4th Tunisian Chemical Society Conference on Coordination Chemistry

JCC 2022

Organized by

Tunisian Chemical Society

RSC LOCAL SECTION TUNISIA

ROYAL SOCIETY OF **CHEMISTRY**
TUNISIA LOCAL SECTION

29 Sep - 02 Oct 2022

Blue Marine Hotel, Yasmine Hammamet, Tunisia

Abstracts of Lectures and Communications
List of Participants

Tunisian Chemical Society - Short Program of JCC 2022

Thursday 29 September 2022	
14.30	**Welcoming participants, distribution of documents and check in**
17.00	**Opening Ceremony**
17.20 – 18.00	**Plenary Lecture 1** (online) **Jochen AUTSCHBACH** *University at Buffalo, State University of New York, USA*
18.00 – 19.00	**Welcome reception**
19.30	***Dinner***
Friday 30 September 2022	
09.00 – 09.35	**Plenary Lecture 2 Anne-Marie CAMINADE** *CNRS, Toulouse, France*
09.35 – 10.10	**Plenary Lecture 3 Eric MANOURY** *CNRS, Toulouse, France*
10.15 – 10.55	**Poster Session 1 (P 1 - P 15) Alphabetical Order**
11.00 – 11.35	**Plenary Lecture 4** (online) **Gillian REID -** *President of the Royal Society of Chemistry* *School of Chemistry, University of Southampton, UK*
11.45 – 12.45	**Oral Communications - Session 1 : OC 02 - OC 05**
13.00	***Lunch***
14.45 – 15.20	**Plenary Lecture 5 Mourad AMARA** *USTHB - Algiers, Algeria*
15.20 – 15.55	**Plenary Lecture 6 Valérie MARAVAL** *CNRS, Toulouse, France*
16.00 – 16.15	**Gathering for the group photo**
16.15 – 17.15	**Oral Communications - Session 2 : OC 07 - OC 10**
17.15 – 17.55	**Coffee break + Poster Session 2 (P 16 - P 30) Alphabetical Order**
18.00 – 18.45	**Oral Communications - Session 3 : OC 11 - OC 13**
19.30	***Dinner***
Saturday 01 October 2022	
09.00 – 09.35	**Plenary Lecture 7 Jason B. LOVE** *University of Edinburgh, UK*
09.35 – 10.10	**Plenary Lecture 8 Isabelle MALFANT** *CNRS, Toulouse, France*
10.15 – 10.55	**Poster Session 3 (P 30 - P 45) Alphabetical Order**
11.00 – 12.45	**Oral Communications - Session 4 : OC 01 + OC 06 + OC 14 - OC 18**
13.00	***Lunch***
FREE AFTERNOON	
Sunday 02 October 2022 (morning)	
09.00 – 09.35	**Plenary Lecture 9 Jean-François NIERENGARTEN** *Université de Strasbourg, France*
09.45 – 11.15	**Oral Communications - Session 5 : OC 20 - OC 24**
11.15	**Closing Remarks, Poster Awards and JCC 2024 Announcements**
12.00	***Lunch, Check Out and Departure***

FOREWORD

On behalf of the JCC 2022 organizing committee, we are very delighted to welcome you in Hammamet for this fourth Tunisian Chemical Society Conference on Coordiniation Chemistry (JCC 2022) 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 fourth JCC 2022 edition, which substitutes the 2021 edition (JCC 2021) upon a disruption due the Covid-19 pandemic, will see the participation of more than 6 African and European countries in addition to the Tunisian universities with more than 100 participants. They will discuss themes involving the science of coordination chemistry carefully distributed over 9 plenary lectures including that of the Royal Society of Chemistry President Prof Gillian Reid, 23 oral communications and about 45 poster presentations.

If you have any feedback about the meeting and its organisation, please send it to us. We will pass anything relevant on to the organising committee of the next JCC meeting.

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

Prof Med Taieb Ben Dhia
JCC 2022 Chair

Dr M.A.K. Sanhoury
JCC 2022 Co-Chair

Prof Hatem Ben Romdhane
President of the
Tunisian Chemical Society

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Thursday 29 September 2022		
14.30	**Welcoming participants, distribution of documents and check in**	
17.00	**Opening Ceremony**	
17.20 – 18.00	**Plenary Lecture 1** (online) **Jochen AUTSCHBACH** *University at Buffalo, State University of New York, USA* Computational studies of spectroscopic and magnetic properties of metal complexes	*Chair:* Med Taieb Ben Dhia
18.00 – 19.00	**Welcome reception**	
19.30	***Dinner***	

Friday 30 September 2022 (morning)		
09.00 – 09.35	**Plenary Lecture 2** **Anne-Marie CAMINADE** *CNRS, Toulouse, France* Phosphorus dendrimers functionalized with nitrogen ligands, and their use in catalysis and oncology	*Chair:* Med Abderrahmane Sanhoury
09.35 – 10.10	**Plenary Lecture 3** **Eric MANOURY** *CNRS, Toulouse, France* Planar Chiral Ferrocenyl P,S Ligands for Asymmetric Catalysis	*Chair:* Ikram Chehidi
10.15 – 10.55	**Poster Session 1 (P 1 - P 15) Alphabetical Order**	
11.00 – 11.35	**Plenary Lecture 4** (online) **Gillian REID** *President of the Royal Society of Chemistry* *School of Chemistry, University of Southampton, UK* Exploring inorganic fluoride complexes towards PET imaging applications	*Chair:* Anne-marie Caminade

Oral Communications - Session 1- chair: *Farhat Rezgui*

	Com.	*Communicating*
11.45 – 12.00	**OC-02**	JOMAA Ikram
12.00 – 12.15	**OC-03**	LABASSI Chiraz
12.15 – 12.30	**OC-04**	GANNOUNI Afef
12.30 – 12.45	**OC-05**	ARGOUBI Samar
13.00		***Lunch***

Friday 30 September 2022 (afternoon)

14.45 – 15.20	**Plenary Lecture 5** **Mourad AMARA** *USTHB - Algiers, Algeria* Complexation phenomena in membrane separations process	*Chair:* Khaled Essalah
15.20 – 15.55	**Plenary Lecture 6** **Valérie MARAVAL** *CNRS, Toulouse, France* Ring *carbo*mers of benzene: synthesis and prospects of applications	*Chair:* Béchir Chaouachi
16.00 – 16.15	**Gathering for the group photo**	
Oral Communications - Session 2 - Chair: *Moufida Romdhani*		
	Com.	*Communicating*
16.15 – 16.30	**OC-07**	HAJJI Ibtissem
16.30 – 16.45	**OC-08**	KECHICHE Azhar
16.45 – 17.00	**OC-10**	MAKHLOUF Jawher
17.00 – 17.40	**Coffee break + Poster Session 2 (P 16 - P 30) Alphabetical Order**	
Oral Communications - Session 3 - Chair: *Latifa Latrous*		
	Com.	*Communicating*
17.45 –18.00	**OC-11**	BEN HAJ FRAJSarah
18.00 –18.15	**OC-12**	JEMAA Imène
18.15 –18.30	**OC-13**	HERMI Sabrine
19.30	***Dinner***	

Saturday 01 October 2022 (morning)		
09.00 – 09.35	**Plenary Lecture 7 Jason LOVE** *University of Edinburgh, UK* Coordination and Supramolecular Chemistry for Electronic Waste Recycling and Rare-Earth Metal Separations	*Chair:* Thouraya Barhoumi
09.35 – 10.10	**Plenary Lecture 8 Isabelle MALFANT** *CNRS, Toulouse, France* Ruthenium Nitrosyl Complexes: Photoisomerisation or Nitric Oxide Photodelivery	*Chair:* Ridha Ben Salem
10.15 – 10.55	**Poster Session 3 (P 30 - P 45) Alphabetical Order**	

Oral Communications - Session 4 - Chair: *Mehrez Romdhane*		
	Com.	*Communicating*
11.00 – 11.15	**OC-01**	ZEROUGH Izid Bih
11.15 – 11.30	**OC-06**	KHALFALLAH Ali
11.30 – 11.45	**OC-14**	AYARI Chaima
11.45 – 12.00	**OC-16**	FRADI Taissir
12.00 – 12.15	**OC-17**	BOUBAKRI Rim
12.15 – 12.30	**OC-18**	NAOUS Mohamed
13.00	***Lunch***	
FREE AFTERNOON		

Sunday 02 October 2022 (morning)		
09.00 - 09.35	**Plenary Lecture 9 Jean-François NIERENGARTEN** *Université de Strasbourg, France* Pillar[5]arene scaffolds for the preparation of advanced materials and bioactive compounds	*Chair:* Rym Abidi

Oral Communications - Session 5 - Chair: *Hichem Ben Jannet*		
	Com.	*Communicating*
09.45 –10.00	**OC-20**	JABLI Souhir
10.00 – 10.15	**OC-21**	KAROUI Brahim
10.15 – 10.30	**OC-22**	ZARROUG Rim
10.30 – 10.45	**OC-23**	MKACHER Hayfa
10.45 – 11.00	**OC-24**	OUNALLI Chayma
11.15	**Closing Remarks, Poster Awards and JCC 2024 Announcements**	
12.00	***Lunch, Check Out and Departure***	

Speakers’ Abstracts

Computational studies of spectroscopic and magnetic properties of metal complexes

Jochen Autschbach

University at Buffalo, State University of New York, USA

Metal complexes exhibit fascinating magnetic and spectroscopic properties, which are strongly influenced by ionic and covalent interactions between the metal and ligands. On-going research projects in our group are devoted to first principles calculations of magnetic resonance parameters (NMR, EPR), magnetic susceptibilities, electronic spectra and optical activity, magnetic circular dichroism, magneto-chiral dichroism, core excitation spectra (XANES), and other types of properties of metal complexes, and how exactly the observed properties relate to the chemical bonding involving the metal. One particular interest is the involvement of the 4f and 5f shells in metal-ligand bonding in lanthanide and actinide complexes, respectively. I will present results from recent computational studies of some of the aforementioned magnetic and spectroscopic properties of metal complexes utilizing quantum chemical methods.

