interstellar conditions.



a) **b)**

Fig. Schematic of the reaction mechanism for peptide bond formation between two amino acids: a) in the gas phase, b) assisted by water.

Key words: Peptide bond, mechanism, Solvent, DFT.

Fluorescent Schiff Base derivative; Boranil: Experimental and theoretical approaches, and textile dyeing exploration

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Luminescent dyes continue to attract strong interest due to their potential application [1, 2, 3, 4]. In this perspective, we synthesized a Schiff base by simple condensation of salicylic aldehyde and p-aminophenol using ethanol as the solvent and its fluorescent boron difluoride complex (Boranil) using BF_3, Et_2O in distilled toluene.[5] Both synthesized compounds chemical structure was resolved using different spectroscopic techniques (Fourier transforms IR, NMR, UV-vis and PL). The fluorescent Boranil was successfully used to dye Cotton Textile. In addition to experimental analysis, density functional theory (DFT) calculations at the B3LYP/6-311 +G (d, p) level were performed on synthesized Schiff base and it's boron difluoride complex to obtain the optimized geometry and spectroscopic and optical properties.[5] Natural Bonding Orbital (NBO), and nature population analysis (NPA) were performed after optimization of geometry at the same basis set (6-311++ G (d,p)) and all the electronic and quantum chemical parameters (FMOs) of the title compounds were calculated at the CAM-B3LYP-D3 method using 6-311++G (d, p).[6] The absorption and emission spectra of the model compounds were also simulated and compared to experimental observations in the DMF solvent. Overall, the DFT calculation results supported the structural and spectroscopic experimental data and confirmed the structure modification of frontier molecular orbitals for BF_2 complexes as well as tunable potentials and energy levels [5]

Key words: DFT calculations, Schiff Base, Boranil, FTIR, Fluorescence NBO, HOMO-LUMO analysis, Optical properties

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Copper (II)-Halide-Based Hybrid Perovskite with an Exceptional Dielectric Phase Transition Induced by a Boat-to-Chair Conformation Change of the Organic Cation

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Hybrid perovskite materials have demonstrated great potential in the field of photoelectronics, environmentally friendly processing and semiconductor applications. On the basis of the high degree of structural flexibility and compatibility, diverse molecular functional materials have been assembled by modifying the length of the organic components and/or dimensionality of the inorganic frameworks. In this work, we present a lead-free organic-inorganic hybrid, (2-chloroethylammonium)$_2$CuBr$_4$, which follows the one-dimensional inorganic frameworks of the corner-sharing CuBr$_6$ octahedra. Strikingly, compound displays a dielectric phase transition at Tc = 243 K, changing from the noncentrosymmetric space group of Pc to the centrosymmetric space group P2$_1$/c upon heating. Crystal structure analyses reveal that an unusual thermally activated conformation change of the 2-chloroethylammonium cations affords the driving force to the phase transition of material. That is, organic 2-chloroethylammonium moieties display a boatlike conformation below Tc, which transforms to a chairlike structure above Tc. Such change is strongly coupled to the dielectric transition along with notable steplike anomalies, which suggest that compound could be used as a potential switchable dielectric material. This zigzag 1D hybrid perovskite-derivative material shows a narrow indirect band gap of 1.66 eV, which is encouraging for optoelectronic and photovoltaic applications.

Keywords: Hybrid perovskites, Crystal structure, Semiconductor materials, chair and boat conformations.

Synthesis and spectroscopic characterization of α-acetoxyphosphonate complexes with tin tetrachloride

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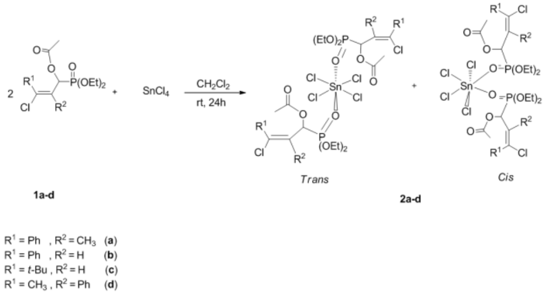
The reaction of tin tetrachloride with a series of variously substituted α-acetoxyphosphonates (L) [1] in anhydrous dichloromethane produces new octahedral tin complexes of the type [$SnCl_4L_2$]. These adducts were characterized by multinuclear (^{1}H, ^{13}C, ^{31}P and ^{119}Sn) NMR and IR spectroscopy. The NMR data show that these complexes exist in solution as mixtures of *cis* and *trans* isomers. It is worth to note that the triplet feature observed in the ^{119}Sn NMR spectra clearly confirms that the ligand is only coordinated through the phophoryl group since if the carbonyl group or the olefin moiety were coordinated the ^{119}Sn NMR spectrum would show only one doublet in the case of a chelate formation through one phosphoryl and one of these functional groups or two signals for *cis* and *trans* isomers in the case of coordination only through these groups. In addition, the ^{13}C NMR spectra as well as the IR data of complexes show that the carbonyl group and olefien carbon absorptions were only very slightly affected, confirming that coordination with tin occurs solely through the phosphoryl group of the phosphonate ligand [2]. The remote substituent effect on the metal ligand interaction was also studied and compared with closely related systems.



Keywords: α-acetoxyhosphonate, tin(IV) complex, ^{31}P and ^{119}Sn NMR.

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Cyclopropenio-imidazol-2-ylidene: The first N-Heterocyclic Carbene bearing a N-cationic substituent

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Over the last two decades, N-heterocyclic carbenes (NHCs) have emerged as a privileged class of ligands in the field of organometallic chemistry.[1] They are defined as neutral species having a divalent carbon atom in a N-heterocycle, and can be considered in a first approximation as phosphine analogues. In recent years, the direct connection of a cationic moiety onto the phosphorous center – leading to α-cationic phosphines – was shown to be a powerful strategy to unveil new reactivity and produce highly efficient catalytic systems.[2]

We present herein the first N-cationic imidazol-2-ylidene, in which one mesityl group has been formally replaced by a stable, aromatic bis(diiisopropylamino) cyclopropenium.[3] The synthetic access toward its imidazolium precursor, its generation and the complete study of its coordination ability and stereoelectronic properties will be described. Preliminary results in gold(I)-catalyzed cyclization reactions will be reported.

Keywords: Carbene, heterocycle, cyclopropenium, ligand, organometallic compound.

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CANDIDA CYLINDRACEA LIPASE CATALYZED THE KINETIC RESOLUTION OF DL-MENTHOL IN PRESENCE OF QUINIDINE AS ADDITIVE.

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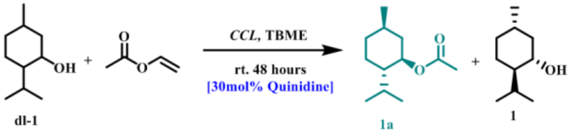
Menthol is the world's most-sold flavor ingredient and can be found in countless everyday products, the worldwide demand of 25,000 to 30,000 metric tons per year already exceeds the available supply and is constantly growing [1]. The l-(-)-Menthol has the best organoleptic performance, since it is widely used in flavor and fragrance industries, foods, cosmetics and pharmaceutics due to its refreshing flavor and cooling effects [2]. The demand on the pure form of l-(-)-Menthol is of an important preoccupation at an industrial level, which explains the research effort to establish efficient routes for yielding it at high purity [3]. One of the efficient routes to obtain it optically active is the biocatalytic process [4]. In this work, we synthesis the pure l-(-)-menthyl acetate via kinetic resolution of dl-menthol by using *Candida cylindracea lipase* catalyzed acylation with vinyl acetate and quinidine as additive in TBME as solvent. In order to valorize this simple and easy methodology under mild conditions we have applied it at large scale. The optimal condition was undertaken and applied to resolve 10 mmol (1.5g) of the racemic menthol. The reaction results are reproduced, and the most important enantiomer l-(-)-1a was obtained quantitatively with ee = 94% and 44% conversion under mild conditions.



1mmole	ee_P= 93%	ee_S= 88%	C=49%	E=80
10mmole	ee_P= 94%	ee_S= 72%	C=44%	E=70
(1.56g)	0.75g (Yield=39%)	0.5g (Yield=32%)		

Key words: l-menthyl acetate. Kinetic resolution. Candida cylindracea lipase. Additive.

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Application of the Doehlert experimental design to optimize hexavalent chromium removal by activated carbon from orange peels

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Wastewater contamination by chromium becomes an important problem due to its widespread applications in industrial processes such as metallurgy, tanning industries, refractories and foundries [1]. Hexavalent chromium is harmful for environment and threatens the human health as it is a carcinogen element. The World Health Organization defined an upper limit of 0.05 mg L^{-1} in drinking water [2]. Different studies were carried out on the efficiency of biochars for heavy metals removal [3, 4]. This work focuses on the efficiency of the response surface methodology to optimize the parameters affecting the chromium removal by adsorption on biochar using orange peels as precursor. Fourier transform infrared spectroscopy (FTIR), BET and SEM were used to characterize the adsorbent. A Doehlert experimental design was applied to determine optimum conditions. Three factors were chosen: the adsorbent amount, pH and the temperature.

The experimental results were analyzed by the ANOVA test and showed that the model regression is well fitted. The determination coefficient R^2 was equal to 0.978 suggesting an excellent relationship between predicted and experimental responses. Graphic analysis of contour plots obtained from NEMROD software showed that the highest removal yield was obtained under the following conditions: an adsorbent dose of 1.26 g L^{-1}, a pH equal to 2.92 and a temperature of 35°C. The adsorption recovery reached 88.5 % under these conditions.

Key words: Biochar synthesis, Experimental design, Hexavalent chromium,

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Facile synthesis of molecularly imprinted polymers for selective extraction of toluene biomarker

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A molecularly imprinted polymer (MIP), obtained by precipitation with 4-vinylpyridine as monomer, ethylene glycol dimethacrylate as cross linking agent and acetonitrile as porogen solvent was prepared. In order to determine the selectivity of this support, batch adsorption tests were conducted to compare the recovery between the imprinted form of the polymer and the non imprinted form (NIP). The characterization results of scanning electron microscopy and nitrogen adsorption desorption measurements showed the presence of agglomerates with irregular shapes. The specific surface area was equal 319 m^2 g^{-1} for MIP and 227 m^2 g^{-1} NIP. The total pore volumes were 0.468 and 0.311 cm^3 g^{-1} for MIP and NI¨P respectively. These results make the material with good characteristics that explain the great capacity of extraction of the analyte.

Key words: MIP synthesis, Selective extraction, toluene biomarker

New hybrid material at the limit of organic and inorganic for environmental applications

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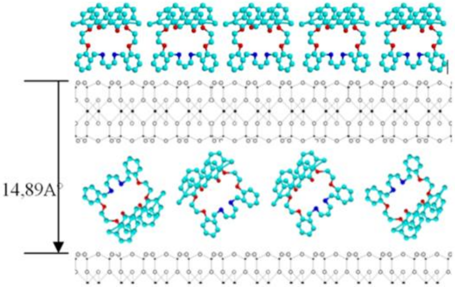
The challenges posed by the protection of the environment challenge chemists through the development of interactive materials (active / intelligent). It is in this context that we have developed new hybrid materials that are systems in which both organic and inorganic species coexist. The interest of these materials lies in the combination of properties provided by each component separately. The new material thus elaborated has higher performances than the elements taken separately. These blends generate very extensive organo-mineral interfaces whose subtle adjustment and sequencing results in variations of shape and functionality at all scales to give rise to multi-scale hybrid materials. The originality of this work consists in making the first clay-calixarenic hybrids by co-grinding in solid phase.The work presented here consists in synthesizing two calixarenic derivatives, studying their complexing and extracting properties vis-a-vis metal cations in order to detect particular selectivities and to use them to prepare clay-calixarenic hybrid materials. The comparison of infrared spectra shows that the reactions did take place. The confirmation of the intercalation of the calixarenes in the interfoliar space of the clay has been demonstrated by X-ray diffraction.



Following a liquid-solid extraction study, the results showed that, generally, the clay has a low extracting power, the calixarenic derivatives extract significantly better than the clay and the hybrid nanocomposites have even higher extraction percentages than the two previous ones. These nanocomposite materials could constitute surfaces as sieves specific for targeted trapping (according to selectivity s) and conditioned re-release.

Enzymatic Deacylation of 1-Phenylethyl Acetate in presence of divers Lewis bases

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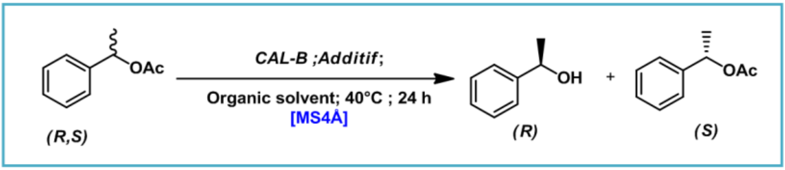
Amongst largely synthetic intermediates employed in pharmaceutical and agrochemical industries are the optically active benzylic acetates. They are as well exploited in asymmetric synthesis as excellent ligands. Divers methods have been developed for their conception, among of them the most practical and interesting is the enzymatic kinetic resolution. In these methods the lipases are needed as key precursors for their high level of efficiency, under mild conditions and eco-compatible of some green chemistry criteria [1]. Although several parameters interact simultaneously, controlling both reactivity and selectivity: such as the enzyme nature, the nucleophile structure, the solvent hydrophobicity. The insertion of additives has also revealed as important parameter affecting the outcome of the enzymatic kinetic resolution [2-3].

In view of these, we report an efficient enantioselective gap of the acyl-moity of phenyl ethyl acetate as model of study, catalyzed by lipase B from Candida Antarctica (CAL-B) in the presence of Lewis bases as additives in non aqueous media. The threshold activity of the introduction of Tertiary amine as well as their structures were studied including the influence of two solvent used (TBME and DIPE).