Phosphorus dendrimers functionalized with nitrogen ligands, and their use in catalysis and oncology

Anne-Marie Caminade

Laboratoire de Chimie de Coordination, UPR 8241 CNRS, 205 Route de Narbonne,
BP 44099, 31077 Toulouse Cedex 4, France

Dendrimers are hyper-branched macromolecules, synthesized step-by-step around a central core, constituted by the association of repetitive branched monomers, which structure is reminiscent to that of trees. Most of their properties are related to the type of their terminal functions [1]. Phosphorus dendrimers are based on a phosphorus atom at each branching point [2]. Such dendrimers are particularly useful as supports of coordination complexes [3]. Different types of ligands have been used, mainly based on phosphines, but nitrogen ligands, especially pyridine-imine ligands, can be also suitable for the complexation of metals. The dendritic copper complexes of such ligands have been shown to be efficient catalysts in O- and N- arylation and vinylation reactions [4], but also in oncology (copper and gold complexes), against various types of cancers [5, 6].

Key words: Dendrimers, Phosphorus chemistry, Nitrogen ligands, Catalysis, Oncology

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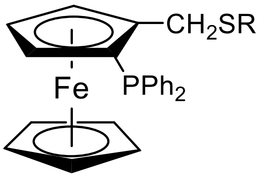
Planar Chiral Ferrocenyl P,S Ligands for Asymmetric Catalysis

Eric Manoury

LCC-CNRS, Université de Toulouse, CNRS, UPS, Toulouse, France

Enantiomerically pure planar chiral ferrocenyl phosphane-thioether ligands [1] have been developed in our team and applied to various asymmetric catalytic reactions : asymmetric allylic substitution (ee up to 93%) [1,2], palladium-catalyzed asymmetric methoxy-carbonylation of styrene derivatives (chemioselectivities up to 100%, regioselectivities up to 98% for the branched isomer, ee up to 17%), [3] and to iridium and rhodium-catalyzed asymmetric hydrogenation of unfunctionalized ketones (global TOF up to $250 \cdot h^{-1}$, TON up to 1500; ee up to >99% at 10°C) [4] and of minimally functionalized olefins ketones (ee up to >98% at RT).[5] A detailed experimental and computational mechanistic study of the iridium-catalyzed asymmetric hydrogenation of ketones will be presented.[6]



Key words: planar chiral ligands, asymmetric catalysis, mechanistic investigations, DFT

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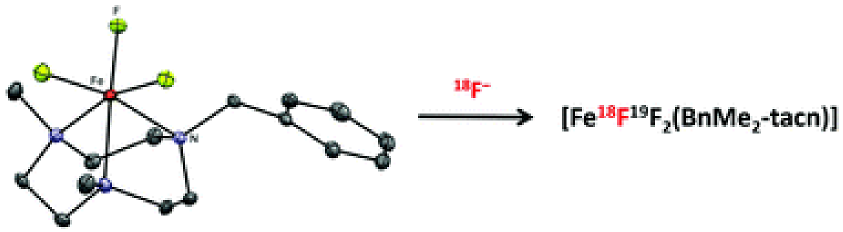
Exploring inorganic fluoride complexes towards PET imaging applications

Professor Gill Reid

School of Chemistry, University of Southampton, UK
& RSC President
Email: g.reid@soton.ac.uk

Coordination complexes bearing fluoride co-ligands often exhibit markedly different properties to those of the heavier halides and the last 15 or so years has seen a surge of new research associated with the chemistry of medium and high oxidation state d- and p-block fluoride complexes.[1] The unexpected stability of the $[MF_3(Me_3\text{-tacn})]^+$ cations (M = Si, Ge) in water[2] prompted the prospect of utilising the inherent strength of certain M-F bonds to create well-defined complexes capable of binding the positron-emitting F-18 isotope, $[^{18}F]F^-$ ($t_{½}$ = 110 mins.).[3,4,5] This presentation will discuss our work on the development of well-defined Ga(III), Al(III) and Fe(III) complexes with a range of neutral and anionic macrocyclic co-ligands, as precursors to F-18 radiolabelled compounds.

Here, the formation of a strong M−F bond using an inherently labile trivalent Group 13 metal ion (M = Al, Ga, In) can allow reactions to proceed fast under relatively mild conditions and are of interest for development of next generation positron emission tomography (PET) imaging agents. The presence of a stable and kinetically robust metal-macrocyclic fragment in these systems plays a key role in facilitating the radiofluorination, achieving high radiochemical yields and good stabilities for the final M-^{18}F species under physiological conditions.[5]



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Complexation phenomena in membrane separations process

Mourad AMARA

Hydrometallurgy and inorganic molecular chemistry lab, Faculty of chemistry, USTHB, Bab Ezzouar, Algiers, ALGERIA, Email :mamara@usthb.dz, moumouradamara@gmail.com, Tél : +213-557-126-222

Membrane separation of chemical species as a clean process becomes extensively employed, its action mechanism is mainly based on fundamentals principles of structural chemistry. Membrane is not only used as a porous material but its surface charge, hydrophilic/ hydrophobic balance, texture and many others physical and chemical properties depending on the medium matrix play a real role as material directly implicated in the transport and separation phenomena of species. The emergence of membranes having specific selectivity imply adoption of a new concept of separation based on the formation of complexes within the membrane material during the process of transport by chelation, conferring on the membrane a highly selective character regarding particular species existing in a very heterogeneous environment. Polymer inclusion membranes (PIM) allow using this phenomenon of chelation and transport by complexation-decomplexation between feed-and-receive interfaces in the direction of transference flow. Polyethyleneneimine (PEI) has been used in this type of membranes for its chelating properties in aqueous media. This polymer behaves as a polyelectrolyte in aqueous solution, its viscosity, protonation rate and conformation depend on pH and ionic strength of water. Maintaining the pH value around pKa = 8.8 leads to a structure containing both amine groups and ammonium groups which thus leading to polarization of the membrane surface. Similarly, more basic pH allows the predominance of amine groups and non-binding doublets of nitrogen and the prevalence of complexation mechanism instead of ion exchange one. At more acidic pH, negatively charged metal-ligand complexes are transported by ion pair mechanism into the membrane bulk.Our work, for more than two decades, has focused on the study of various aspects of acid-base and complexing behavior of PEI in aqueous solutions and inside membranes or ion exchange resins as a surface modifier and as facilitator of ion transport by complexation. Other molecules have also been used to provide synergy with PEI or as alternatives such as polyvinylpyrrolidone (PVP) for Co, thiourea for the separation of Cu and Ag, D2EHPA for the transport of Cr, or the extraction of REE as well as other agents.

Key words: Polyethyleneimine, complexation, membrane separation, ion exchange

Ring *carbo*-mers of benzene: Synthesis and prospects of applications

Valérie Maraval

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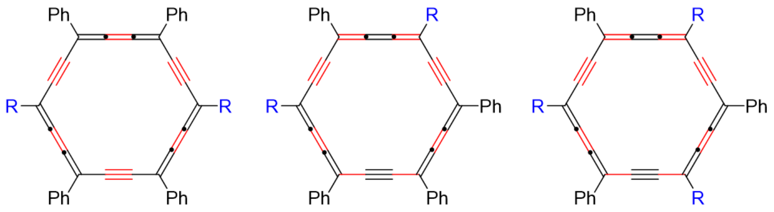
The chemistry of *carbo*-benzenes and related derivatives have progressed in the last 20 years through the synthesis of more than 50 representatives of this unique family of compounds.[1] *Carbo*-mers, which are formally obtained by systematic insertion of dicarbon units into each covalent bond of a parent Lewis structure,[2] exhibit unique features making them attractive for various applications. Depending on the nature and number of the substituents R, and their position on the hexagonal C_{18} *carbo*-benzene ring, charge transport,[3] two-photon absorption,[4] photosensitization,[5] or mesogenic properties have been evidenced.[6]



The multi-step synthesis strategies giving access to these different series of *carbo*-benzenes will be described, and illustrated by the presentation of selected examples of applications.

Key words: Acetylenic chemistry, *carbo*-mers, charge transport, chromophore.

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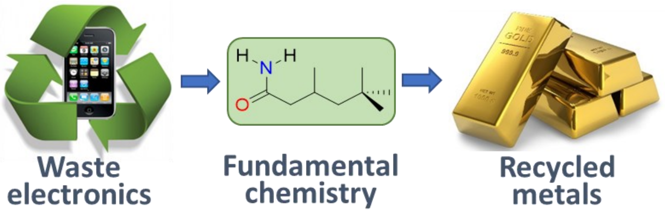
Coordination and Supramolecular Chemistry for Electronic Waste Recycling and Rare-Earth Metal Separations

Jason B. Love

EaStCHEM School of Chemistry, University of Edinburgh, Edinburgh EH9 3FJ, UK.

Metals are ubiquitous in modern technology and their recycling from sources such as electronic waste, magnets, and high-performance materials is crucial to achieve circular economy visions and to ensure that wastes are both minimised and environmentally benign.[1]In this presentation, the application and significance of coordination and supramolecular chemistry in metal recycling processes will be highlighted.[2] New solvent extraction and precipitation routes to the selective separation of gold and other metals from electronic waste will be described,[3] along with the selective precipitation of light rare-earth elements using a unique supramolecular encapsulation strategy.[4] These case studies rationalise the need to understand the mode of actionin separations processes at a fundamental chemical level and the ability to exploit ligand design to achieve new and useful separations technologies.



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Ruthenium Nitrosyl Complexes: Photoisomerisation or Nitric Oxide Photodelivery

Isabelle Malfant and Pascal G. Lacroix

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Photoactive nitrosyl ruthenium complexes have 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.

- **Ru-NO / Ru-ON photoisomerisation**

Few years ago, we have observed a *quasi*-complete photoswitching process with the population of the metastable state MS1 after irradiation of a crystal of $[Ru^{II}Cl(NO)(py)_4](PF_6)_2.0.5H_2O$ at λ = 473 nm [1, 2]. We have targeted the role devoted both to the intramolecular electronic properties and the solid state environment.

$$[\mathrm{Ru\text{-}(\mathbf{NO})}] \leftrightarrow [\mathrm{Ru\text{-}(\mathbf{ON})}]$$

- **NO photorelease**

The challenge is to design ruthenium-nitrosyl complexes delivering NO in the therapeutical window (Near Infrared Region) having large two photon absorption cross-section and efficient NO quantum yield. We are currently developing new systems based on $[Ru^{II}(Cl_2/bpy)(NO)(R\text{-}tpy)](PF_6)_n$ delivering NO in the NIR region [3, 4] with significant bactericidal effect. [5]

$$[\mathrm{Ru\text{-}(\mathbf{NO})}] \rightarrow [\mathrm{Ru\text{-}(\mathbf{solvent})}] + \mathrm{NO}^{\bullet}$$

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Pillar[5]arene scaffolds for the preparation of advanced materials and bioactive compounds

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One important aspect of modern chemistry is directed towards the synthesis of complex nanomolecules that exhibit specific properties for applications in materials science and biology. However, the preparation of complex nanostructures combining the required functional groups remains often difficult and requires a large number of synthetic steps thus limiting both their accessibility and applicability. Our research group has shown that the preparation of easily accessible nanoscaffolds allowing for the grafting of one or more molecular entities is an appealing strategy to generate sophisticated nanomolecules. Overall, one of our main concerns is to increase the complexity of the molecular structures without increasing the synthetic difficulties. This is an important challenge for synthetic organic chemistry in general. As part of this research, we became interested in pillar[5]arene[1] as compact scaffolds for the construction of nanomaterials. Our latest advances in this particular field will be presented.

Keywords: supramolecular chemistry, macrocyclic compounds, rotaxanes,

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Oral Communications' List

(alphabetically authors' name)

Nr	Communicatings’s Names	Ref
1	**S. Argoubi**, M.A. Sanhoury, E. Manoury, I. Chehidi *FST - Tunis* Tin(IV) chloride complexes with fluorinated phosphoramidates: Synthesis and multinuclear (^{1}H, ^{19}F, ^{31}P and ^{119}Sn) NMR characterization	**CO-05**
2	**C. Ayari**, A.A. Alotaibi, M.A Baashen, K.M. Alotaibi, K.H. Alharbi, A. Othmani, W. Fugita, C. Ben Nasr, M.H. Mrad *FSB - Bizerte* Synthesis of new homopiperazine-1.4-diium tetrachloridromercurate(II) monohydrate $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$, crystal structure, Hirshfeld surface, spectroscopy, thermal Analysis, antioxidant activity, electric and dielectric behavior	**CO-14**
3	**S. Ben Haj Fraj**, J. El Haskouri, M.H.V Baouab *FSM - Monastir* Rapid capture and visual detection of fluorescent Schiff base modified dialdehyde nanocellulose-based sensors for metal ions detection	**CO-11**
4	**R. Boubakri**, K. Kaabi *FSB - Bizerte* Synthesis, single crystal structural investigation, Hirshfeld surface analysis, thermoanalysis and spectroscopic study of a new Cu(II) transition-metal complex	**CO-17**
5	**T. Fradi**, O. Noureddine, F. Ben Taheur, T. Roisnel, N. Issoui, H. Nasri *FSM - Monastir* Magnesium(II) (DMAP) complex with the meso-tetra(para-chlorophenyl)porphyrin: X-ray crystallography, spectroscopic, electrochemical properties, DFT, DOS and MEP calculations and biologic activities	**CO-16**
6	**A. Gannouni**, R. Kefi *FSB - Bizerte* X-ray crystallography, spectral analysis, DFT studies, and molecular docking of $(C_9H_{15}N_3)[CdCl_4]$ hybrid material against methicillin-resistant staphylococcus aureus (MRSA)	**CO-04**
7	**I. Hajji**, F. Aloui *FSM - Monastir* Synthesis, characterization and photophysical properties of π-conjugated architectures	**CO-07**
8	**S. Hermi**, C. Ben Nasr, M.H. Mrad *FSB - Bizerte* The coordination behavior of two new complexes, $[(C_7H_{10}NO_2)CdCl_3]n$ (I) and $[(C_7H_9NO_2)CuCl_2]$(II), based on 2,6-dimethanolpyridine; Elaboration of the structure and Hirshfeld surface, optical, spectroscopic and thermal analysis	**CO-13**

Nr	Communicatings's Names	Ref
9	**S. Jabli**, M. Chaabene, T. Roisnel, F. Molton, F. Loiseau, P. Jehan, R. Ben Chaabane, H. Nasri *FSM - Monastir* Synthesis, molecular structure, spectroscopic characterization, of a new magnesium(II) porphyrin complex with DMAP axial ligand antifungal activity	**CO-20**
10	**I. Jemaa**, I. Opalinski, S. Papot *LNCM - Monastir* Synthesis of mechanically interlocked component:[1] rotaxane	**CO-12**
11	**I. Jomaa**, N. Issaoui, H. Marouani *FSB - Bizerte* Experimental, computational, and in silico analysis of $(C_8H_{14}N_2)2[CdCl_6]$ compound	**CO-02**
12	**B. Karoui**, M. Rzaigui, S. Akriche *FSB - Bizerte* Synthesis and characterization of a new hexaborate stabilized by organic cations	**CO-21**
13	**A. Kechiche**, M. Guergueb, O. Noureddine, F. Loiseau, N. Issaoui, H. Nasri *FSM - Monastir* Synthesis, spectroscopic characterization, molecular structure and catalytic studies of a chromium(III) porphyrin complex with axial cyanate ligands	**CO-08**
14	**A. Khafallah**, S. Mazzouzi *FSG - Gabès* Critical micelle concentration of alkylbetainthioates surfactants	**CO-06**
15	**C. Labassi**, N. Fournier, M.L. Efrit, J.L. Fillaut, R. Gatri *FST - Tunis* Synthesis of photoactivatable diaryltetrazoles for bioorthogonal 1,3-dipolar cycloaddition reactions	**CO-03**
16	**J. Makhlouf**, W. Smirani Sta, A. Valkonen *FSB - Bizerte* Growth, single crystal investigations, DFT studies, molecular dynamics simulations and molecular docking, of novel thiocyanic complex with zinc transition metal precursor	**CO-10**
17	**H. Mkacher**, F. Ben Taheur, N. Amiri, F. Loiseau, F. Molton, T. Roisne, I. Turowska-Tyrk, H. Nasri *FSM - Monastir* Reaction of DMAP and HMTA with the (Triflato) *meso-tetra*(*para*-methoxyphenyl)porphyrinto manganese(III) complex. Spectroscopic, and structural characterizations - Antibacterial, antifungal and antioxidant activities	**CO-23**