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Reactivity of some anhydrides in the enzymatic acylation reactions of chiral alcohols

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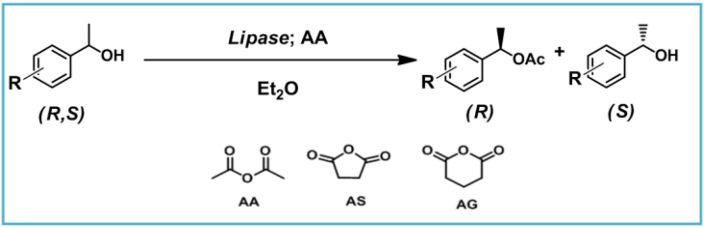
The development of efficient catalytic systems under green chemistry conditions to access chiral molecular bricks is of considerable interest in many fields. Our contribution in the field is reflected in the study of enzymatic kinetic resolution of chiral secondary benzylic alcohols with various aliphatic acid anhydride and cyclic acid anhydride acylating agents. These acylating agents are widely used as irreversible acyl donors in kinetic enzymatic resolution reactions.

The practical and advantageous use of cyclic anhydrides makes it easy to recover by a simple liquid-liquid extraction, each enantiomer of the substrate was obtained without requiring the use of chromatographic separations. This makes it an economical process in volatile organic solvents, in perfect agreement with the concern of developing an eco-compatible chemistry.



We have developed a study regarding the kinetic resolution of aryl-alkyl-ethanols with an anhydride in the presence of CAL-B [1]. The main purpose of this work is to demonstrate the influence of the acylating agent's nature. Moreover, the secondary products formed during the acylation reaction on the reactivity. In addition of the enzymatic selectivity. In order to conduct this study an examination of few parameters were done: the nature of the enzyme, the structure of the alcohol as well as the nature of the acylating agent.

Key words: anhydride, chiral alcohol, enzymatic acylation, CAL B.

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X-RAY STRUCTURAL STUDY, IR CHARACTERIZATION AND THERMAL STUDIES OF NEW COORDINATION COMPLEXE

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The complex $[Zr(C_{12}H_{17}N_4O_4S_2)_2]^{+2}$. $2(NO_3)^{-}$ (1) was studied by X-ray diffraction on single crystal. The crystallographic measurements were carried out at 293 K on an APEX2 CCD automatic diffractometer using molybdenum Kα radiation (λ= 0.71073Å) and a graphical monochromator equipped with a cryogenic system allowing low temperature recording **[1]**. The coordination polyhedron of the metal ion Zr(II), of the type [ML4] (L= $N_{sulfanilamide}$, $O_{sulfanilamide}$), has a distorted pyramidal geometry. This polyhedron is generated from an equatorial plane (ZrN3), comprising three nitrogen atoms (N1, N3, N4) belonging to three ligands chelates sulfanilamide; the axial position involves the oxygen atom (O1) from a fourth sulfanilamide ligand (Figure 2). The Zr atom and the three nitrogen atoms that define its coordination environment are almost in the same plane. The sulfanilamide ligand in this molecule is "bidentate"**[2]**.

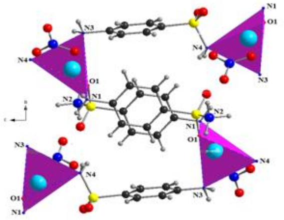

Figure 1. The spiral form described by the compound (1): $[Zr(C_{12}H_{17}N_4O_4S_2)_2]^{+2}.2(NO_3)^{-}$ according to plan (b, c)

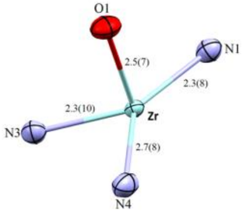

Figure 2. Environment of zirconium within the compound (1)

The structural description is enriched by an infrared spectroscopic study to highlight the main bands of chemical functions. ATG measurements have explained the mechanism of thermal decomposition of the compound.

Key words: Single-crystal, X-ray study, hydrothermal synthesis, chelates.

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COORDINATION COMPLEXES WITH THE ANTIBIOTIC "SULFANILAMIDE"

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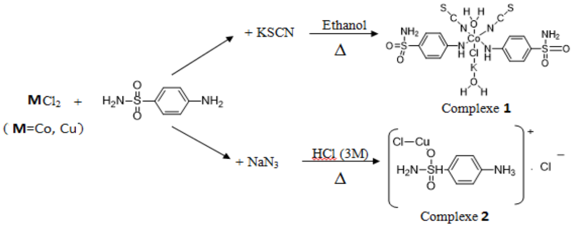
It is well known that sulfonamide derivatives through exchanges of different functional groups without modification of the -S(O)2N (H)- function, can exhibit a wide variety of pharmacological activities. In addition, some metal complexes of these ligands have been prepared to promote rapid healing of burns in humans and animals [1].

This framework explains why an increasing attention is given to the function sulfanilamide and these derivatives, as well as their coordination with the different metallic atoms to have a new range of complexes which can have reactivity biologically interesting. In this context, the work presented in this thesis aims to design new molecular complexes characterized by the coordination of the sulfanilamide ligand by different ways of these two functions [2] .

The combination of the sulfanilamide ligand with the co-ligand KSCN, in the presence of the Co(II) ion, led to the production of a new molecular complex of formula: K CoCl $[(C_6H_8N_2O_2S)\ SCN.\ H_2O]_2$ (1). In a second step the effect of the solvent also in the presence of the Cu (II) ion led to a second new molecular compound of formula $[CuCl\ (C_6H_9N_2O_2S)]^+.\ Cl^-$ (2). The two crystal structures of sulfanilamide complexes (1) and (2) were determined by single crystal X-ray diffraction.



Key words: Complexes, sulfonamide, syntheses, X-ray diffraction.

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EFFICIENCY OF DIFFERENT INORGANO-ORGANO-CLAYS IN THE ADSORPTION OF AN ANIONIC DYE FROM WASTEWATERS

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The soil is a complex system consisting of one mineral part and another organic part. The mineral part results from the fragmentation of the rocks into finer and finer particles and form a stack of clay leaves. The organic part is the result of chemical and biological degradation of plants, animal tissues, and natural and artificial debris.

The products of the decomposition of rocks and organic matter mix to form organo-mineral aggregates that give the soil their structure.

The interest of this study is to create a soil model: consisting of an organic part which is the humic acid, and of a mineral part represented by the double lamellar hydroxides (HDL). This is intended to try to understand the interactions and mechanisms that occur during ion exchange, transport or element migration.

We are interested in our work on the synthesis of $MgRFeCO_3$ double lamellar hydroxides at different molar ratios R = 2, 3, 4 by coprecipitation at constant pH (pH = 10). These materials will be modified by humic acid by different methods to note: anion exchange, coprecipitation, rehydration calcination in humic solution.

Then the base materials and modified products called "hybrids" will be used for the adsorption of the anionic dye Orange II. These precursor materials will be characterized by various techniques: FTIR, RDX, BET, MEB.

Key Words : Dépollution, adsorption, hydroxydes doubles lamellaires, orange II.

Host−Guest Interactions Accompanying the Encapsulation of doxorubicin within dendritic macromolecular cavities.

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One of the reasons why supramolecular structures containing cavities represent an important branch of supramolecular chemistry [1] is because of the high tunability of the cavity size and shape that can be obtained by varying the nature of the constituting monomers and of their sequencing [2]. Cavities inside macromolecular structures can be rigid, like in cyclodextrins or cucurbiturils, or flexible, like in calixarenes, as a result of the complex pattern of intra- and inter-molecular interactions. In particular, non-rigid structures with readily functionalized end-groups are versatile systems for host-guest chemistry applications, particularly in the bio-medical field, where new and effective classes of active compounds with antiviral, bactericidal and anticancer activities can be prepared [3]. Falling in this category, dendrimers, or arborols, are a special class of flexible polymeric molecules with unique properties and structures, we present theoretical results based we present theoretical results based on density functional theory to study the encapsulation drug inside macromolecular cavities.

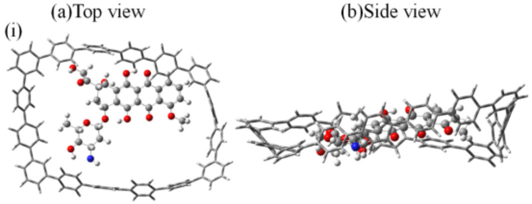

Figure 1: Top and Side Views of optimized structures of doxorubicine inside dendrimer (C, O, H, N and S atoms are represented as: gray, red, white, blue, yellow).

Keywords : Dendrimers, DFT, anticancer drugs..

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SYNTHESIS AND CHARACTERIZATION OF NEW SYMMETRICAL 1,3-dialkyl-5,6-dimethylbenzimidazolium

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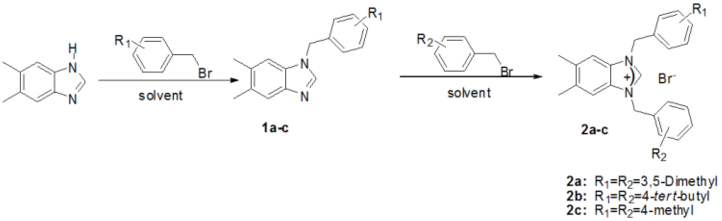
N-Heterocyclic Carbenes (NHCs) are nowadays ubiquitous ligands in organometallic chemistry as well as catalysis due to their unique properties[1]. Steric and electronic properties of NHCs can be tuned in a wide range by change of substituents and backbones[2]. We herein report the synthesis of N-substituted 5,6-dimethylbenzimidazole **1a-c** which were obtained from the reaction of 5,6-dimethylbenzimidazole with alkyl bromides. Subsequent treatment of the resulting *N*-alkyl-5,6-dimethylbenzimidazole with bulky alkylated benzyl bromides (**a:** R_1= R_2= 3,5-dimethylbenzyl; **b:** R_1= R_2= 4-tertbutylbenzyl; **c:** R_1= R_2=4-methylbenzyl) afforded the corresponding 1,3-dialkyl-5,6-dimethylbenzimidazolium **2a-c** with high yields (>86%) (Figure1). A series of new N-Heterocyclic Carbenes (NHCs) ligands **2a-c** have been characterized by appropriate spectroscopic techniques (IR, ^{1}H NMR, ^{13}C NMR, HRMS) and microanalysis[3].



Keywords: N-substituted 5,6-dimethylbenzimidazole, 5,6-dimethyl benzimidazole, alkyl bromides, 1,3-dialkyl-5,6-dimethylbenzimidazolium.

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SYNTHESIS, CRYSTAL STRUCTURES AND CHARACTERIZATIONS OF TWO NEW COPPER(II) COMPLEXES INCLUDING THIOHENEACETIC ACID AND IMIDAZOLE LIGANDS

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Two new thiopheneacetic – based copper (II) complexes, namely bis(1*H*-imidazole)-(2-thiopheneacetato-O,O^i) (thiopheneaceato-O)-copper(II), $[\mathrm{Cu}(\mathit{HTAA})_2(\mathrm{imd})_2]$ **(1);** bis(1*H*-benzimidazole-$_k N^3$)bis(2-thiopheneacetato-O,O^i)copper(II), $[\mathrm{Cu}(\mathit{HTAA})_2(\mathrm{bimd})_2]$ **(2),** (*HTAA* is thiopheneacetic acid ($C_6H_5O_2S$), imd is imidazole ($C_3H_4N_2$) and bimd is benzimidazole ($C_7H_6N_2$)), have been synthesized and characterized by **FT–IR** spectroscopy, and single crystal X-Ray diffraction. X-Ray diffraction analysis shows that complexes **1** and **2** have mononuclear units with the general formula $[\mathrm{Cu}(\mathit{HTAA})_2\mathit{L}_2]$ (*L* is imd or bimd), in **1** Cu^{+2} ions is surrounded by tow *HTAA* and tow imd ligands with the distorded square bipyramidal coordination, Discrete monomeric units of **1** form a one-dimensional network via hydrogen bonds through nitrogen atoms and acetate oxygen atoms of the neighbouring molecules. Complex **2** consist of individual molecule in wish the Cu^{+2} lies on a center of symmetry; two thiopheneacetat and tow benzimidazole ligands surround the copper center forming an octahedral CuN_2O_4 core. Both the *HTAA* and bimd ligands are arranged in *trans* positions. Each *HTAA* ligand is coordinated in a bidentate manner to the Cu^{2+} ion through the carboxylate O atoms (O1, O2,O3 and O4), creating a four-membered chelate ring, while the bimd ligands behave in a monodentate manner, coordinated through the N1 and N3 atoms. The coordination mode of carboxylate group in complex **2** were revealed by Fourier transform IR (FT–IR) spectroscopy.

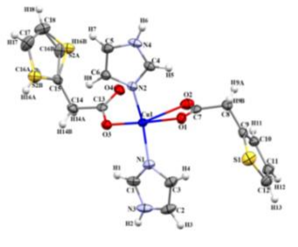

Fig1: Molecular structure of $[\mathrm{Cu}(\mathit{HTAA})_2(\mathrm{imd})_2]$ **(1)**

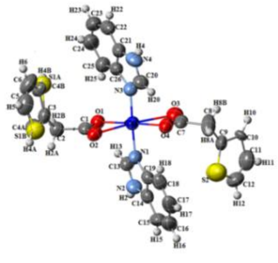

Fig2: Molecular structure of $[\mathrm{Cu}(\mathit{HTAA})_2(\mathrm{bimd})_2]$ **(2)**

Keywords: Sulphur ligands, Coordination compound, Structural determination, X-ray diffraction

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The study of different enzyme inhibition with some compounds by molecular modeling

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[2]University of Tlemcen-AlGERIA
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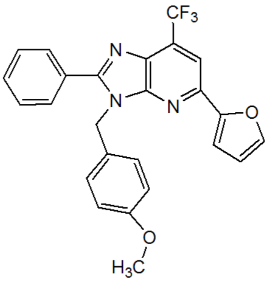
A series of nitrogen heterocycles including the derivatives of 1-deazapurines, were studied for miscellaneous enzyme inhibition activities in search of the potent enzyme inhibitor. The hyperactive enzymes like carbonic anhydrase-II, phosphodiesterase-I, xanthine oxidase, α-glucosidase, and β-glucuronidase were selected for the study.
The compounds 11 and 12 were found the most potent against carbonic anhydrase-II, α-glucosidase and β-glucuronidase in comparison to their standard compounds. These selective inhibitors can be used as lead compounds for development of drugs against various diseases associated with these enzymes (1). For this reason, this study was undertaken by molecular modeling using MOE (Molecular Operating Environment) software (2) to predict their interaction with these enzymes.