Nr	Communicatings's Names	Ref
18	**M. Naous**, H. Zoubir, B. Bounaceur, A. Halfadji *University of Oran, Algeria* Elimination of chromium VI from wast water by recyclable nanoparticles Fe_3O_4 @CnTAB	**CO-18**
19	**C. Ounalli**, M. Essid, S. Abid, Z. Aloui *FSB - Bizerte* Synthesis, crystal structure, vibrational and optical properties of new Bi(III) halide complex (tris(2-Amino-5-(methylthio)-1,3,4-thiadiazol-3-ium) hexachlorobismuthate(III)): $(C_3H_6N_3S_2)_3$ $BiCl_6$	**CO-24**
20	**R. Zarroug**, B. Ayed *FSG - Gabès* Crystal structure, stability and binding interactions with bio-macromolecules of new phosphotetradecavanadate with 4-methylimidazolium	**CO-22**
21	**I. Zerough**, M. M'Haiham, K. Ebeid, M.T. Ben Dhia, M.A.K. Sanhoury *FST, University Al Aasriya, Nouakchott, Mauritania* Synthesis and characterisation of zinc(II) complexes with phosphoramidates bearing a long alkyl chain of the types $(RO)_2P(O)NR'_2$	**CO-01**

Oral Communications' Abstracts

Program of

Friday

30 September 2022

Experimental, computational, and in silico analysis of $(C_8H_{14}N_2)_2[CdCl_6]$ compound

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[b)] University of Monastir, Laboratory of Quantum and Statistical Physics LR18ES18, Faculty of Sciences, Monastir, 5079, Tunisia

The crystal structure of a novel compound $(C_8H_{14}N_2)_2[CdCl_6]$ is discussed based on single crystal X-ray diffraction. This compound crystallizes in the triclinic system, with the space group P1 and the lattice parameters obtained are a = 7.5482(8)Å, b = 8.495(1)Å, c= 10.4656(12) Å, α = 101.649(3), β = 100.006(3), γ = 112.971(3), V = 580.92(11) Å^3 and Z = 1. The compound is built up from inorganic layers formed by $CdCl_6^{4-}$ anions and ammonium groups. The organic entities are located between these layers and are linked to the anions through N-H…Cl and C-H…Cl hydrogen bonds generating a three-dimensional network, which stabilizes the crystal packing. The surface mapped over the d_{norm} support the X-ray structural analysis and highlights the hydrogen bonds as the main intermolecular contacts. An infrared spectrum was registered to reveal the vibrational modes of the various characteristic groups of the title compound. The non-covalent interactions were studied through AIM and RDG analysis. Subsequently, DFT and TD-DFT calculations were carried out to study the molecular structure, vibrational and electronic properties of the investigated molecule. In silico investigation was performed via molecular docking analysis to explore the anticipated antibacterial activity possessed in the title compound.

Keywords: Bis(m-xylylenediaminium), hexachlorocadmate(II), DFT calculations, Molecular docking.

Synthesis of Photoactivatable Diaryltetrazoles for Bioorthogonal 1,3-Dipolar Cycloaddition Reactions

Chiraz Labassi[a,b], Nicolas Fournier[b], Mohamed Lotfi Efrit[a], Jean-Luc Fillaut[b], Rafik Gatri[a]

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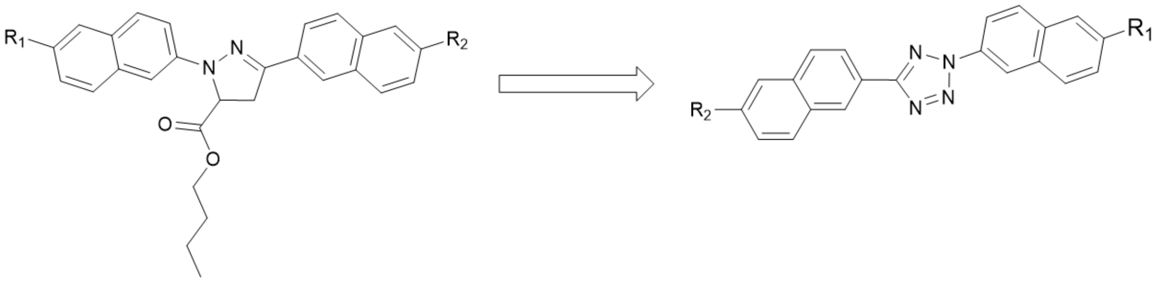
The concept of “photoclick chemistry”already inspired numerous researchers, who exploited for the synthesis of adducts or the functionalization of biocompatible materials. Our interest is to study the reactivity of diaryltetrazoles with butylacrylate. In fact a series of substituted diaryltetrazoles was synthesized inorder to generate pyrazolines derivative via the NITEC[1] (nitrile imine-mediated tetrazole-ene cycloaddition) reaction. The formed pyrazolines will be used as ligands for heavy metal complexation reactions.



NITEC Reaction

Key words: NITEC, Cycloaddition, Pyrazoline, diaryltetrazoles.

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X-ray crystallography, spectral analysis, DFT studies, and molecular docking of ($C_9H_{15}N_3$)[$CdCl_4$] hybrid material against methicillin-resistant staphylococcus aureus (MRSA)

Afef Gannouni, Riadh Kefi

Laboratoire de Chimie des Matériaux, Faculté des Sciences de Bizerte, 7021 Zarzouna, Tunisie

The ($C_9H_{15}N_3$)[$CdCl_4$] complex was synthesized and characterized by X-ray crystallography, FT-IR vibrational analysis, UV, thermal, and photoluminescence spectroscopic investigations. The crystal structure crystallizes in the monoclinic space group C2/c with Z=4 and the lattice parameters a = 12.6686(13) Å, b = 16.7728(16) Å and c = 6.9751(7) Å.The thermal analysis (ATD/TG) reveals the decomposition of the title compound at 100 °C. Density functional theory (DFT) results obtained using the ωB97XD and B3LYP-D3 computational methods were compared with the experimental geometric data of the crystalline molecule. To comprehend the type and degree of intermolecular interactions of the investigated complex, Hirshfeld surface (HS) analysis was performed. Molecular docking conducted with the 6U3Y, 1SAX, and 2D45 receptors show optimal postures with comparably fascinating binding affinities of -5.2 kcal.mol^{-1}, -5.6 kcal.mol^{-1}, and -5.7 kcal/mol respectively. The results of the molecular docking analysis showed that the target receptor proteins and the ligand have excellent potential for binding. Three of the proteins used in this obviously succumbed to the fact that the ($C_9H_{15}N_3$)[$CdCl_4$] complex is reported to be an effective inhibitor of enzymes in almost all situations and an activator in some cases.

Keywords: ($C_9H_{15}N_3$)[$CdCl_4$] complex, crystal structure, spectroscopy, electronic properties, molecular docking.

Tin(IV) chloride complexes with fluorinated phosphoramidates: Synthesis and multinuclear (^{1}H, ^{19}F, ^{31}P and ^{119}Sn) NMR characterization

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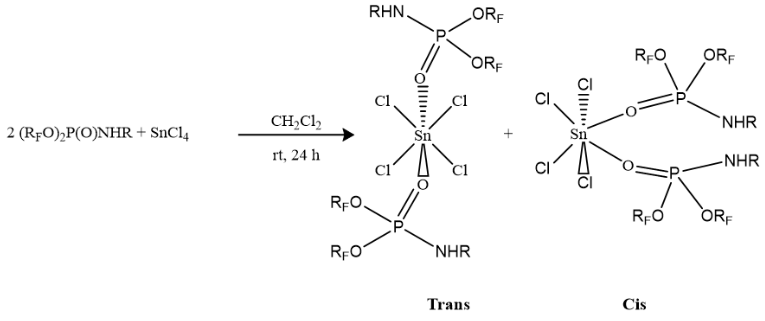
The study of tin compounds continues to provide fundamental insights into the Lewis acid-base model, the reactivity and the Lewis acid catalytic properties of tin (IV) species [1-3]. Recently, we have described the synthesis of new tin complexes with fluoroalkyl phosphoramidates ($(R_FO)_2P(O)NR)$) having secondary amino groups as potential ligands [4]. It was shown that the stability of such complexes depends on the nature of substituents on the phosphorus atom. In the present work, we report on the synthesis of new octahedral tin tetrachloride complexes with a novel series of fluorinated phosphoramidates with the general formula [$SnCl_4L_2$] (L= $(R_FO)_2P(O)NHR$)).These ligands were designed in order to see the effect of the presence of NH groups on their coordination properties. The adducts were characterized with multinuclear (^{1}H, ^{19}F, ^{31}P, and ^{119}Sn) NMR. The NMR data show that these complexes exist in solution as a mixture of *cis* and *trans* isomers. In addition, the solution behavior of these complexes in the presence of excess ligand was investigated with variable temperature NMR using the coalescence temperature method and compared with closely related complexes.



R= C_6H_5-C_2H_4, C_6H_5-CH_2, $CH_3(CH_2)_3$-, $(CH_3)_2$-CH-, C_6H_{11}-.
R_F=$C_6F_{13}CH_2CH_2$, $C_2F_5CH_2$, CF_3CH_2.

Keywords: Phosphoramidate, tin complex, ligand exchange, ^{119}Sn NMR.