Key words: Molecular modeling, DFT (density functional theory), Drug research, Derivatives of 1-Deazapurines



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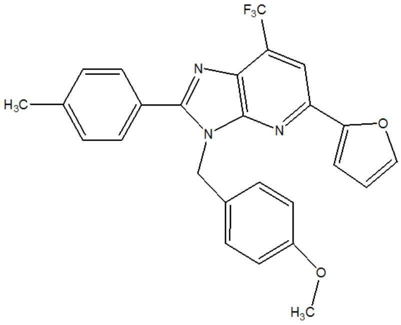

Ligand_12

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Molecular structure, Mulliken charge and frontier molecular orbital analysis on 3-nitroaniline and 4-methoxy-3-nitroaniline using density functional theory

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Aniline and its derivatives have been widely used as starting materials in a vast amount of plastics, organic semiconductors, agricultural, pharmaceutical, catalytic, chemical and many other industrial processes [1]. The understanding of their molecular properties as well as the nature of reaction mechanisms they undergo has a great importance. Hence, the investigation on the structures of aniline and substituted anilines are still being carried out, increasingly. The inclusion of a substituent group in aniline leads to the variation of charge distribution in the molecule and this greatly affects the structural, electronic and vibrational parameters [2].
In this work, the geometry optimization of 4-methoxy-3-nitroaniline and 3-nitroaniline was carried out by Gaussian 09W program [3] using B3LYP functional and 6-311G(d,p) basis set. We analyzed gap energy of the frontiers molecular orbitals and the molecular dipole moment changes due to the effect of the substitution of hydrogen atom in relative position 4 by a methoxy group in the 3-nitroaniline molecule.

Key words: 4-methoxy-3-nitroaniline, 3-nitroaniline, DFT calculations

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Synthesis and characterization of new tin(IV) chloride complexes of *O,O'*-dialkyl-*N,N'*-dialkylphosphoramidates

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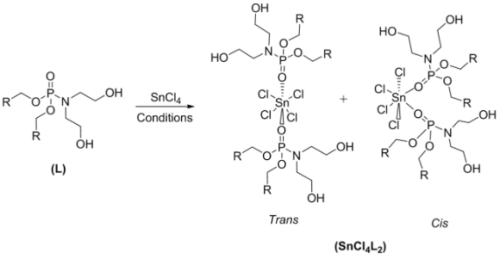
The chemistry of phosphoramidates is recently developed due to their biological activity [1] and also their interesting coordination chemistry [2]. Some of these compounds were used as *O,O*'-donor ligands for rare earth metal cations [3]. In partculary, the coordination compounds of organotin(IV) are a matter of interest in recent researches [4,5].They have been, also,extensively used as wood preservatives, agrochemical fungicides and biocides [6]. We described, previously, the synthesis of a series of *O,O*'-dialkyl-*N,N'*-dialkylphosphoramidates ligands (L) [7] and we report, herein, their reaction with tin tetrachloride to produce new octahedral tin complexes of the type [$SnCl_4L_2$] (Scheme 1). These adducts were characterized, at the present, by multinuclear (^1H, ^{13}C, ^{31}P and ^{119}Sn) NMR, and IR spectroscopy. The NMR data show, as expected, that these complexes exist in solution as mixtures of *cis* and *trans* isomers with a slow ligand exchange on the *cis* isomer at room temperature.



Scheme 1

Keywords : *O,O*'-dialkyl-*N,N'*-dialkylphosphoramidates ligands, octahedral tin complexes, ^{119}Sn NMR.

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Analytic and therapeutic evaluation of platelet-rich plasma on the skin wound healing process: A comparative experimental study in sheep

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The therapeutic evaluation of the biological effect of platelet-rich plasma (PRP) used as a surgical adjunct to maintain the inflammatory process and to potentiate tissue healing, make the subject of recent research in regenerative medicine. This study was designed to evaluate the healing activity of PRP by its topical application on the skin experimentally injured in a sheep model. The study was conducted on 9 adult and clinically healthy males sheep. PRP was obtained by a protocol of double centrifugation of whole blood from each animal. After sterile skin preparation, full-thickness excisional wounds (20 mm x 20 mm) were created on the back of each animal. The animals were randomly divided into three equal groups of three sheep for each. In Group I, the wounds were treated with PRP, in Group II; wounds were treated with Asiaticoside; in Group III, wounds were treated with saline solution. The different treatments were administered topically every 3 days. Morphometric measurements of the contraction surface of the wounds and histopathological biopsies were carried out at the 3rd, 7th, 14th, 21st, and 28th days of healing. The results of the morphometric data obtained revealed that it was significant differences recorded at the 7th and 14th day of healing in favor for animals of Group I. Semi-quantitative histopathological evaluation showed that PRP reduces inflammation during 3 first days post-surgical and promotes epithelialization in 3 weeks of healing. We concluded that topical administration of PRP obtained by double centrifugation protocol could potentially improve the skin healing process in sheep.

Keywords: healing, platelet-rich plasma, sheep, skin

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Investigation of the charge transfer and transport in MEH-PPV:BMN composite

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In conjugated polymer based optoelectronic devices (light emitting diodes and solar cells), transfer and transport of the charge are two essential processes which could be responsible for better performance of the device. We have investigated the effect of incorporation of BMN small organic molecule into the polymer MEH-PPV matrix on the optical, morphological and electrical properties.

Key words: conjugated polymer, charge transfer, electrical properties.

Synthesis and characterization of a low-spin iron(III) *meso*-tetra(para-tertbutylphenyl)porphyrin complex with the Bis(Pyrazol) ligand: X-Ray diffraction, DFT, Magnetic and cyclic voltammetry studies

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Porphyrins, aromatic tetrapyrrole macrocycles are molecules widely represented in the living areas. Metalloporphyrins are of particular attention due to the interdisciplinary research fields involved, such as advanced materials or biological processes. Especially, iron(III) porphyrins have been the subject of several studies due to their significant applications in biological functions, catalysis and ptophysical properties. The iron porphyrin compounds play also important roles in oxygen transfer and as storage agents in hemoglobin and myoglobin and as electron carriers in cytochrome c. The object of this communication concerns the synthesis, the UV, IR, SQUID, DFT and the molecular structure of a new Pyrazoliron(III) porphyrin coordination compound with a formula :
$[Fe(TBPP)(Pyzr)_2].SO_3CF_3$ where TBPP is the dianion of the para-tetratert-butylphenylporphyrin. The SQUID data indicates that the title complex is a low-spin (S =1/2) iron(III) porphyrin species. The X-rays molecular structure shows that the Fe(III) of the $[Fe^{III}(TBPP)(Pyrz)_2]$ ion complex, one counter ions SO_3CF_3. The central ion Fe3+ is hexacoordinated by two NH-bonded axial Pyrazol ligands and the four pyrrole N atoms of the porphyrin ligand.

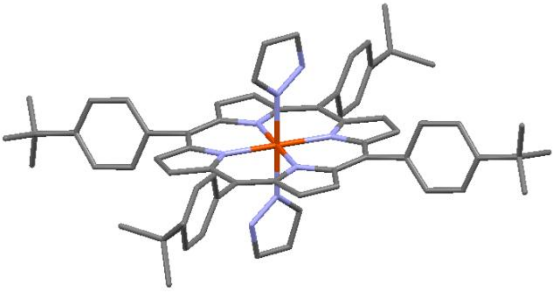

Fig.1. Representation ORTEP of the structure of the complex ion $[Fe^{III}(TBPP)(Pyrz)_2]$.

Elimination des colorants textiles par adsorption et oxydation avancée

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Dyes are widely used in printing, food, cosmetic and clinical industries, but especially in the textile industries for their chemical stability and ease of synthesis and color variety. However, these dyes are the source of pollution once evacuated into the environment.

The experiments, conducted in (JAR-test) with a stirring of 100 Tour / mn, contact time 2 hours. The analysis is done by DCO-meter

The experimental results show that the orpiment doses are pH = 2; the mass of activated carbon m = 1.5, the temperature

Then study the degradation of methyl violet textile dye by the process of Fenton in aqueous medium in the presence of an oxidizing hydrogen peroxide and iron as a catalyst

This study makes it possible to follow the influence of certain parameters such as pH; dye concentration, oxidant concentration, catalyst concentration and temperature on degradation kinetics.

The results show that the best dose for a good degradation are pH = 3, [fe2 +] = 7mg / l, [H2O2] = 10 mg / l

Finally apply these optimal dose obtained on the real water of textile to know the effect of salts.

Keywords: Dyes, adsorption, methyl violet, fenton process

AN ELECTROCHEMICAL STUDY ON THE COPOLYMER FORMED FROM PIPERAZINE AND ANILINE MONOMERS

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A study on the electrochemical oxidation of piperazine and its electrochemical copolymerization with aniline in acidic medium is presented. It was found that the homopolymerization of piperazine cannot be achieved under electrochemical conditions. A combination of electrochemistry, in situ Fourier transform infrared (FTIR), and ex situ X-ray photoelectron spectroscopy (XPS) spectroscopies was used to characterize both the chemical structure and the redox behavior of an electrochemically synthesized piperazine–aniline copolymer. The electrochemical sensing properties of the deposited material were also tested against ascorbic acid and dopamine as redox probes.

Keywords: copolymer; polyaniline; piperazine; FTIR in situ

SYNTHESIS OF SOME SALEN-BASED TRANSITION METAL COMPLEXES AND EVALUATION OF THEIR BIOLOGICAL PROPERTIES

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Metal complexes derived from Schiff bases have attracted much attention due to their remarkable application in several domains [1]. In fact, they exhibit a wide range of biological activities, *viz*., antimicrobial [2,3] and anticancer [4] …etc. They also used as catalyst in synthetic chemistry [5,6].

Owing to this diversity of applications, our studies were conducted to synthesize some tetradentate ligands based transition metal complexes and screen them for their biological and electrochemical behavior.

This work deals with the synthesis of metal complexes based Schiff base. Biological and electrochemical investigations were also performed. All complexes have shows moderate antioxidant and antibacterial activities. Among obtained complexes Cu-complex and Zn- complex have shown respectively an excellent antioxidant and antibacterial activities.

Keywords: Schiff base, metal complexes, electrochemical, antioxidant activity, antibacterial activity.

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Comparaison between amine and alcohol addition on tri-coordinated phosphorus compounds

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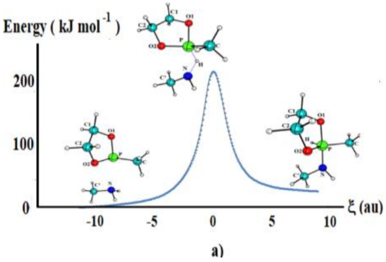
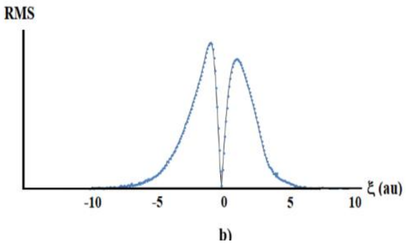
The oxidative addition of aliphatic alcohols[1-2] and amines on monocyclic phospholanes leads both to pentacoordinated phosphorane with P-H bond. Although the two mechanisms are not similar, even if it proceed in both cases through the intermediacy of phosphonium species and an oxidation degree change in the central phosphorus atom.

In this study, we will focus on the main differences caracterizing this two mechanisms : one or two-step mechanism, biphilic behavior of central phosphorus atom, stereochemistry of final product and activation barrier energy.

Key words: transition state, IRC, energetic profile, phosphorane



a) Energy profile of 1-4 isomer formation.



b) Corresponding reaction force.

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Synthesis, characterisation and biological activities of 2, 5-disubstituted 1, 3, 4-Oxadiazoles and their Zinc (II) complexes

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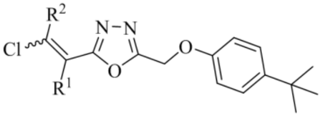
Aromatic 1, 3, 4-oxadiazoles are an important group of π-conjugated heterocyclic compounds. Moreover, these heterocyclic scaffolds have also proven important biological activities [1] but also have been used as laser dyes, photographic materials or scintillators during past decades [2]. In recent years, their use has grown rapidly in the application of some 1, 3,4-oxadiazoles in coordination chemistry and structural studies of supramolecule polymers [3]. The Zn2+ is actively involved in various biological processes in several organs, e.g., brain, pancreas, spermatozoa, vesicles of presynaptic neurons, etc., and plays pivotal roles in controlling gene transcription and metalloenzyme function in either a free state or a sequestered form [4]. In this work, we describe the synthesis of a novel series of Zinc (II) complexes of an asymmetrical 2,5-disubstituted 1,3,4-oxadiazoles derivatives. These new complexes ($[ZnCl_2\ L]$) ($L = p\text{-}tBuPhOCH_2CON_2C{=}CHCR^1{=}CR^2Cl$) are fully characterized by IR, UV-visible, Fluorescence and NMR spectroscopies. Comparative study of biological activity of both ligands and Zinc (II) complexes will be presented.

$$ZnCl_2 + L \longrightarrow ZnCl_2L$$



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SUPRAMOLECULAR POROUS ARCHITECTURES BASED ON IONIC H-BONDS: SYNTHESIS, PORE TUNABILITY AND SORPTION PROPERTIES

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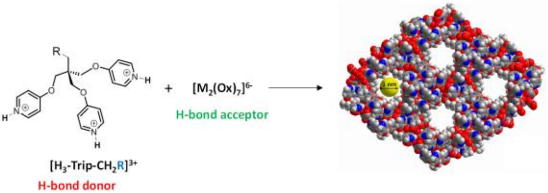
Microporous hydrogen-bonded frameworks are an emerging class of materials reminiscent of metal–organic frameworks (MOF) and covalent organic frameworks (COF), for which high surface area and potential in the fields of gas sorption, catalysis and separation have been highlighted recently.[1] An emerging trend towards the development of such porous architectures consists in using preformed complexes to assemble with organic molecules via ionic H-Bonds.[2-4] In this strategy, metal-organic units with given geometries and linking abilities form the network nodes, and contribute to govern the net topology through their association with organic linkers (Figure).

In this poster, recent results obtained using metal-oxalate complexes and organic cations as building-blocks will be presented. Two families of robust supramolecular porous architectures showing tunable pore sizes and functionalities together with interesting sorption properties will be highlighted.[3,4] A special attention will be devoted to a supramolecular material showing a potential porosity of 60%, chirality, and channels decorated with free pyridyl groups. Guest sorption experiments through reactions with these pyridyl groups will be illustrated.[4]



Key words: Open-framework, supramolecular architectures, sorption properties

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Synthesis and biological activity of new β–aminovinylimines and their zinc(II) complexes

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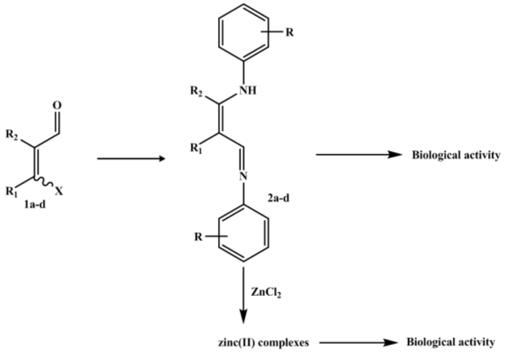
Nowadays, There is an increasing academic, commercial and biochemical interest on the metal complexes of organic chelating ligands[1]. Schiff bases and their metal complexes had a variety of applications including biological [2], clinical, analytical and industrial in addition to their important roles in catalysis and organic synthesis [3–5]. They are important intermediates in a number of enzymatic reactions involving interaction of an enzyme with an amino or a carbonyl group of the substrate [6]. In this work, we report the synthesis, characterization and the antimicrobial activity of new β-aminovinylimines compared to their new Zinc(II) complexes. The adducts have been characterized in solution using NMR, IR and UV-Vis spectroscopies.



Keywords: β-aminovinylimines, Zin(II) complex, characterization, antimicrobial activity

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Comparative study of the dynamics of the photoionisation of two diarylketone molecules: the case of benzophenone and fluorenone

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The benzophenone molecule, a diarylketone (Figure 1a), is a paradigmatic organic molecule where the singlet-to-triplet energy transfer is especially efficient [1]. The floppy character of this molecule plays a significant role in this behaviour, which is dramatically perturbed when a more rigid diarylketone molecule, such as fluorenone (Figure 1b), is considered [2]. Single photon ionization and subsequent unimolecular ion decomposition were studied on jetcooled benzophenone and fluorenone separately, using VUV synchrotron radiation in a photoion/photoelectron coincidence setup. Slow PhotoElectron Spectra (SPES) were recorded in coincidence with either the parent or the fragment ions for $h\nu<12.5$ eV. Dissociative ionization is observed for benzophenone only. The full interpretation of the measurements, including the identification of the neutral and ionic species when dissociative ionization is at play, benefits of high level *ab-initio* computations for determining the equilibrium structures and the energetics of the neutral and ionized molecules and of their fragments. Electronically excited states of the parent molecular ions were calculated also. The calculation scheme, adopted here, associates: *i)* optimization of molecular structures at the PBE0 level; *ii)* single point energy calculations using the (R)CCSD(T)- F12 technique on the optimized structures to take the electron correlation into account; *iii)* combination of points *i)* and *ii)* with IC-MRCI excited state calculations.

Key words: VUV synchrotron radiation, ab-initio calculation, (R)CCSD(T)- F12,

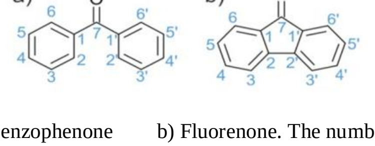

Fig. 1 a) Benzophenone b) Fluorenone. The numbers identify the C atoms

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EFFECT OF THE BINARY AND TERNARY EXCHANGES ON CRYSTALLINITY AND TEXTURAL PROPERTIES OF X ZEOLITES.MODIFICATION CHARACTERISATION AND APPLICATION

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The ionic exchange of the NaX zeolite[1,2] by Cu^{2+} and/or Zn^{2+} cations is progressively driven while following the development of someof its characteristic: crystallinity by XR diffraction, profile of isotherms, RI criterion, isosteric adsorption heat and microporous volume using both the Dubinin–Radushkevich (DR) equation and the t-plot through the Lippens–de Boer method which also makes it possible to determine the external surface area[3,4,5].
Results show that the cationic exchange process, in the case of Cu^{2+} introduced at higher degree, is accompanied by crystalline degradation for Cu(x)X, in contrast to Zn^{2+}-exchanged zeolite X. This degradation occurs without significant presence of mesopores, because the RI criterion values were found to be much lower than 2.2. A comparison between the binary and ternary exchanges shows that the curves of CuZn(x)X are clearly below those of Zn(x)X and Cu(x)X, whatever the examined parameter.
On the other hand, the curves relating to CuZn(x)X tend towards those of Cu(x)X. This would again confirm the sensitivity of the crystalline structure of CuZn(x)X with respect to the introduction of Cu^{2+} cations. An original result is the distortion of the zeolitic framework of X zeolites at middle exchange degree, when Cu^{2+}competes with another divalent cation, such as Zn^{2+}, for the occupancy of sites distributed within zeolitic cavities. In other words, the ternary exchange accentuates the crystalline degradation of X zeolites. An unexpected result also is the no correlation between crystal damage and the external surface area.

Key words: Adsorption,crystallinity, ion exchange, zeolite.

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SYNTHESIS AND CHARACTERIZATION OF A NEW COORDINATION COMPOUND BASED ON THIOCYANATE AND NICKEL METAL

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Several hybrid compounds are synthesized based on thiocyanate and metal due to their interesting properties [1]. In this context, a new compound $Ni(SCN)_4 (C_5H_{13}N_2)_2$ was prepared based on 2-methylpiperazine, nickel and thiocyanate. The preparation leads to the formation of a single crystal with a monoclinic crystalline system. His space group is $P2_1/c$. These mesh parameters are as follows a = 7.2267 (4) 13.0449 (6) 12.4047 (6) and β (°) = 106.298 (3)°. Different techniques analysis are used to characterize it as infrared, UV-visible and thermal analysis. Antibacterial activity and magnetic property are also investigated. Thermal analysis shows a partial decomposition. The hybrid indicates antibacterial activity and a weak antiferromagnetic interaction.

Key words: Thiocyanate, nickel, antibacterial activity, magnetic activity

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SYNTHESIS, DESIGN AND SPECTROSCOPIC CHARACTERIZATION OF A NOVEL HETEROBIMETALLIC L-ARGININE COMPLEX WITH BIOCHEMICAL PROPERTIES

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The self-assembly of the transition metal complexes with L-Arginine are currently attracting much attention. In particular, a considerable effort has centered on the synthesis of the copper(II)-Arginine complexes owing to their intriguing design and biological applications [1]. Controlling the self-organization and molecular interactions is therefore an extremely topical field of researches that aims to obtain supramolecules with original topologies and possessing attractive physical and/or biological properties. It is in this context that Yamauchi et *al.* were interested in the study of a series of compounds of $[Cu(L\text{-}Arg)_2]_m(X).nH_2O$, containing different counter-anions X_m^- [2], which demonstrated that the architecture of the self-organization of Cu(II)-Arginine complexes is strongly influenced by the nature of the incorporated counter-ions. Meanwhile, heterometallic μ-oxo-bridged complexes containing M-O-M' motifs are of special interest due to the possible "synergetic" interplay of the two M/M' metal ions that improves their catalytic, magnetic, optical or biochemical properties, compared to those of the monometallic compounds. Heterometallic μ-oxo-bridged complexes can also be served as models for the active sites of metalloproteins and metalloenzymes [3]. One of the powerful strategies for elaboration of such advanced multifunctional materials is the use of metal oxy-anion. However, to the best of our knowledge, no studies on the Cu(II)–Arg–$X_{(counter\text{-}ion)}$ systems, involving metal oxyanion as counter-ions, have been reported in the literature. Therefore, the extended studies in this field seem to be very interesting. On the basis of the aforementioned points, we present here the synthesis, design and spectroscopic characterization of a novel (Cu^{II}/Re^{VII})-heterobimetallic complex with L-Arginine ligand, namely *trans*-$[Cu(L\text{-}Arg)_2(ReO_4)_2]$. The obtained results will be discussed and presented in details. The biochemical properties of the novel compound were also investigated via free radical scavengers and ferric reducing power (FRP), showing promising antioxidant activities in a concentration-dependent fashion.

Keywords: Heterobimetallic complex; L-arginine; Chiral; Antioxidant activities.

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A One-Dimensional Lead-Free Perovskite-Derivative $(C_7H_8NO_2)_2BiI_5$: Crystal Structure and Optical Properties

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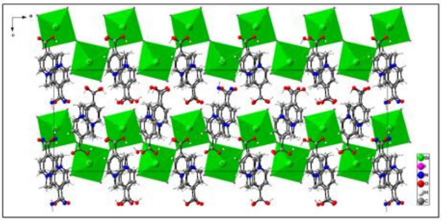
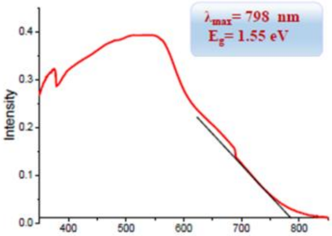
Lead-free organic-inorganic hybrid perovskites have recently attracted intense interest as environmentally friendly, data storage and ferroelectric field-effect transistors. Hybrid organic–inorganic perovskite materials combine the characteristics of organic and inorganic components and thus might be promising candidates to obtain semiconductor materials. Here, we reported a new one-dimensional (1D) zigzag chainlike hybrid material of $(C_7H_8NO_2)_2BiI_5$, in which the corner-sharing octahedral bismuth halide chains are surrounded by organic cations of 1-methyl-4-carboxyl-pyridinium. This unique zigzag 1D hybrid perovskite-derivative material shows a narrow direct band gap of 1.55 eV, which is encouraging for optoelectronic applications. Importantly, it behaves as a typical semiconducting material and displays obvious photoresponse in the visible-light range. This work opens a potential pathway for the further application of 1D lead-free hybrids.





Keywords: Lead-free, Hybrid perovskites, Crystal structure, Semiconductor materials, Optical band gap.

ESTIMATION OF MOLECULAR DIFFUSIVITY IN AQUEOUS SOLUTION OF SOME AZO DYES: A QSPR MODELS

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Diffusion coefficient is one of the most important transport properties of the fluids in the environment. The experimental determination of diffusion coefficients can be considered difficult, time-consuming, besides being costly. However, an alternative standard is the use of models relating the diffusion coefficient and molecular properties. In this study, we tried to estimate the molecular diffusivity (D_m) of some azo dyes by several empirical methods: Wilke-Chang, Stokes-Einstein, Wilke-Chang, Hayduke-Laudie, Scheibel and molecular weight equations. The volume (V_M) of the solute is required to estimate this parameter. Classical LeBas method is commonly used. However, this method may represent a boring and time-consuming task, depending on the nature and number of compounds to be calculated. Another way to address the problem consists in the use of theoretical semi-empirical (AM1, RM1, PM3 and PM6) molecular volume (V_M; Å3) and polarizability (α; Å^3), which demonstrated to estimate the diffusion coefficients within an acceptable average error.
Single and Multiple Linear Regression (SL;MLR) were both used to correlate experimental diffusion coefficient (D_{exp}) with semi-empirical physicochemical calculated parameters such as: Molecular volume (V_M ;A° ^{3}), Molecular surface area (S; A°^{2}), Miller polarizability (α_{Miller}; Å^3), Molar refraction (R_D), Molecular weight (M_W), Ionization potential (PI; eV), HOMO-LUMO energies (eV), Polar surface area (PSA), Hydration energy (E_H; Kcal/mol). According to these results, the Linear Regression methods were seen to be statistically valid to calculate molecular diffusivity with an average correlation coefficient of 0.99. The resulting model involves variables easily obtained, can be useful to estimate easily the diffusion coefficients of azo dyes compounds in water that cannot be easily measured, either by physicochemical or electrochemical methods.

Keywords: Diffusion coefficient, linear regression, semi empirical, QSPR

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Optimization of the electrodeionization process: Design considerations

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Electrodeionization (EDI) is a separation process combining electrodialysis (ED) and ion-exchange (IEX); the resulting hybrid process gained increasing attention for removal/ recovery of ions from water [1, 2].

Ion-exchange mixed bed is the primary deionization technology associated with ultra-pure water production. The discontinuity of the process and the need for high-purity regenerating chemicals constitute serious disadvantages. Likewise, ED is not an economical process for treating diluted solutions. High resistances, energy consumption and polarization are the main drawbacks [3]. The EDI process eliminates these problems and can be considered, in principle, as an electrically regenerated IEX process or as an ED system whose conductivity and selectivity are aided by the presence of IEX particles in the dilute compartment.

The optimization of the EDI resin bed has been and remains a serious challenge for the design. What is the best design? Thin or thick cell, Single or mixed bed… This research work deals with this optimization problem.

It is based on the comparison of five different configurations (homogenous/mixed, cationic, anionic, inert and two layers ordered bipolar beds). We have also investigated the effect of the inter-membrane space on the process efficiency under different operating conditions using resin beds thicknesses of 2, 4 and 6 mm.

This study showed that the introduction of the resins in the desalting compartment has significantly reduced the resistance of the system particularly in the ordered bed, and a remarkable, empirical equation describing the EDI efficiency as functions of flow rate and cell thickness is established.

Key words: Electrodeionization, Efficiency, Ion exchange, Electrodialysis.