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Synthesis, characterization and photophysical properties of π-conjugated architectures

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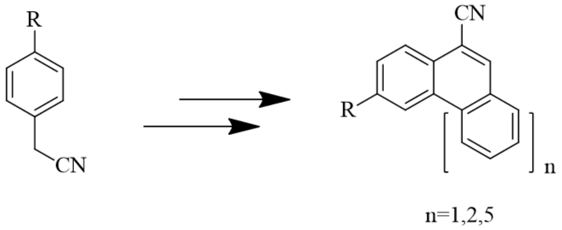
Polycyclic aromatic hydrocarbons (PAHs) represent an important class of compounds that have two or more fused benzene rings. They have received considerable attention due to their fascinating chemistry [1], their specific structure and photoelectric properties [2]. They have also led to many applications in electronic devices and proved to among the most important semiconductors [3,4]. Here, we report the synthesis of novel π-conjugated architectures by incorporating donor and acceptor groups at selected positions of the aromatic rings, aiming to use them in optoelectronic applications. The compounds were obtained in good yields through a short approach involving mild and easy experimental conditions. The absorption, emission and electrochemical properties of the target molecules have been investigated in solution and a remarkable behavior has been noted.

Keywords: Condensation, Photooxidation, photophysical properties.



Scheme 1: Synthesis of new polycyclic aromatic hydrocarbons

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SYNTHESIS, SPECTROSCOPIC CHARACTERIZATION, MOLECULAR STRUCTURE AND CATALYTIC STUDIES OF A CHROMIUM(III) PORPHYRIN COMPLEX WITH AXIAL CYANATE LIGANDS

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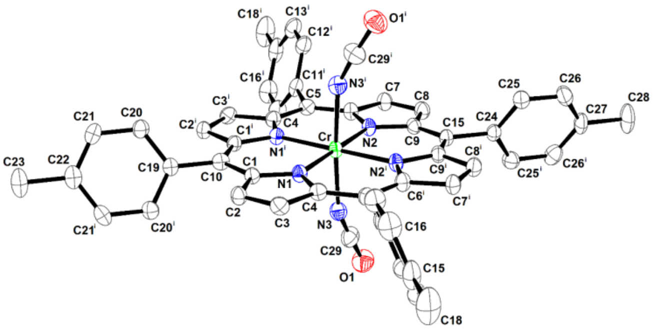
We report in this communication the synthesis and the spectroscopic, structural, and electrochemical characterization of a new chromium(III) coordination compound namely the bis(cyanato[*meso*-tetratolyporphyrinato]chromate(III) (cryptand-222)potassium dihydrate with the formula $[K(crypt\text{-}222)][Cr^{III}(TTP)(NCO)_2]^{\bullet}2H_2O$ (complex **I**). This compound crystallizes in the orthorhombic crystal system with the non-centrosymmetric space group $C222_1$. The chromium and the potassium atoms are located at special positions in a two-fold axis. The crystal lattice of complex (**I**)is stabilized by O—H···O, C—H···O, C—H···N and C—H···π intermolecular contacts involving the negatively charged $[Cr^{III}(TTP)(NCO)_2]^{-}$species, the $[K(crypt\text{-}222)]^{+}$ counterions and the two non-coordinated water molecules. Further insights on these weak intermolecular contacts are provided by the Hirshfeld surface analysis. Molecular electrostatic potential (MEP) theoretical calculation on complex (**I**) are reported. The new Cr(III) complex was efficient as a catalyst in the decomposition of the Rhodamine B (RhB) dye by hydrogen peroxide. This coordination compound was also tested as a photocatalyst of the photodecomposition of the RhB dye by molecular oxygen.



Ortep drawing of the $[Cr^{III}(TTP)(NCO)_2]^{-}$ complex ion with thermal ellipsoids drawn at 30% probability. The hydrogen atoms are omitted for clarity and only the major position of the disordered cyanate axial ligand is shown.

Keywords: Chromium(III) porphyrin complex; X-ray molecular structure; Photophysical properties; Cyclic voltammetry; FMOs calculation analysis; Photodegradation.

Growth, Single crystal investigations, DFT studies, Molecular Dynamics Simulations and Molecular docking, of novel thiocyanic complex with Zinc transition metal precursor

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The present work undertakes the study of novel thiocyanic complex, which have been obtained due to the interaction of cationic entities with the thiocyanate ligands. In fact, these latter are added to a transition metal leading to the production of novel solid-state complex that was studied and characterized by single crystal X-ray crystallography. However, $(C_{11}H_{18}N_2O)[Zn(SCN)_4]$ crystallizes in orthorhombic system with the non-centrosymmetric space group $P\ 2_12_12_1$. Infrared spectrum was registered to revel the vibrational modes of the compound, add to the study of the optical properties using a polar solvent to carry out the UV–visible analysis. Thermogravimetric analysis techniques (TGA) and thermo-differential analysis techniques (DTA) were carried out to account for the thermal decomposition of complex. Furthermore, the antibacterial properties were determined against some bacteria. In order to gain insights into the role of weak molecular interactions in the complex that influence the self-assembly process and crystal packing, Hirshfeld surface analysis and DFT calculation were also performed. Furthermore, molecular docking and molecular dynamic simulations were performed for the compound against different antibacterial targets to identify to which target the compound show the best binding affinity. The MurF enzyme, which catalyzed the last cytoplasmic step of bacterial peptidoglycan synthesis, among the target was revealed to show better interactions with the enzyme and formed strong and stable intermolecular complex.

Keywords: Metal, Thiocyanate, Crystal structure, Antibacterial activities, DFT calculations, Molecular docking, Molecular dynamics simulation.

Rapid capture and visual detection of fluorescent Schiff base modified dialdehyde nanocellulose-based sensors for metal ions detection

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In this paper, a novel fluorescents probes: **[PDA-DANC],[SAL-PDA-DANC], [ClSAL-PDA-DANC], [BrSAL-PDA-DANC]** was successfully synthesized based on dialdehyde nano-cellulose (DANC). The characterization and structural identification were carried out by FT-IR as well by XRD spectroscopy and EDX, the particle size of nanocellulose was determined by DLS analysis, the morphology and thermal stability was evaluated by SEM and TGA respectively. All the products synthetized exhibited a remarkable “turn off” with some metal ions. This behavior was studied by UV-VISIBLE and PL Spectroscopy.

Keywords: Nano-cellulose, Schiff Base, Sensors, Metal iondetection.

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Synthesis of mechanically interlocked component:[1] rotaxane

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The structures known as molecular machines can move in response to an external stimulus. Some of these machines are interlaced molecules. These structures are characterized by interactions involving mechanical bonds. The synthesis strategies of these molecules are still limited. As a result, the Programmed Molecular Systems group at IC2MP has been interested in creating novel syntheses for these compounds using the active metal recognition technique. Therefore, this work has three goals: first, we investigated how adding a second macrocycle affects lasso creation. This was carried out by the sequential addition of Cu(I) in the reaction medium. Then, we undertook the possibility of using an encumbered pyridine instead of a second macrocycle. Finally, we considered the rotaxanation reaction using a new stopper with an ester function activated by a nitro electro attractor group in the para position of the terphenyl. Cu(I) was successively added, which led to the progressive production of [1] rotaxane over time. The latter is primarily created in respect to threads that are not entangled. [1] rotaxane is obtained with a yield of 19%. However, sequential addition lasso training does not improve yield much, and it is time-consuming. We have chosen as encumbered pyridine for this study: 2,6-di-tert-butyl-4-methyl-pyridine. There has been significant deinterlacing formation. After purification, we obtained only 9% of [1]rotaxane. We carried out a trans-amidation reaction by substituting the ester with a stopper amine already synthesized in the laboratory. Following up with HPLC revealed that the transient lasso had disappeared and a new product had created. The 1H NMR spectra appears to match a deinterlaced molecule's spectrum. The attack of the amine from within the cavity is the only explanation for how the deinterlaced structure formed. The positioning of the macrocycle on the wire and the bulkiness of the ester must facilitate the development of the deinterlaced.

Understanding the behavior and selectivity of this reaction for the production of deinterlaced structure is required for the synthesis of a new [1]rotaxane.

Key words: rotaxane, molecular lasso, interlocked molecules

The Coordination Behavior of Two New Complexes, $[(C_7H_{10}NO_2)CdCl_3]_n$(I) and $[(C_7H_9NO_2)CuCl_2]$ (II), Based on 2,6-Dimethanolpyridine; Elaboration of the Structure and Hirshfeld Surface, Optical, Spectroscopic and Thermal Analysis

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Two new complexes have been synthesized and characterized: $[(C_7H_{10}NO_2)CdCl_3]_n$(I) and $[(C_7H_9NO_2)CuCl_2]$ (II). Single crystal X-ray diffraction revealed that in compound (I), 2,6-dimethanol pyridinium acts as a monodentate ligand through the O atom of the hydroxyl group. Contrarily, the 2,6-dimethanol pyridine ligand interacts tridentately with the Cu(II) ion via the nitrogen atoms and the two oxygen (O, O’) atoms of the two hydroxyl groups. The structure’s intermolecular interactions were studied using contact enrichment ratios and Hirshfeld surfaces. Following metal coordination, numerous hydrogen connections between entities and parallel displacement stacking interactions between pyridine rings dictate the crystal packing of both compounds. The aromatic cycles generate layers in the crystal for both substances. Powder XRD measurements confirmed the crystalline sample phase purity. SEM confirmed the surface homogeneity, whereas EDX semi-quantitative analysis corroborated the composition. IR spectroscopy identified vibrational absorption bands, while optical UV-visible absorption spectroscopy investigated the optical properties. Finally, the thermal stability of the two materials was tested using TG-DTA.