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A DENSITY FUNCTIONAL THEORY EXPLORATION OF THE ELECTRONIC−STRUCTURAL PROPERTIES OF DIVALENT FIRST-ROW TRANSITION METAL CATIONS COMPLEXES WITH GLDA

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In the aqueous media free metal ions catalyze many reactions disadvantageous for man. Therefore it is necessary to control accessibility and a number of metal ions both during technological processes and in their final products. This aim could be achieved owing to metal ions complexation by the compounds characterized by complex formation ability. Therefore, the chelating agents belonging predominantly to two different groups i.e. aminopolycarboxylates (APCAs) and polyphosphonates are commonly used [1,2]. APCAs containing carboxylic groups connected to one or a few atoms of nitrogen are able to complex metal ions by formation around them one or a few stable heteroatom rings. This phenomenon is called chelating. Forming of stable complexes with metal ions is the base of their application for analytical and industrial purposes. The complexes formed due to chelation are dissolved in water and metal ions found in them do not exhibit such chemical activity as uncomplexed ions. Because of the importance of chelating agents they are produced and used in large quantities and their behaviour as well as their effect on the environment have received considerable attention.

In the present study the structural and bonding characteristics of the GLDA complexes of Divalent First-Row Transition Metal Cations were investigated by means of density functional theory computations. The computed molecular geometries were compared to those in the crystal. We focus on the metal–ligand interactions and analyse the bonding using energy partitioning analysis and AIM method.

Key words: DFT, AIM, GLDA

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Synthesis and structural study of $(C_9H_{24}N_2)_3V_{10}O_{28}.7H_2O$

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The compound has been prepared by slow evaporation at room temperature and its structure was elucidated using single-crystal X-ray diffraction. It crystallizes in the monoclinic system, C2/c space group with the cell parameters: a=20.861(2)Å, b=29.170(2)Å, c=10.362(8)Å, β=115.53(4)°, Z=4 and volume V=5690.3(8)$Å^3$.

The asymmetric unit is formed by one half centrosymmetric decavanadate group, one cation $(C_9H_{24}N_2)^{2+}$, one half centrosymmetric organic cation $(C_9H_{24}N_2)^{2+}$ and four water molecules (Fig 1).

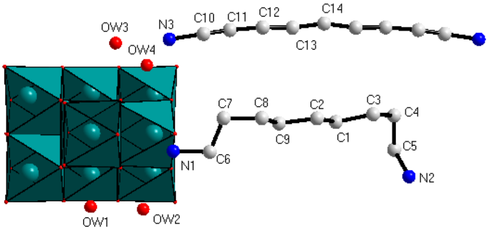

Fig 1. Asymmetric unit of $(C_9H_{24}N_2)_3V_{10}O_{28}.7H_2O$

Key words: Decavanadate, Synthesis, Crystal structure.

Experimental and theoretical study of quinoline derivatives obtained by slight modifications of the standard Skraup reaction

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In order to explore the role of glycerol in the Skraup reaction in producing complex structure quinolines, synthesis of some quinoline-5-carboxylic acid glycerol esters, from the commercially available anilines (3-aminobenzoic acid derivatives), has been carried out using the slightly modified Skraup reaction (excess of glycerol). It has been found that the use of an excess of glycerol in reaction with 3-aminobenzoic acid with I2 as oxidant in concentrated H2SO4, results in the formation of two acyclic isomers (a, b) of the corresponding glycerol ester one of which is predominant and a third cyclic isomer (c) obtained in the form of traces. While obtaining the acyclic isomers is quite expected, the formation of the cyclic one was unsuccessful despite various attempts. To support the experimental results, theoretical computations have been carried out at DFT level and using the B3LYP/6-31++G(d,p) method. The calculations show that the cyclic isomer is predicted at very higher energy than its acyclic congener, sustaining its failed formation.

Key words: Glycerol esters, Isomers Quinoline derivatives, Skraup reaction, DFT calculations

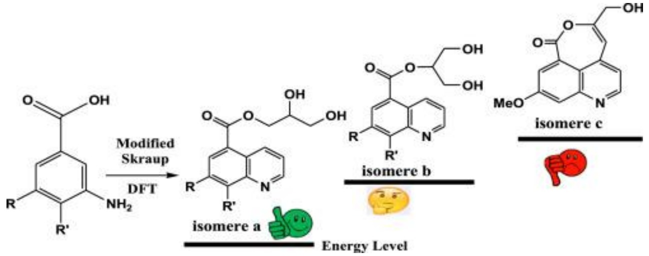

Fig. 1 Isomers Quinoline derivatives

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Application of raw sawdust and olive pomace and their derived biochars in the removal copper from aqueous solution

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Over the last decades, groundwater and soil pollution has dramatically increased as a result of the release of different contaminants in the environment, such as pesticides and Metal Trace Elements (MTE). In particular, the presence of MTE in water is due to the massive use of mineral fertilizers in agriculture, mining activities as well as the discharge of wastewater in the natural environment. Sorption is being one of the most used techniques to remove these pollutants from water. Recently, more attention is given to the development of low cost,bio-based and sustainable sorbents. It is the case of biochar, a highly porous and carbonaceous material obtained through the pyrolysis of biomass.

Against this backdrop, the aim of this work is to study the performance of two raw organic wastes (sawdust and olive pomace) and their derived biochars in terms of copper removal from aqueous solution. The sorption capacities of the four studied sorbents were assessed using the batch technique. For each sorption experiment, 25mL of copper solution (0.2 to 0.6 mmol/L) and 0.5 to 4g/L of sorbent were added into the vessels. The suspensions were shaken for different durations (15 min to 8h), at pH values varying from 3 to 10, then filtered and the copper concentration in solution analyzed by ICP-OES. Our results indicate that, regardless of sorbent nature, the uptake of Cu from solution increases with pH and is maximum at pH 7. The most efficient sorbent dose corresponds to 1 g/L. Under these experimental conditions and for $[Cu^{2+}]=10^{-4}$mol/L, raw olive pomace retained higher amounts of copper than raw sawdust (50% and 20% of Cu initial concentration respectively). After the artisanal pyrolysis of the two feedstocks at 300°C for two hours, the sorption capacities of both raw sorbents significantly increased. Thus, the highest removal yields of copper were obtained for the biochar derived from sawdust (about 90% of the introduced Cu) while the olive pomace-derived biochar exhibited lower affinity (60%).

Synthesis, crystal structure, vibrational spectroscopy, optical investigation and DFT study of a novel hybrid material: 4,4’-diammoniumdiphenylsulfone iodobusmuthate

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Single crystals of a new organic-inorganic hybrid compound ($C_{12}H_{13}N_2O_2S$) BiI4 (I) (Abbreviation (**HDDP) BiI4**) was synthesized and characterized by DTA-TG measurement, FT-IR spectroscopy and optical absorption. Its structure has been solved by single crystal X-ray diffraction at 150 K. The compound crystallizes in the monoclinic system and P21/c space group with a = 7.8282(3) Å, b = 12.2162(5) Å, c = 21.7696(9)Å, β = 95.005(2) and V = 2073.91(14) Å^3. The structure consists of edge-sharing BiI_6^{3-} octahedra chains extended along the a-axis. These chains are linked via the 4-4'diaminodiphenyl sulfone cations by hydrogen bonds. The different components are connected by a network of N/C-H…I hydrogen bonds and halogen-halogen interactions. Theoretical calculations were performed using density functional theory with the B3LYP/LanL2DZ level for studying the molecular structure and vibrational spectra of the title compound. Good consistency is found between the calculated results and the experimental structure, IR spectra. The optical properties in the UVevisible region have been explored by the UV evisible absorption. This material shows two absorptions bands centred at 256 nm and 287 nm respectively. The simulated spectra satisfactorily coincide with the experimental spectrum.

Keywords: organic/bismuth (III) iodide hybrid, X-Ray diffraction, SEM, EDX, DSC, Hirshfled surfaces

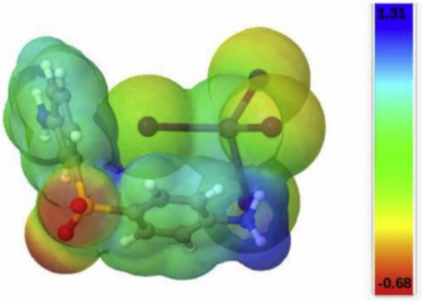

Figure: Electrostatic potential (red: negative potential, blue: positive potential).

Ortho-Phenyl dialkylphosphonium sulfonate compounds : Two rotamers in equilibrium

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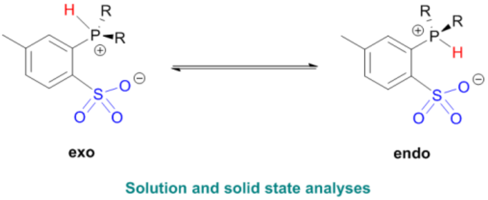
ortho-Phenyl phosphonium sulfonate compounds are important molecules in Pd and Ni polymerization chemistry. In 2002, Drend and al discribed a catalyst system with a mixture of a Pd precursor and a phosphonium-sulfonate compound [1]. Since then, the chemistry of this type of ligand has been developed and improved, but the phosphonium-sulfonate compounds were often ill-defined.
Broad NMR resonances and additional unassigned signals have been reported, but no more detail explanation has been proposed.
Thanks to our study of four phosphonium-sulfonate compounds, we prove the presence of two rotamers in equilibrium in solution, which explain the often observed NMR fluxionality.
Our investigations are supported by multinuclear VT-NMR, IR, X-ray diffraction and theoretical calculations [2].



Key words: NMR, phosphonium sulfonate compounds, rotamers, equilibrium, cristal structure.

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SYNTHESIS, CRYSTAL STRUCTURE AND HIRSHFELD SURFACE ANALYSIS, PHOTOPHYSICAL PROPERTIES OF CADMIUM(II)-TETRACHLOROPHYENYL PORPHYRIN WITH MORPHOLINE AXIAL LIGAND

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In this work we report the synthesis of the cadmium(II)-*meso*-tetrachlorophyenyl porphyrin with the morpholine *O*-donor axial ligand. The [Cd(TClPP)(morph)] complex adopt a distorded five-coordinate square pyramidal geometry indicated by a major *doming*, a moderate *ruffling* and *saddle* distortions of the porphyrinato core. The supramolecular architecture are dominated by intermolecular N−H···Cl and C−H···Cl interactions formed between the morpholine and the chlorine atom of the adjacent *meso*-phenylporphyrin of complex(I). Hirshfeld surface analysis was carried out to understand the nature of intermolecular contacts, where the fingerprint plot provides the information about the percentage contribution. The photophysical properties have been also study.

Keywords: Cadmium(II) porphyrin/ Crystal structure/ Hirshfeld surfaces/ Fluorescence/ Singlet Oxygen.

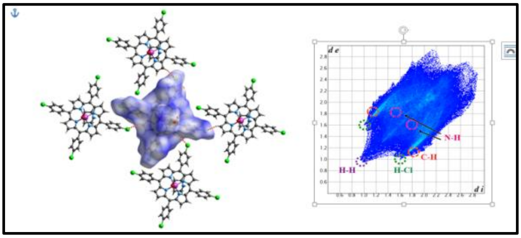

Fig. 1. a) Hirschfeld surfaces mapped over d_{norm} for the title compound and b) Tow-dimensional fingerprint plot with a d_{norm} of the title compound.

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Synthesis and electrochemical behaviour of new ferrocenylphosphonates and their tin(IV) complexes

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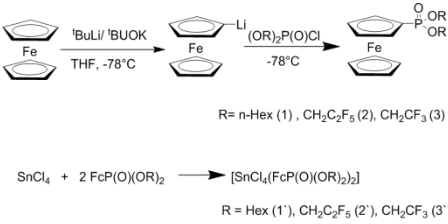
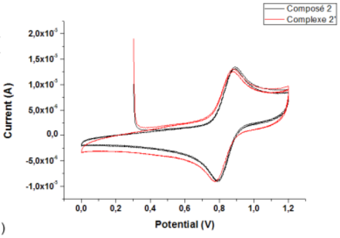
Ferrocene derivatives are extensively used in many areas of chemistry, such as catalysis, material science, and bioorganometallic chemistry[1,2]. One of the reasons for their attractiveness is the fact that their redox state can be easily varied, which allows for a number of their applications in analytical and supramolecular chemistry[3]. The redox potential depends on the electronic effect of the ring substituents on ferrocene. Electron-withdrawing substituents increase the oxidation potential (decrease the reactivity towards oxidation), while electrondonating substituents decrease the oxidation potential and thus enhance the reactivity of ferrocene[4-6,]. In this work, we report on the synthesis and electrochemical study of fluoroalkyl and non-fluorinated long chain group ferrocenylphosphonates and their tin(IV) complexes. The results show that fluoroalkyl groups render the reverse one-electron transfer oxidation reaction more diffuclt ($\Delta E_{1/2}$ = 310-330 mV) as compared to non fluorinated alkyl groups ($\Delta E_{1/2}$ = 215 mV). In addition, the $\Delta E_{1/2}$ between the ferrocenylphosphonate and its tin tetrachloride complex is only 5-10 mV, indicating the small effect of the coordination of the phosphoryl group on the potential of the ferrocene/ferrocenium couple. This would suggest a fast exchange, which is consistent with the small chemical shift and the rapid ligand exchange on the *cis* isomer as observed with ^{31}P NMR spectroscopy.





Keywords: Fluoroalkyl, lithiation, ferrocene, ferrocenylphosphonate, cyclic voltammerty.

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Synthesis of new 3-[3-(4-hydroxy-2-oxo-2-H-chromen-3-yl) -1-yl) -1-methyl-3-phenyl-propylidene-amino] -2-phenyl-thiazolidine-4- one in Eco-friendly Media-Greener and their antibacterial and acetylcholinesterase activities

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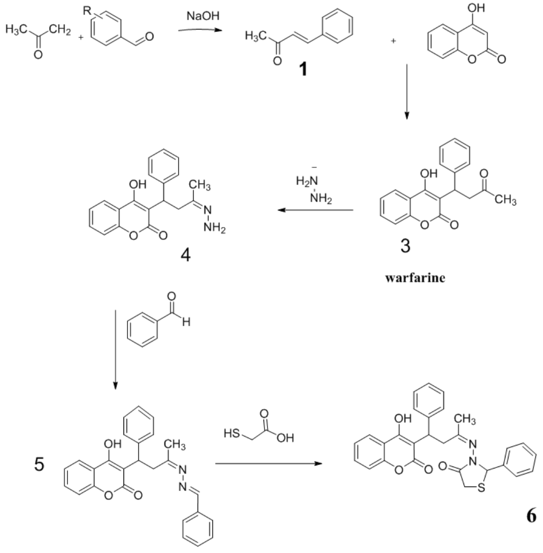
A series of 3-[3-(4-hydroxy-2-oxo-2-H-chromen-3-yl) -1-yl) -1-methyl-3-phenyl-propylidene-amino] -2-phenyl-thiazolidine-4- one **6** were synthesized following several reactions.

We first synthesize benzalacetone **1** using acetone and aromatic aldehydes. Compounds **1** react with 4-hydroxycoumarin to give warfarin **3** which was treated by hydrazine to led to compound **4**. Compound **5** is obtained by condensation between compound **4** and aromatic aldehydes. Finally, the treatment of compound **5** by thioglycolic acid led to compound **6.**

The new compounds were characterized by ^{1}H NMR, ^{13}C NMR, FT-IR spectroscopic methods and elemental analysis. Antimicrobial properties [1,2] of new synthesized compounds are investigated and results are submitted for their activities against three Gram positive and two Gram negative bacteria by well diffusion method.



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EVALUATION OF AROMATICITY OF CLOSED-SHELL AND OPEN-SHELL SINGLET INDENOFLUORENE ISOMERS USING MAGNETICALLY INDUCED CURRENTS

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The aromaticity of recently-synthesized indenofluorene isomers [1] is investigated at the density functional theory level by focusing on their NMR signatures. The NMR shielding constants are calculated by using the Gauge Including Atomic Orbital method, a selection of exchange-correlation functionals (B3LYP, BHandHLYP, as well as the HF method), and the 6-311+G(2d,p) basis set. Both spin-restricted and spin-unrestricted treatments have been considered to highlight the difference between closed-shell singlets and singlet diradicals. The NMR chemical shifts were then estimated using, as reference, the TMS shielding tensors calculated at the same level of theory. All calculations were performed using the Gaussian 16 program package. It turns out that the calculated ^{1}H and ^{13}C NMR chemical shifts are in good agreement with experiment, showing the reliability of the method in view of subsequent analyses. These are carried out by considering the spatial distributions of the magnetically induced currents (MICs), as calculated with the GIMIC method [2]. These MICs and their differences between spin-restricted and spin-unrestricted treatments are then interpreted in terms of the bond current strengths and the current gradients, which indicates the bond aromaticity and enable to analyze the spatial distributions of the diatropic and paratropic currents, respectively [2]. Finally, the spatial correlation between the open-shell and closed-shell character, the aromaticity, and the second hyperpolarizabilities [3] are discussed.

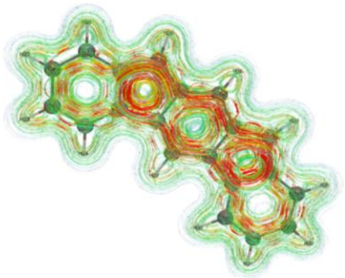

Fig.1 3D streamline plot of the MIC density for indenofluorene **3** calculated at the B3LYP/6-311+G(2d, p) level.

Key Words: Indenofluorene, NMR, magnetically induced currents, aromaticity

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New hydrido bridged bimetallic platinum complex $[Pt_2(\mu\text{-}H)(\mu\text{-}PPh_2)_2Br_2(PPh_3)_2]$

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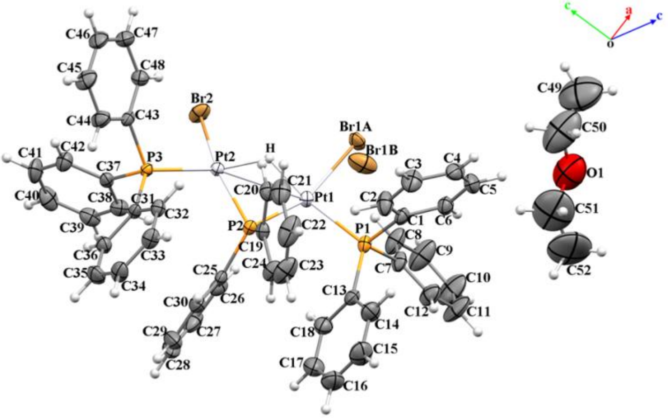
Transition metal hydrides play a central role in many homogeneous catalytic reactions (Bertolasi et al., 1993), they are very important in hydrogenetaion or hydroformylation Their characterization is commonly carried out by NMR spectroscopy, X-Ray analysis or neutron diffraction (Ciriano et al., 1978)
Hydrides of Pt(II) are the most numerous (Leoni et al ., 1995) of any transition metal hydride group ; In addition to the presence of the hydride ligand the complexes invariably have a coordinated phosphine, the pure complexes are usually both air stable and kinetically inert (Roundhill., 1978) we report here the synthesis and structural analysis of a new hydrodo bridged diplatinum complexe $[Pt_2(\mu\text{-}H)(\mu\text{-}PPh_2)_2Br_2(PPh_3)_2]$
The title compound is composed of a triangle formed by two platinum atoms and one phosphorus (P2), the coordination sphere of each platinum is completed with a terminal phosphine (P1, P3) and two bromides (Br1, Br2)



Key words : Platinum complexes, phosphine ligands, hydrido bridge

COUPLING OF BIOSTIMULATION AND FENTON-LIKE TREATMENT FOR REMEDIATION OF PETROLEUM HYDROCARBONS-CONTAMINATED SOIL

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This work deals the influence of coupling of Fenton-like oxidation in two molar ratios H_2O_2 / Total Fe / EDTA, 15/4/4 and 20/1/1 and a biological treatment which consists in stimulation of soil by the appropriate nutrients using molar ratio C / N / P of 100/10/1, on the effectiveness o of a soil remediation polluted by total petroleum hydrocarbons (TPHs) at a rate of 3.0 ± 0.1% in gas-solid microcosms under aerobic conditions. The contribution of microorganisms was studied using abiotic and biotic systems under the same conditions. The temperature and the pH being kept constant throughout the treatment.

The highest removal efficiencies of soil TPHs of 83.3% and 84% are obtained for the two molar ratios H_2O_2 / Total fe / EDTA of 15/4/4 and 20/1/1 respectively.

Key words: Fenton-like, Biostimulation, Biodegradation, Petroleum hydrocarbons

Réduction énantiosélective de cétones aromatiques par catalyse avec le complexe de ruthenium.

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Chiral secondary alcohols are valuable synthetic intermediates in the pharmaceutical, agrochemical, and flavor industries [1]. Asymmetric transfer hydrogenation in water is an alternative method to perform reactions under mild conditions with high enantioselectivities and have been widely employed for the preparation of chiral alcohols. In this area we have studied catalysts for ATH reduction of ketones in water and reported on ruthenium-based catalysts which are reusable both with the same substrate or changing the ketone for each reduction without a loss of enantioselectivity [2].Various ligands for the ruthenium-catalyzed enantioselective reduction of ketones in water have been investigated. Multi-substrate reactions have been carried out for the comparison of various proline amides and aminoalcohol ligands. Two sets of six aromatic ketones have been selected in order to evaluate the enantiomeric excesses of all the resulting alcohols by a single chromatographic analysis. The proline amide derivative prepared from (1R, 2S)-cis-aminoindanol revealed as the best ligand for most of the ketones used in the multi-substrate reductions. This ligand has been employed for the enantioselective reduction of a variety of other aromatic ketones and in all cases the enantiomeric excesses were improved compared to those obtained with phenylprolinamide used in our previous work.

Keywords: asymmetric catalysis; hydride transfer; multi-substrate screening; reduction; ruthenium

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Synthesis of enantiopure heteroaryl carbinols by biocatalysis under mild and eco-friendly conditions.

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Stereoselective reductions of heteroaryl ketones containing furan, thiophene, chroman, and thiochroman moieties are of utmost importance in organic synthesis since the resulting chiral alcohols are used as antioxidants, or building blocks. [1] Asymmetric reduction of ketones with chemical catalyst or biocatalyst is a promising route for the production of enantio enriched alcohols. In the context of developing green and sustainable chemical processes, biotechnologies are attractive alternatives.

The biocatalytic reduction of ketones was performed using medlar *(Mespilus germanica. L)* fruit grown in large amounts in Algeria.[2] Variety of heterocyclic aromatic ketones was reduced with medlar as catalyst in aqueous media. Prochiral ketones containing furan, thiophene, chroman, and thiochroman moieties are reduced with up to 98% ee. High enantioselectivities have been observed especially for the bioreduction of tetralone and thiochromanone with respectively 89% and 98% ee. These chiral benzylic alcohols are used as synthon-key in various syntheses of the many drugs.

In conclusion, Bio-reduction catalyzed by medlar fruits provides an attractive approach to access chiral alcohols with excellent enantiomeric excess. These results show that *medlar* fruits have enzyme system with ability to enantioselective reduction of ketone. Indeed, fruits represent an alternative source of "new" enzymes for use as catalysts in organic synthesis.

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High-Pressure Reactors Platform: Catalytic Reactions

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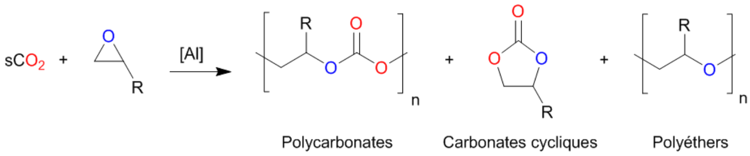
The team Catalysis and Fine Chemicals of the Laboratoire de Chimie de Coordination (LCC) is structured around the design and syntheses of homogeneous, single-site and heterogeneous catalysts. In order to run different catalytic tests, we are equipped with 12 reactors: 1 homogeneous pilot reactor, 2 heterogeneous reactors, 1 supercritical CO_2 reactor, and 8 homogeneous reactors. This poster will present our high-pressure reactors platform through examples illustrating the team's main scientific themes. First, we will discuss the carbonylation reaction of MeOH, with Rh catalysts, carried out in a continuous pilot reactor [1]. We will then introduce the hydroaminomethylation reaction in high-pressure reactors [2].Next, we will examine the operational conditions for the copolymerization of epoxides and supercritical CO_2 (sCO_2) catalyzed by single-site Al catalysts.



Lastly, we will broach the methanation reaction of CO_2 catalyzed by a heterogeneous nickel catalyst supported on a metal oxide. This reaction is carried out in a heterogeneous reactor with in-line sampling (GC-TCD).

$$4\,H_2 + CO_2 \longrightarrow CH_4 + 2\,H_2O$$

Key words: High-pressure reactors, catalysis.

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METALLOPORPHYRINS AS LIGANDS OF G-QUADRUPLEX NUCLEIC ACIDS: SYNTHESIS TOWARD ANTIVIRAL ACTIVITY

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G-quadruplexes are four-stranded nucleic acid structures that form in guanine-rich regions. Four guanines interact through Hoogsteen hydrogen bonds and form G-quartets that further undergo π-stacking interaction between each other creating the four-stranded nucleic acid. G-quadruplexes are involved in fundamental processes of life (transcription, translation, telomere maintenance …). These peculiar structures, as relevant pharmacological targets, can be targeted by synthetic molecules.

The presence of G-quadruplex structures in the genome of some viruses such as HIV-1, papillomavirus, Epstein-Barr virus, Ebola, Marburg, was recently evidenced (1,2). In the case of HIV-1 the G-quadruplex structures locate in crucial regions for the viral cycle (initiation of reverse transcription, promoter regulation) (3,4). We showed previously that G-quadruplex ligands based on metalloporphyrins inhibit HIV-1 infection *in vitro*. The compounds have IC_{50} values similar to that of AZT, the reference compound, and do not show any cytotoxicity toward the host cells (5).

We report the preparation of functionalized derivatives of the most active gold porphyrin (6) with a biotin moiety. The resulting hybrid molecule will allow the study of the mechanism of action of this G-quadruplex ligand inside HIV-1 infected cells.

Key words: metalloporphyrin, G-quadruplex, antiviral.

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CHEMICAL CHARACTERIZATION OF HEAVY ORGANIC MATERIAL ISSUED FROM DIFFERENT CRUDE OILS

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Wax deposition is one of the serious problems in oil industry. Indeed, paraffinic waxes present in petroleum crude can precipitate when temperature decreases during oil production, transport or storage.

These deposits are mainly composed by n-paraffins and branched paraffins. The precipitation of these paraffins is responsible for changes in the waxy crude oil properties, including gelation of oil and an increase in viscosity.

For this, the proper characterization of the composition of the waxes present in the oil is one of the major obstacles in dealing with this issue.

In this context we are interested in the characterization of paraffins, after isolation from different crude oils using precipitation method and purification by column chromatography.

Key words: crude oil, paraffins, precipitation, deposit.

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Synthesis and characterization of nano magnetic material based on (carbon nanotubes / γ-FeOOH): Application for the removal of congo red of dye from contaminated water

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Water pollution by dyes has been a worldwide problem. Colour is the first contaminant to be recognised in wastewater. Dyes are used in different industries such as paper, plastics, food cosmetics, leather, pharmaceutical dyes tuffs textiles etc. to colour the product. Various techniques have been developed for decontamination purposes. However, adsorption process seems to be among the most effective methods yielding therefore to remove dyes from aqueous environments [1], while several studies have already been done in this field using several materials as adsorbents. Indeed, the performance and the efficiency of this adsorption technique depend generally and preponderantly on the nature of the support used as adsorbent.

Synthetic γ-FeOOH is one of the most important phases of iron oxides because of its application as an adsorbent for various toxic cations and anions due to chemical reaction occurring at specific surface sites. In another side of view, double walled carbon nanotubes shows good mechanical, electrical properties and especially a large surface area [2]. Prior to this, carbon nanotubes are nanomaterials which have undergone considerable development in recent years due to their remarkable potential for nanoscale applications, with a fibrous form, large external surface accessible, and a well-developed mesopore As a starting point as an hypothesis, the combination of magnetic properties and adsorbent properties within the same material is an interesting challenge that could overcome the problems of recovery of adsorbents loaded with pollutants.