Keywords: coordination compound; X-ray structure; Hirshfeld surface study; IR spectroscopy; UV-visible absorption; TG-DTA

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01 October 2022

Synthesis and characterisation of zinc(II) complexes with phosphoramidates bearing a long alkyl chain of the types $(RO)_2P(O)NR'_2$

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Phosphoramidates are increasingly attracting considerable attention due to their potential applications in industry as flame retardants, in medicine as prodrugs, in catalysis and synthesis as long alkyl chain ligands [1, 2]. On the other hand, phosphoramidates are prevalent in the coordination chemistry of both transition and main group metals [3], having found important applications in the field of bioinorganic chemistry [4]. Recently, we have described the synthesis and coordination chemistry of phosphoramidates containing fluoroalkyl [5] or sulfoximine [6] groups. In this work, we report on the synthesis of zinc(II) complexes with phosphoramidates bearing long alkyl chain of the types $(RO)_2P(O)NR'_2$ (R = n-butyl, n-hexyl or n-heptyl; R'_2N = pyrrolidinyl, piperidinyl or morpholinyl). These complexes were fully characterised by multinuclear (^1H and ^{31}P) NMR, IR spectroscopy and conductivity measurements. The effect of phosphophorus substituents on the stability of the complex formed will be also discussed.

$$ZnCl_2 + 2\,(RO)_2P(O)NR'_2 \xrightarrow[\text{rt/24 h}]{EtOH/CH_2Cl_2} \left[ZnCl_2((RO)_2P(O)NR'_2)_2\right]$$

(R = n-Butyl, n-hexyl or n-heptyl; R'_2N = Pyrr, Pip or Mor)

Keywords: Phosphoramidate, cyclic amine, zinc complex, ^{31}P NMR.

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Critical Micelle Concentration of Alkylbetainthioates Surfactants

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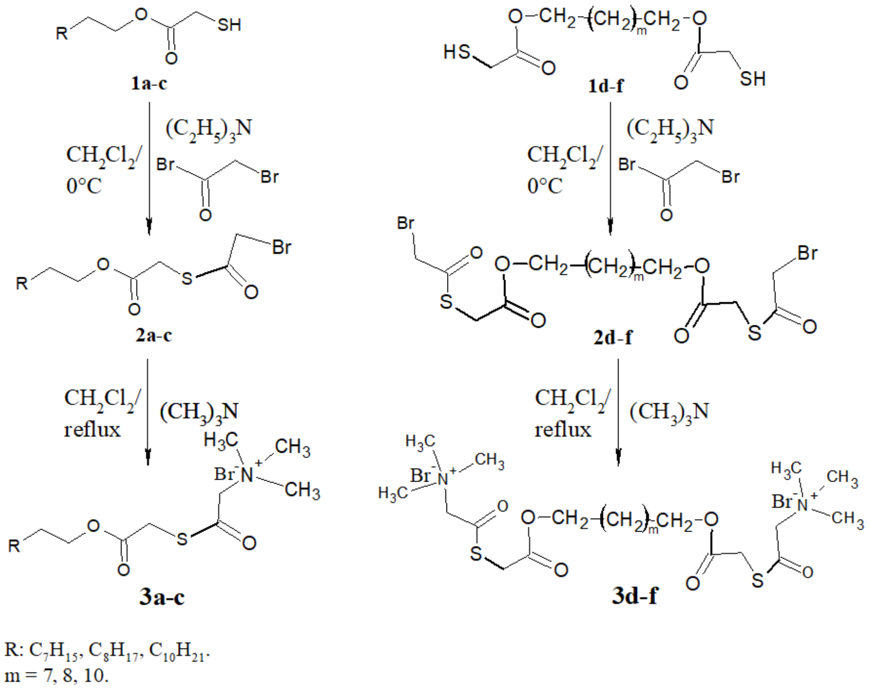
The synthetic procedure for the preparation of betainthioates series carrying a single hydrocarbon chain (**3a-f**) are depicted in Scheme 1. The starting compounds, alkyl sulfanylacetate **1a-c** and alkyl-α,ω-diyl bis(sulfanylacetate) **1d-f** were prepared by esterification reaction of mercapto acetic acid with respectively alcohol and diol. These compounds were reacted with excess of bromoacetyl bromide in triethylamine to afford respectively alkyl [(bromoacetyl)sulfanyl]actate **2a-c** and alkyl–α,ω-diyl bis{[(bromoacetyl) sulfanyl]acetate} **2d-f**. The reaction of bromoacetyl **2a-c** and bis bromoacetyl 2d-f with excess of trimethylamine in dry of dichloromethane give respectively, mono-tetramethylammonium bromide **3a-c** and bis- tetraethylammonium bromide **3d-f** in good yields [1]. These compounds can be used as ligands in the extraction of metal ions.



Scheme 1: Synthesis of surfactants **3**

Keywords: monotailed, bolaphiles, cationic, surfactants, betainthioates.

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Synthesis of New Homopiperazine-1.4-Diium Tetrachloridromercurate (II) Monohydrate $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$, Crystal Structure, Hirshfeld Surface, Spectroscopy, Thermal Analysis, Antioxidant Activity, Electric and Dielectric Behavior

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Using acid-base assays and simple slow evaporation method at ambient temperature, we were successful in producing of novel salt with the chemical formula $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$. According to single-crystal X-ray diffraction data, the crystal packing was regulated by H-bonds and by coulomb interactions (also called electrostatic interactions) between distinct entities, which formed a 3D network. The 2D fingerprint plots and the Hirshfeld surface were utilized to examine the effect of intermolecular interactions. FTIR spectroscopy, PL spectroscopy, thermal analysis and electrical conductivity experiments were also carried out. The antioxidant activity was done.

Key words: Photoluminescence, FT-IR, Chloromercurate (II), Dielectric Analysis, Antioxidant activity.

Magnesium(II) (DMAP) complex with the *meso*-tetra(*para*-chlorophenyl)porphyrin: X-ray crystallography, Spectroscopic, Electrochemical properties, DFT, DOS and MEP calculations and Biologic activities

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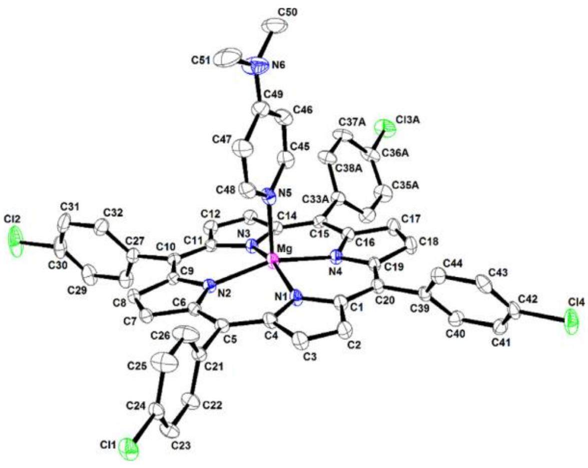
Porphyrins and metalloporphyrins, are aromatic tetrapyrrolic macrocycles species very widely represented in living media. They participate, in many biological processes such asin the hemoglobin, the myoglobin and cytochromes. Studies of magnesium(II) porphyrin complexes are important given the fact that these complexes structurally gather at the active site of chlorophyll which is a complex of Mg(II) with chlorine. In this communication we describe the synthesis of the (DMAP)[*meso*-tetra(*para*-chlorophenyl)porphyrinato]magnesium(II) complex with the formula [Mg(TClPP)(DMAP)] (**I**). This species was characterized by UV-visible, IR, ^{1}H NMR, fluorescence, and mass spectrometry. The molecular structure of (**I**) was determined and described by single crystal X-ray diffraction analysis and Hirshfeld surfaces computational method. To gain further insights into the reactivity of (**I**), a density of states (DOS) and a molecular electrostatic potential (MEP) theoretical calculation were carried out. Furthermore, the antifungal and the antioxidant activities of the free base H_2TClPP porphyrin, the [Mg(TClPP)] starting material and [Mg(TClPP)(DMAP)] (**I**) were also tested.

Keywords: Magnesium(II) porphyrin complex; X-ray molecular structure; Photophysical properties;Cyclic voltammetry; Biological activity.



Ortep diagram of the [Mg(TClPP)(DMAP)] complex.

Synthesis, Single Crystal Structural Investigation, Hirshfeld Surface Analysis, Thermoanalysis and Spectroscopic Study of A New Cu(II) Transition-Metal Complex

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A new complexe, $[Cu(dimpyr)_2(H_2O)_2](NO_3)_2.2H_2O$, with the monodentate ligand 2-amino-6-methylpyrimidin-4-(1H)-one (dimpyr) is prepared and characterized by single crystal X-ray diffraction, elemental analysis and IR spectroscopy. The Cu(II) cation is tetracoordinated, in a square plan fashion, by two nitrogen atoms from the pyrimidine ring of the organic ligand and two oxygen atoms of two coordinated water molecules. In the atomic ar- rangement, the CuO_2N_2 square planes are interconnected via the formation of O-H…O hydrogen bonds involving both coordinated and free water molecules and NO^{3-} nitrate anions to form inorganic layers parallel to the (a, b) plane at z = (2n + 1)/4. The vibrational absorption bands were identified by infrared and Raman spectroscopy. Intermolecular interactions were investigated via Hirshfeld surfaces. The compound were characterized by thermal analysis to determine their thermal behavior with respect to temperature.

Key words: coordination compound, X-ray structure, Hirshfeld surface, DTA-TGA.

ELIMINATION OF CHROMIUM VI FROM WAST WATER BY RECYCLABLE NANOPARTICLES Fe_3O_4@CnTAB

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Hexavalent chromium CrVI is a common industrial pollutant that poses serious threats to ecosystems[1]. It is classified in the Group 1 by the Cancer Research Agency (IARC)[2]. The World Health Organization (WHO) guideline is 0.05 mg/L for total chromium[3]. Hence, the imperative of using an analytical method for the extraction and determination of Cr VI, which must be simple, inexpensive, non-polluting, fast and above all selective and efficient. Fe_3O_4 magnetite nanoparticles (NPMs) are potential adsorbents for water treatment as they combine the advantages of easy handling and large surface areas for the adsorption of pollutants. Surface modification of NPMs with trimethyl ammonium alkyl bromide (CnTAB) effectively reduces particle size and improves its stability in solution. In this work we propose to study the the cationic surfactant chain length (trimethlyl ammonium alkyl bromide CnTAB, with n=10, n=14 and n=16) effect on the adsorption capacity of CrVI by magnetite nanoparticles coated with cationic surfactant Fe_3O_4@CnTAB. This study was motivated by the promising results obtained recently by several researchers[5]. First we started with the synthesis and functionalization of magnetite nanoparticles functionalized by CnTAB. The synthesis method is a co-precipitation of ferrous salt and ferric salt in a single step in the presence of CnTAB surfactant. The products were characterized by XRD and IRTF. Finally, the extraction of Cr VI metal was realized by adsorption on NPMs and its transformation into Cr III. The assay is carried out by UV spectroscopy. The optimization of the adsorption is carried out by varying of the medium pH, the contact time, the adsorbent amount and the influence of the presence of salt. To test the efficiency and selectivity of our CrVI adsorption and analysis protocol, we chose a real sample: Sebkha water from Oran (Dayat el Morsli) after filtration. The results show that: a longer chain surfactant gives more extraction.

- a high percentage of adsorption in a acid medium.
- More quantity of adsorbent offers more interaction surface.
- The method is effective even in the presence of salts.
- The method is relatively very fast. In fact, only a few minutes (8 minutes) of contact for a maximum extraction (95%).

Key words: Chromium; pollution; recyclable magnetite nanoparticles; adsorption extraction; CTAB.

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02 October 2022

SYNTHESIS, MOLECULAR STRUCTURE, SPECTROSCOPIC CHARACTERIZATION, OF A NEW MAGNESIUM(II) PORPHYRIN COMPLEX WITH DMAP AXIAL LIGAND ANTIFUNGAL ACTIVITY

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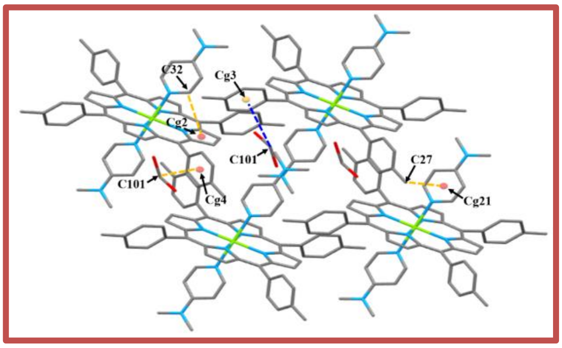
Investigations on magnesium(II) porphyrin complexes has a particularity importance given the fact that these complexes are structurally similar to the active site of chlorophyll which is a complex of Mg(II) with *chlorine* (a reduced porphyrin). Consequently, an important number of studies have been devoted to synthetic Mg(II) metalloporphyrins to understand the very complicated mechanism of the chlorophyll photosynthesis. A new magnesium(II) metalloporphyrin namely the bis(4-dimethylaminopyridine)[*meso*-tetra(*p*-tolyl) porphyrinato)]magnesium(II) dichloromethane disolvate complex with the formula $[Mg(TTP)(DMAP)_2]^{\bullet}2CH_2Cl_2$ (**I**) has been synthetized and fully characterized by UV-Vis, fluorescence, IR, ^{1}H NMR spectroscopy and mass spectrometry. The cyclic voltammetry data of **I** is also reported. Crystallographic study of this monocrystal metalloporphyrin was performed on a Bruker APEXII CCD diffractometer. The product crystallizes in the triclinic system with the space group *P-1* and the lattice parameters are: a = 10.7646(11) Å; b = 10.8804(11) Å; c = 13.1589(13) Å; α = 75,028 (3)°; β = 87.745(3)° ; γ = 68,827(2)°. The bioactivity of the free base porphyrin H_2TTP, the [Mg(TTP)] starting material and $[Mg(TTP)(4\text{-}DMAP)_2]\bullet 2CH_2Cl_2$ (**I**) was evaluated *in vitro*, by examining their inhibitory effect against three strains of *Candida.*

Keywords: Magnesium(II) porphyrin complex; X-ray molecular structure; Photophysical properties;Cyclic voltammetry; Antifungal and Biological Activities.



Packing diagram of (**I**) showing C—H-Cg π intermolecular interactions.

Synthesis and characterization of a new hexaborate stabilized by organic cations.

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A new mixed ligand cobalt-hexaborate $[C_6N_2H_9]_2\{Co[B_6O_7(OH)_6]_2\}\cdot 4H_2O$ (2A6MPCoB6) was synthesized in aqueous solution with slow evaporation method in presence of boric acid, cobalt chloride and organic amine ($C_6H_8N_2$). The structure was determined by X-ray diffraction on single crystal and characterized by IR absorption spectroscopy, UV-Vis spectrophotometry, spectrofluorimetry, thermogravimetric analysis and impedance spectroscopy complex. Single crystal X-ray show that 2A6MPCoB6 crystallizes in the triclinic system with $P\bar{1}$ space group and mesh parameters: a=8.064 (3) Å; b=9.129 (3) Å; c=11.607 (4) Å; α=95.212 (4)° ; β =95.269 (5)°; γ=97.268 (4)°, V= 839.5 (5) Å^3 and Z=1. The form unit consists of two cations $(C_6H_9N_2)^+$, the anionic complex $\{Co[B_6O_7(OH)_6]_2\}^{2-}$ and four molecules of crystallizing water. These groups are strongly linked between them by multiple intermolecular interactions (electrostatic, hydrogen and Vander-Waals bonding) to form a three-dimensional supramolecular stacking. In addition, spectroscopic investigations have revealed the principal vibrations modes, electronic, optical, luminescent and electric properties of the studied compound.

Key words: Hexaborate, X-ray-diffraction, Infrared spectroscopy, Thermal analysis, Impedance spectroscopy.

Crystal structure, stability and binding interactions with bio-macromolecules of new phosphotetradecavanadate with 4-methylimidazolium

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Polyoxovanadates (POV), as a relevant subfamily of polyoxometalates (POM), have attracted increasing attention over the years due to the variable oxidation states that vanadium can adopt and the various spheres of coordination demonstrated by vanadium oxide polyhedra, which gives them the ability to form an exceptional variety of different architectures [1]. In contrast to molybdates and tungstates, which are typically based on [MoO6]/[WO6] octahedra as fundamental building units, POVs show more structural flexibility and feature tetrahedral [VO4], square pyramidal [VO5], and octahedral [VO6] coordination modes.[2,3]. In order to obtain new materials with news structures and interesting properties, we report in this work for the first time the synthesis, characterizations, crystal structure and stability of the novel bicapped Keggin phosphotetradecavanadates with organic cations $(C_6H_5N_2)_6(NH_4)[H_2PV_{14}O_{42}].4H_2O$ crystallized in a monoclinic system, P21/n space group with the cell parameters : a = 12.3187 (3) Å, b = 115.1592 (3) Å, c = 32.7674 (8) Å, β = 90.762 (2)° and Z = 4.