The synthesis of (DWNTCs / γ-FeOOH) by refluxing process. Herein, the synthesized adsorbent was characterized via Fourrier Transform Infrared Spectroscopy (FTIR), X-ray diffraction (DRX), BET, zeta potential and transmission electron microscopy (TEM), where the adsorption of congo red on (DWNTCs / γ-FeOOH) has been carried out by studying the adsorption kinetics, pH, mass and the initial concentration. The results indicated that the maximum adsorption rate is 16 $mg.g^{-1}$ at pH 7 with 100 mg of (DWNTCs / γ-FeOOH), and an initial orange methyl concentration of 10 $mg.l^{-1}$. In addition, the adsorption process describes a second-order kinetic model, where the modeling of adsorption isotherms showed that the Freundlich one seem to be the adequat model describing the adsorption process with $R^2 = 0.97$.

Keywords: Carbon nanotubes, α-FeOOH, methyl orange

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Silver–N Heterocyclic Carbene Complexes: Synthesis, Characterization, and Antimicrobial Properties

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Among the NHC-metal complexes, Ag–NHC complexes have been utilized for several purposes. These include carbine transfer reagents to prepare other NHC–metal complexes, catalysis and interesting biological activity [1]. NHC–silver complexes are easily prepared by a one-pot reaction of a benzimidazolium salt with silver compounds; silver oxide is the most commonly used. The reactions can be carried out at room temperature, solvent pretreatments and strong bases are not required, chirality can be retained [2]. In this contribution, we reported the synthesis, characterization of Ag(I) complexes of benzimidazolylidene ligands

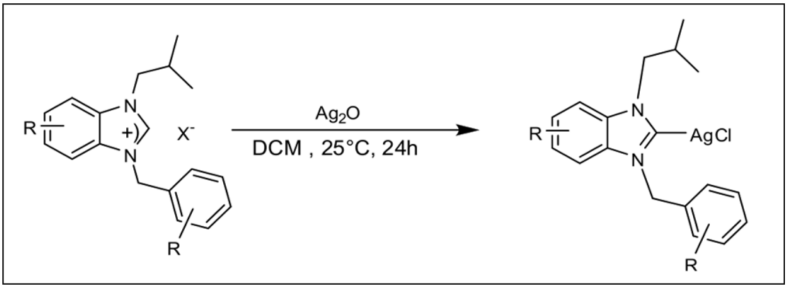

Fig.Synthesis of Ag-NHC complexes

Key words: Silver, N-heterocyclic carbenes, biological activity.

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Luminescence properties of Nd^{3+} doped $Ca_8NaBi(PO_4)_6F_2$ microrod powder for Near-infrared light emitting system

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The rapid advancement of bioimaging field demands the development of biocompatible bioprobes [1,2]. Compared with the conventional biological labels, such as organic dyes and quantum dots, rare earth doped inorganics powder possess several advantages like, lower toxicity, photo stability, high thermal and chemical stabilities, high luminescence quantum yield and sharp emission bands [3]. Therefore, inorganic compounds doped Nd^{3+} emitting in the wavelength range near 1 µm are currently of interest for their potential use in different field such as biological imaging, IR scintillator in the medical radiation monitoring and optical amplification[4.5]In this work, we report for the first time, Nd^{3+} doped Sodium Bismuth fluorapatite,$Ca_8NaBi(PO4)_6F_2$ ((NaBi)FAp) with strong NIR emission properties. The new phosphor Nd:(NaBi)FAp was prepared using the modified Pechini method, Well crystallized microparticles of size around 200 nm with rod morphologies. The Rietveld refinement with high-resolution indicate that this compound crystallizes in the hexagonal system with space group $P6_3/m$, Z = 1 and unit cell parameters a= 9.39806 Å, c= 6.90399 Å, V= *528.05* (7) Å^3, The 4f (C_3) sites are statistically occupied by Ca, Bi and Na, while 6h (C_s)sites are occupied by Ca and Bi . Under 808nm excitation the microparticles exhibit strong near infrared emission at 1,05 µm. 20% Nd^{3+} :(NaBi)FAp have the highest emission intensity among all samples. the shape of $^4F_{3/2}$ - $^4I_{11/2}$ transition prove that there is a redistribution of ions Nd^{3+} over the two sites (C_s and C_3) with increasing doping level. the relative intensity of luminescence decreases as the temperature elevates from 10k to 300k.These apatite phosphors are promising materials for near- infrared solid-state lighting applications.

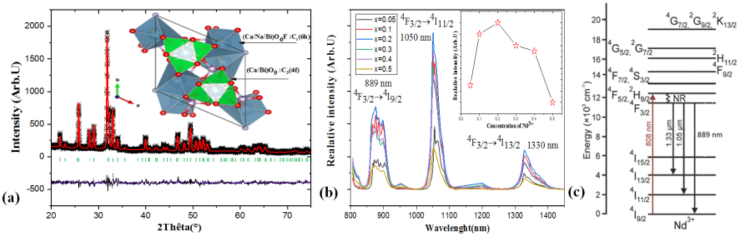

Fig.(a) Rietveld refined XRD pattern of the matrix $Ca_8NaBi(PO_4)_6F_2$, Inset: the unit cell structure of (NaBi)FAp indicating the positions of various metals coordination polyhedron in a unit cell. **(b)** RT luminescence spectra (λex = 808 nm) of xNd:(NaBi)FAp (x=0.05,x=0.5) in the range from 0.8 to 1.45 µm**,** Inset: the Relative luminescence intensity of the line at 1050 nm versus Nd^{3+} concentration in (NaBi)FAp **(c)** Simplified energy level diagram, excitation and infrared emission schemes for Nd^{3+} doped (NaBi)FAp.

Key words: Neodymium, Sodium Bismuth fluoroapatite, Pechini Process, Microrods particle, Luminescence, Near-infrared emission.

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Nucleophilic Aromatic substitution of a methoxy group by dimethylamine on the 2-methoxy-5-nitro and 3,5-dinitrothiophene: A DFT Study

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The S_NAr mechanism of the substitution reaction of the methoxy group by a secondary amine on the 2-methoxy-5-nitrothiophene molecule was investigated using theoretical DFT calculations. The hypothesis of a zwitterion formation during the kinetically determining step has been confirmed [1,2]. However, our calculations have shown that the structure of this reaction intermediate is much more diffuse than commonly accepted. Its geometry can be described as one situation in which the nitrogen of the nucleophilic entity is not totally bound to the carbon whereas the oxygen of the leaving group is about to separate from the substrate. The transition state corresponding to the formation of the zwitterion has a barrier of 17.78 kcal mol^{-1} in methanol. Three pathways have been studied to describe the second step leading to the formation of methanol or methoxyammonium. The most probable route uses, in a first sequence, a second amine molecule to convert the zwitterion, a dipolar compound, into a hydrogen bonding association of a carbanion located on the carbon C5 carrying the nitro group and an ammonium with a weak activation barrier of 2.25 kcal mol^{-1}. The electron density supplement provided by the nucleophile is stored at the oxygen atoms of the 5-nitro group in position α of the sulfur atom. The presence of a second nitro group in position β modifies the structure of this carbanion by locating the negative charge on the carbon C3 carrying the second nitro group. To visualize the reaction mechanism, we propose an innovative technique called Reactive Internal Reaction Coordinate (RIRC) that traces the reaction path in a 3D figure as a variation of the energy according to the most active internal coordinates in the transition state zone of influence.

Key words: Zwitterion, thiophene, carbanion, RIRC, IRC, Wiberg index

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CONTRIBUTION OF LEWIS ACID SITES (Si AND Al) OF TUNISIAN ACID ACTIVATED CLAY TO THE SYTNHESIS OF SAME -1,3-DIOXOLANE

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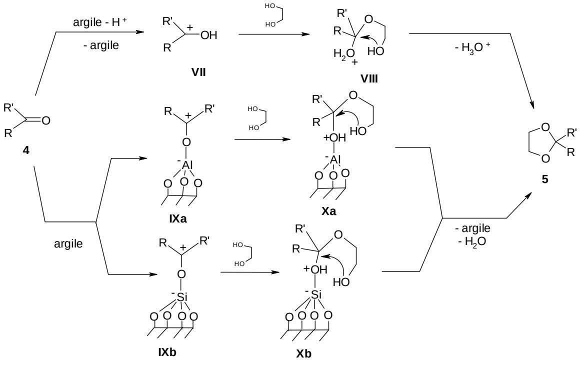
As part of the development of Tunisian natural resources, we used raw clay from the Gabes region of South East Tunisia [1]. Activation of the **H_B** purified clay with HCl (3N) while hot for 0.5 h strongly increases the adsorption, which promotes its catalytic role by decreasing its cation exchange capacity [2].
Dioxolanes were synthesized by the acetalization of various carbonyl compounds with ethylene glycol in the presence of green heterogeneous catalyst as acid activated clay **$H_{0.5}$** without solvent and under autogenous pressure.
The clay exhibits weak Lewis acid sites on its surface, due to the presence of electron-deficient orbitals of the silicon and aluminum atoms. Therefore, silicon and aluminum atoms could also enable the acetalization reaction. As an example, aluminate intermediates are the key intermediate for the reaction.



Key words: acetalyzation, acid activated clay, carbonyl compound, dioxolane, Lewis acid sites (Si and Al).

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Theoretical Study of Quinoline Derivatives Involved In Neurodegenerative Diseases.

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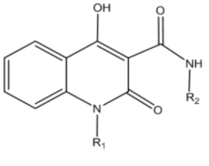
Neurodegenerative diseases include more than 600 affections that alter the structures of the brain, the best known being Alzheimer's disease and Parkinson's disease. Neurodegenerative diseases form a heterogeneous and complex group of evolving chronic diseases, characterized by a progressive dysfunction of the nervous system, caused by a deterioration in the functioning of nerve cells, especially neurons. A series quinoline derivative has been synthesized with a very high heterocyclic class in a wide range of biological activities. the derivatives have been shown to be selective inhibitors of acetylcholinesterase (AChE) with IC50 values [1].

This work is to study the inhibition of acetylcholinesterase (AChE) which is an enzyme involved in the Alzheimer's disease by methods of molecular modeling. These results will probably help in the development of an effective therapeutic tool in the fight against the development of Alzheimer's disease .Our goal of research is to study the inhibition of acetylcholinesterase (AChE) by molecular modeling methods.

key words: acetylcholinesterase (AChE), Alzheimer's disease, quinoline derivatives, Molegro.



Compounds	R_1	R_2	IC50 (μM)
Ligand -1	H	$-NH_2$	179
Ligand -2	CH_3	$-NH_2$	□ 400
Ligand -3	H	$-C_2H_4NHC_2H_4NH_2$	172
Ligand -4	CH_3	$-C_2H_4NHC_2H_4NH_2$	142
Ligand -5	H	$-C_2H_4NHC_2H_4NHC_2H_4NH_2$	77.2
Ligand -6	CH_3	$-C_2H_4NHC_2H_4NHC_2H_4NH_2$	102

THE DIFFERENT LIGANDS AND THEIR RESPECTIVE IC50 VALUES

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ASYMMETRIC HYDROGENATION OF KETONES WITH IRIDIUM COMPLEXES WITH CHIRAL PLANAR FERROCENYL PHOSPHINO-THIOETHER LIGANDS

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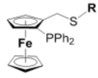
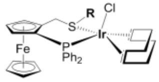
Various chiral ferrocenyl phosphine-thioethers ligands have been synthesized in both racemic and enantiomerically pure form [1]. Iridium complexes with these P,S ligands were tested in the hydrogenation of prochiral ketones.



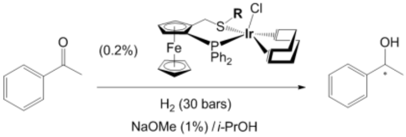
1^R



2^R

(R = Et, Ph, *t*Bu, Bz,)

Optimization of the conditions (additive, solvent, pressure) led to a highly active catalytic system with good levels of enantioselectivity depending on the R substituent on sulfur (77% for R=Bz at rt) [2].



Furthermore an experimental and computational study of the mechanism of this catalytic system has been carried out. We propose a mechanism via an anionic Iridium (III) tetrahydride establishing the important role of the strong base and of the counter cation in the ketone hydrogenation reaction [3].

Keywords: asymmetric hydrogenation, iridium, P,S ligands, strong base

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ELIMINATION OF HEAVY METAL FROM WASTEWATER BY COMPLEXATION WITH DAWSON-TYPE NANO-POLYOXOMETALATES

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Nowadays water pollution is one of the major concerns of our society, because of the continuous degradation of the quality of drinking water, surfaces and rejections.

Heavy metals such as Hg, Pb, Cd, Co, Fe, Cu…etc. are among the most common pollutants in areas with a strong urban and industrial agglomeration. In fact, industrial wastewater from the iron and steel complex collects these various pollutants in a significant quantity. These are a major problem for the environment and public health.

To contribute to the elimination of these heavy metals, we propose to complex the cadmium "Cd" in aqueous medium by two lacunar polyoxometalates Dawson type $(P_2W_{15}Mo_2)^{10-}$ and $(\alpha_2P_2W_{17})^{10-}$ used as ligands.

The parameters influencing the formation of complexes $(P_2W_{15}Mo_2Cd)^{8-}$ and $(\alpha_2P_2W_{17}CdO_{61})^{8-}$ such as pH of the reaction medium, time and temperature were studied.

The stoichiometry and stability constants of these formed complexes have also been studied. The results obtained showed that these complexes formed are very stable in an aqueous medium giving sufficiently high stability constants which are β_1= 1,074.10^4 for $(P_2W_{15}Mo_{21}Cd)^{8-}$ and β_2 = 5,74.10^5 for $(\alpha_2P_2W_{17}Cd)^{8-}$.

Key words: Water pollution, heavy metals, complexation, Cadmium, Polyoxometallates.

SYNTHESIS AND DEVELOPMENT OF A NOVEL IRON PHOSPHOTUNGSTIC CATALYST FOR THE REMOVAL OF AN ORGANIC POLLUTANT FROM WASTEWATER

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Wastewater discharged by the petrochemical, agro-food and textile industries causes a great deal of nuisance to the environment and public health. Certain pollutants present in these waste waters, especially dyes, are found in liquid discharges destined for groundwater, rivers and seas.

These waters must therefore be treated before their final discharge, for environmental and legal reasons. It therefore becomes necessary, to develop effective and specific processes for their elimination. Among these processes, advanced oxidation processes (AOPs) in homogeneous phase which can be a promising alternative. This study investigates the removal of a dangerous dye, Congo Red (R.C) in aqueous media by a modified advanced oxidation process using a Dawson-type synthesized phosphotungstic catalyst $(\alpha_2P_2W_{17}O_{61}Fe)^{7-}$, which has specific physicochemical properties as a catalyst in the presence of an oxidant hydrogen peroxide (H_2O_2), it is the modified system (H_2O_2 / $P_2W_{17}O_{61}Fe$). The advantage of this system is that reaction by-products are very low in toxicity.

The optimization of the operating conditions for the elimination of Congo red was carried out by varying the following parameters:

Initial pH of the solution to be treated, concentration of the oxidant (H_2O_2), mass of catalyst $(\alpha_2P_2W_{17}O_{61}Fe)^{7-}$, concentration of the dye (R.C), effect of temperature, effect of the nature of catalyst. Under optimal conditions the discoloration efficiency of Congo red is 95%.

Keywords: water pollution, homogenous catalysis, hosphotungstic material.

SYNTHESIS AND CHARACTERIZATION PHYSICO-CHEMICAL OF A NEW DECAVANADATE $[(C_6H_{12}N(OH)]_3[V_{10}O_{28}]\cdot 10H_2O$

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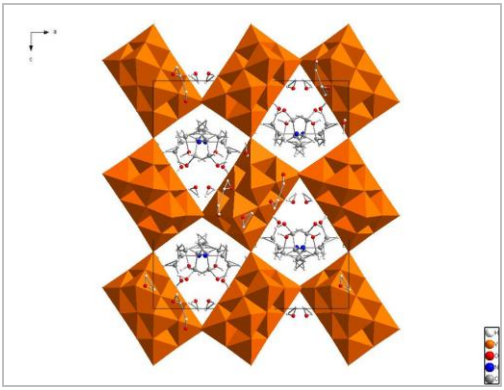
Polyoxometalates (POMs) as early-transition-metal oxide clusters have received much attention in various fields such as catalysis, ion exchange, electrochemistry, magnetism and medicine for their enormous variety of structures and unique properties **[1-3]**.

In order to obtain new materials with novel structures and interesting properties, we report in this work for the first time the synthesis, characterizations and crystal structure of the novel decavanadate $[(C_6H_{12}N(OH)]_3[V_{10}O_{28}]\cdot 10H_2O$, crystallized the orthorhombic system with the Pbca space group and cellular constants of a = 16.8955 (3) Å, b = 13.4818 (2) Å, c = 19.320 (4) Å and Z = 8

Key words: Synthesis, Characterization, X-ray diffraction



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On the relationship between corrosion inhibiting effect and molecular structure of Curcumin: DFT studies

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From the present study, it has been established that the mechanism of inhibition involves electron donation to the Fe surface by the electron. However, it has also been discovered that the inhibitor can not only give up electrons to the metal, but can also accept electrons from the isolated pair of Fe, leading to the formation of a feedback link [1]. The formation of a feedback bond can be analyzed by considering a quantitative relationship between E_{HOMO}, E_{LUMO} and the experimental inhibition efficiency. In order to gain more information about the mode and type of adsorption of curcumin on the iron surface, the clusters have played a strong role to explain this phenomenon [2].

Keywords: surface of iron, adsorption, DFT calculations, E_{HOMO}, E_{LUMO}, cluster

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Reactivity of β,β' dihydroxy sulfides towards tin tetrachloride and phosphoryl chloride

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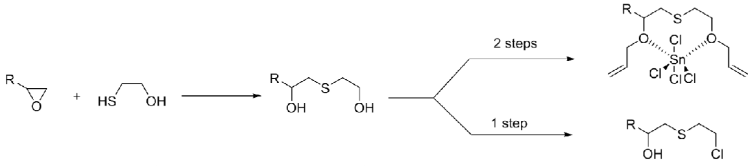
Epoxides are among the most versatile intermediates in organic synthesis. Their nucleophilic opening leads to a large number of 1,2-difunctionalized systems[1]. Ring opening of epoxides by thiols constitutes a convenient, practical and widely employed method for the synthesis of β-hydroxysulfide moieties, which are useful as intermediates in organic chemistry[2] especially in the preparation of important naturally occurring products and a variety of compounds with pharmacological and/or biological activities[3]

Herein, we report on the synthesis of novel substituted 1,5-bis(allyloxy) obtained from the products of opening of epoxides by mercaptoethanol[4]. The study of coordination chemistry of these 1,5-bis(allyloxy) sulfides as new ligands towards 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 reaction of these diols towards phosphoryl chloride did not take place and the chlorinated derivative was obtained.



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

Keywords: Epoxide, Thioethers diol, 1,5-bis(allyloxy) sulfides, tin complex, phosphoryl chloride

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Push-Pull Oligocarbazole Dyes-Sensitized Solar Cells : Determination of Active Electrons Intramolecular Path

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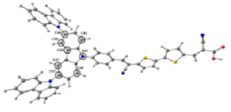
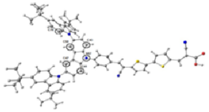
Dye sensitized solar cells (DSSC) as a new type of photovoltaic devices were given full attention since the first work of O′Regan and Gratzel in 1991. Their principle advantages are a good efficiency and a lower cost compared with conventional photovoltaic devices based on inorganic semiconductors and silicon. A push-pull configuration, based on a dipolar electron donor D, π-bridge spacer and electron acceptor A (D-π-A) system, the acceptor ligand being anchored to the semiconductor surface.

All molecular calculations were performed in the gas phase, in dichloromethane and in methanol solutions using the density functional theory (DFT and TD-DFT) method implanted in the Gaussian (09) program package with the hybrid B3LYP and CAM-B3LYP exchange correlation functionals using the 6-311G (d) basis set.

In this work [1], we presente a theoretical study of oligocarbazole based organic dyes for solar-cell devices. The good agreement between the experimental and TD-DFT calculated absorption spectra allowed us to provide a detailed assessment of the main spectral features of a series of dyes.


SD1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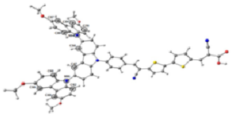
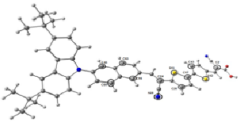
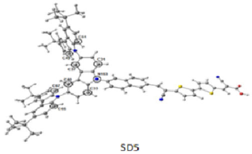

SD3


SD4


SD5

From the present study, we can note some general trends regarding the effect of the dependence of π-conjugation length and the influence of hydrogen substitution by electron donor groups such as (tBu and OCH_3). Increased conjugation length resulted in a more red-shifted spectral response in the case of SD4 and SD5.The dye with the methoxy group showed better absorbance efficiency than the dye with naphtyl unit and the two other dyes SD1-2, due to a larger dipole moment of the dye and the low gap energy. We have noticed that the SD3 dye has the good performance. In this case it will be a good candidate as dye sensitizer DSSC.

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Evaluation of pollutant loading and geochemical characterisation of petroleum exploitation solid wastes

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During the drilling phase in petroleum exploration, the cuttings of drilled rocks are transported from the well to the surface by a circulating fluid called mud. Once they have been brought to the surface, the cuttings are separated from the synthetic fluid and dried.

The management of those generated solid wastes is one of the emerging problems of oil and gas companies.

The purpose of the present study is to evaluate the pollutant loading of the cuttings generated from a drilled well in a southern Tunisian oilfield and to perform treatment tests using stabilization/solidification method.

The analysis of leachates by ICP-OES revealed relatively high heavy metals concentration values especially for Zn, Cu and Pb. The concentration of TPH determined by Rock-Eval pyrolysis exceeded the pollution indicative value. A geochemical study has been conducted to identify the source of hydrocarbon contamination using GC and GC-MS.

A series of treatment tests of the drill cutting has been performed using mixes containing different ratios of cement, lime and sodium silicate. Total petroleum hydrocarbons and heavy metals content of the obtained leachates have also been determined.

The drill waste disposal strategy to be adopted in the concerned oilfield is being derived in a large part from the results of the present study.

Key Words: Drill cuttings, ICP-OES, GC-MS, stabilization/solidification, leachates.

Synthesis and Characterisations of Photoreactive Ruthenium Nitrosyl Complexes

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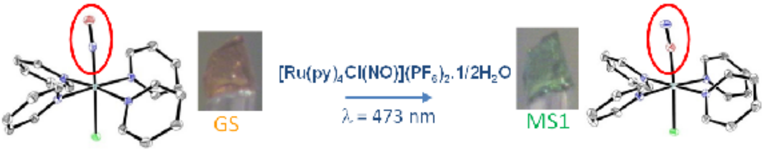
Photoactive ruthenium nitrosyl complexes deriving from $[Ru^{II}Cl(NO)(py)_4]^{2+}$ have recently witnessed an increasing interest in relation to their capability for providing solid state photo-switches with high yields or their ability to release the biologically active $NO^{\bullet}$ radical [1, 2].

Insight on our recent work in the two domains will be presented:

▶ Ru-NO / Ru-ON photoisomerisation

$$[Ru^{II} - NO] \xrightarrow{h\nu} [Ru^{II} - ON]$$

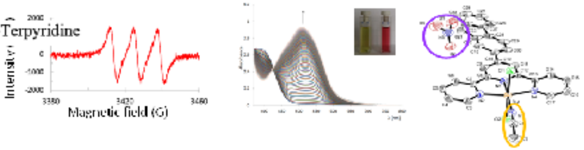


▶ NO photorelease

$$[Ru - NO] \xrightarrow{h\nu} [Ru - solvent] + \boldsymbol{NO^{\bullet}}$$

trans/*cis*-(Cl,Cl)- $\mathbf{[Ru^{II}(FT)Cl_2(NO)]^+}$ + CH_3CN → *trans*-(Cl,Cl)- $\mathbf{[Ru^{III}(FT)Cl_2(CH_3CN)]^+}$ + $NO^{\bullet}$

FT : Fluorene-Terpyridine



NO Signature by EPR at 810 nm Griess Test at 405 nm Photoproduct

Key words: Ruthenium Nitrosyl Complexes, .Photoisomerisation, NO-release

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A DFT RELATIVISTIC STUDY OF CYANIDE AND ISOCYANIDE CERIUM(III) AND URANIUM(III) COMPLEXES.

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The chemistry of cyanide complexes of the f-elements[1] witnessed significant recent advances, showing in particular the remarkable ability of the cyanide ligand to stabilize uranium compounds in their lowest and highest oxidation states and its capacity to adopt two distinct ligation modes, namely cyanide M−CN or isocyanide M−NC, towards trivalent f-ions.
We have investigated theoretically the tris(cyanide) complexes $[ML_2X_3]^{2-}$ (M = Ce^{3+}/U^{3+}; L = $C_5H_4Me/N(SiMe_3)_2$; X = CN/NC), using relativistic DFT[2] computations, focusing on cyanide (CN^-) and isocyanide (NC^-) coordination competition and differences between their electronic structures. X-ray crystal data reveal distinct coordination modes of the CN group towards uranium and cerium metal centers. Interestingly, in the case of the cerium complexes, and contrarily to the uranium ones, the coordination mode of the cyanide ligand depends on the co-ligand L attached to the metal. The observed coordination in these tris(cyanide) complexes is driven by the binding energies of the CN^-/NC^- groups to the metals. The solvent is shown to play a determining role for the chosen coordination. The developed methodology can help to confirm a cyanide or isocyanide coordination mode when X-ray crystal data are not conclusive or to predict the configuration of a complex to be synthesized.

Key words: Cyanide, f-complexes, Ln(III)/An(III) differentiation, CN-coordination isomerism, DFT calculations.

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Synthesis and biological evaluation of possible anti-cancer coumpounds: Zinc (II) Phthalocyanines

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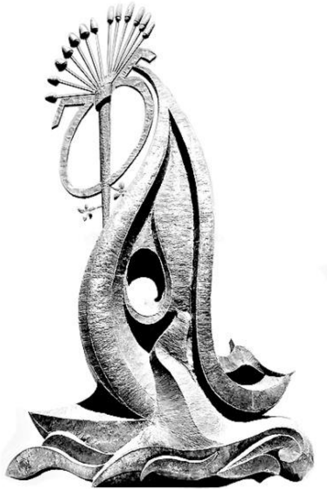
This work focuses on the synthesis and characterization of new tetrasubstituted zinc (II) phthalocyanine-based organic material, their electronic properties and the evaluation of their anticancer activities.

Methallophthalocyanines are a macrocyclic compounds. Their structure involves a metal atom inserted into a cavity surrounded by four isoindole units linked by aza nitrogen atoms. To achieve this objective, we have taken into account the choice of functional groups introduced on the peripheral part of the macrocycles since it affect specifically the physicochemical properties of the phthalocyanine molecules. The selected metal is the zinc, a diamagnetic metal, ionized and bonded to the rest of the molecule by two dative bonds and two coordination bonds.

The followed methodology to obtain the desired macrocycles begins with a base catalyzed nucleophilic aromatic nitro displacement of 4-nitrophthalonitrile (starting material prepared according to the protocols described in the literature) with three alcohols. The obtained compounds are three phthalonitriles substituted in the position 4 serving as precursors for the cyclotetramerization reaction leading to three news zinc phthalocyanines. One of them contains four carboxylic acid groups while the two others contain vinyl derivatives.

The novel molecules have shown the importance of the substitution effect and the significance effect of the nature of the inserted central metal. Indeed, they have a high solubility in the majority of organic solvents and exhibit very significant inhibition effects against human cancer cells: MDA-MB-231 breast cancer and U266 multiple myeloma.



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