Key words: Synthesis, Characterization, X-ray diffraction, phosphotertradecavanadate

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Reaction of DMAP and HMTA with the (Triflato)*Meso*-Tetra(*para*-methoxyphenyl)porphyrinto Manganese(III) Complex. Spectroscopic, and Structural Characterizations - Antibacterial, Antifungal and Antioxidant activities

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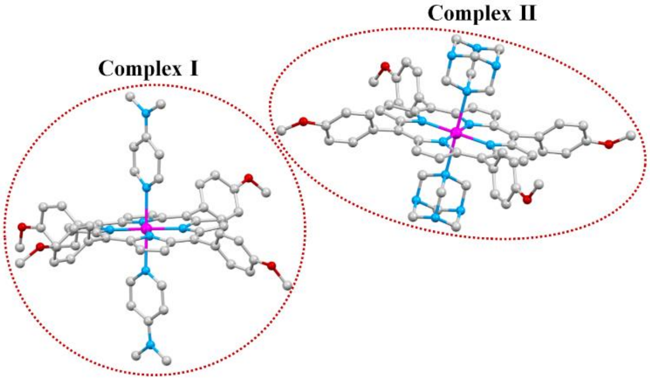
Manganese porphyrins have been of interest to researchers since the early 1960's when the pioneering work of Boucher[1–4]can be cited. In the early 1960s and 1970s, the great interest in these metalloporphyrins stemmed from (i) the role of manganese in the release of oxygen from water in photocatalysis reactions[5] and (ii) the important catalytic properties of these compounds which can mimic those of P450 cytochromes[6]. In the present work we have synthesized two new six-coordinated manganese(III) porphyrin coordination compounds namely the bis(4-dimethylaminopyridine)[(*meso*-tetra(*para*-methoxyphenyl)porphyrinato)] manganese(III) chloroform desolate (**I**) and the bis(hexamethylenetetramine)[(*meso*-tetra(*para*-methoxyphenyl)porphyrinato)]manganese(III) dichloromethane disolvate (**II**).Both crystal structures were determined and described by single crystal X-ray diffraction analysis and Hirshfeld surfaces computational method. Those complexes were characterized by UV-visible, IR, mass spectrum, cyclic voltammetry. The role of these complexes as Antibacterial, Antifungal and Antioxidant agents was also performed.



Molecular structure of ion complexes I and II

Key words: Manganese(III) porphyrin; Single crystal X-ray molecular structure; UV-visible; IR; cyclic voltammetry, Antibacterial activities, Antifungal activities, Antioxidant activities.

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Synthesis, crystal structure, vibrational and optical properties of new Bi(III) halide complex *(tris*(2-Amino-5-(methylthio)-1,3,4-thiadiazol-3-ium) hexachlorobismuthate(III)): $(C_3H_6N_3S_2)_3BiCl_6$

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The new organic–inorganic hybrid zero-dimensional bismuth-chloride based compound : $(C_3H_6N_3S_2)_3BiCl_6$, was synthesized by slow evaporation at room temperature. Single-crystal X-ray diffraction analysis indicates that the compound belongs to the triclinic crystal system with the centrosymmetric space group $P\bar{1}$. The asymmetric unit contains one octahedral geometry of $[BiCl_6]^{3-}$ and three protonated cations $(C_3H_6N_3S_2)^+$. In the crystal structure, the isolated $[BiCl_6]^{3-}$ anions are linked to organic cations via N-H…Cl and C-H…Cl hydrogen bonds. Vibrational assignements of $(C_3H_6N_3S_2)_3BiCl_6$ are interpreted by FT-IR and Raman spectroscopic studies. The crystal packing is stabilized by N/C-H…Cl interactions whereas the Van Der Waals contacts play a key role in the consolidation of the 3D packing as verified by Hirshfeld surface analysis in combination with 2D fingerprint plots. The two-dimensional fingerprint plots reveal that the structure is dominated by Cl…H/H…Cl, H…N/N…H and H…H contacts. The crystal exhibits the thermal stability up to 270 ºC using thermal analysis. The fluorescence measurements show two blue peaks which are attributed to band to band and excitonic emissions within the chlorobismuthate octahedron.

Keywords: Bi(III) complex, X-ray diffraction, optical properties, synthesis of organo bismuthate compound

Poster Communications' List

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C. Ayari, M.H. Mrad, F. Lefebvre, V. Ferretti, C. Ben Nasr *FSB - Bizerte* Crystal structure, Hirshfeld surfaces, computational study and physicochemical characterization of 2,5-di-tert-butylanilinuim chloride: $[C_{14}H_{24}N]Cl$	**PC 01**
S. Ben Haj Fraj, S. Agren, J. El Haskouri, M.H.V Baouab *FSM - Monastir* Green Synthesis and characterization of disubstituted Imidazoles derivatives by an ecofriendly and efficient heterogenous nano-catalytic: Nanocellulose based magnetic nanocomposite	**PC 02**
R. Boubakri, K. Kaabi *FSB - Bizerte* Crystalline structure and physico-chemical stady of a new Co(II) transition-Metal complex with the countercation ligand 4-amino-2,6-dimetylpyrimidium	**PC 03**
H. Fouzai, Z. Barhoumi, N. Amdouni *FST - Tunis* Micellization and aggregation in aqueous amphiphilic ionic liquid and anionic polymer	**PC 04**
T. Fradi, H. Nasri *FSM - Monastir* Synthesis of the pyrazole magnesium(II) meso-tetrakis-(4-chlorophenyl) porphyrin) complex. Spectroscopic, cyclic voltammetry investigations and X-ray molecular structure	**PC 05**
A. Gannouni, R. Kefi *FSB - Bizerte* Single crystal investigations, Hirshfeld surface analysis, DFT studies, molecular docking, physico-chemical characterization and biological activity of a novel non-centrosymmetric compound with copper transition metal precursor	**PC 06**
O. Gatri, M.L. Efrit *FSB - Tunis* Synthesis of new S, N-Heterobidentate Ligands: *N*-(carbamothioyl)benzimidate	**PC 07**
K. Guiza, R. Ben Arfi, K. Mougin, A. Ghorbal *FSG - Gabès* Elaboration and characterization of ecofriendly keratin/cellulose-based composites for oil/organic solvent absorption	**PC 08**
I. Hajji, F. Aloui *FSM - Monastir* Nitrile grafted [7] Helicenes through a photocyclization pathway of di-bromo-phenanthrene: Synthesis and photophysical properties	**PC 09**

Communicatings' Names	**Ref**
K. Hamrouni, F. Aloui *FSM - Monastir* Photochemical evaluation of nitrile α, β-insaturated through a photooxidation pathway in benzo[c]phenanthrenic	**PC 10**
K. Hamrouni, F. Aloui *FSM - Monastir* Synthesis, characterization and chiroptical properties of a new thiahexhelicene	**PC 11**
M. Harzallah, N. Issaoui, M. Medimagh, B. Ayed *FSG - Gabès* Study of functional theories of the density of non-covalent interactions in [1-(2-aminoethyl) pipezinium] tetrabromidomercurate(II) monohydrate : Analyzes of molecular structure, ELF, RDG, AIM, MEP , HUMO-LUMO and molecular docking studies	**PC 12**
S. Hermi, C. Ben Nasr, M.H. Mrad *FSB - Bizerte* Elaboration, crystal structure, physico-chemical characterization and theoretical investigation of a new non-centrosymmetric Sn(IV) complex $(C_4H_{12}N_2)[SnCl_6]\cdot 3H_2O$	**PC 13**
S. Jabli, T. Roisnel, F. Molton, F. Loiseau, H. Nasri *FSM - Monastir* Preparation, spectroscopic characterization and molecular structure of the (3,5-lutidine) (MESO-tetratolylporphyrinato) magnesium(II) complex	**PC 14**
Z. Jebali, H. Farkous, M. Radjai, S. Boufi, H. Majdoub, M. Boutahala *FSM - Monastir* Enhanced dye removal by diatomite/cationic nanoholocellulose nanocomposite: Modeling, kinetics, equilibrium, thermodynamics, and reusability Studies	**PC 15**
I. Jomaa, N. Issaoui, H. Marouani *FSB - Bizerte* The coordination behavior of a new hybrid compound $(C_6H_{14}N)2[CdCl_4]$: Structural features, physicochemical characterization and theoretical study	**PC 16**
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C. Labassi, N. Fournier, M.L. Efrit, J.L. Fillaut, R. Gatri *FST - Tunis* Synthesis of new fluorescent pyrazolines via the NITEC reaction	**PC21**
N. Mahbouli Rhouma , F. Mezzadri, G. Calestani, M. Loukil *FSS - Sfax* Synthesis, characterisation, and optical properties of the novel organic-inorganic hybrid material bis (4-fluorobenzylammonium) tetrachloridozincate(II): $[C_7H_9NF]_2ZnCl_4$	**PC 22**
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F. Mannai, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* Rheological and physicochemical properties of polysaccharides extracted from *Opuntia* (Cactaceae)	**PC 24**
H. Mkacher, F. Molton, F. Loiseau, H. Nasri *FSM - Monastir* Synthesis, spectroscopic and structural of manganese(III) porphyrin complex: $[MnIII\ (TTP)(DMAP)_2](SO_3CF_3)\cdot 3/2(CHCl_3)$	**PC 25**
R. Omrani, N. Jebli, Y. Arfaoui, A. Ben Akacha *FST - Tunis* Synthesis, X-ray structure, DFT investigation and molecular docking of novel ligand: A cyclic polyamide with anti HIV-1 (RT), antiplatelet and anticoagulant activities	**PC 26**
Y. Oueslati, A. Valkonen, W. Smirani *FSB - Bizerte* Growth, single crystal investigation, Hirshfeld surface analysis, DFT studies, molecular docking, physico-chemical characterization and, in vitro, antioxidant activity of a novel hybrid complex	**PC 27**

Communicatings' Names	**Ref**
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I. Rajhi, M.T. Ben Dhia, M. Abderrabba, S. Ayadi *FST - Tunis* Fractionation, characterization and biological activities of Tunisian *Capparis spinosa* L.	**PC 29**
D. Sghairi, M.A. Sanhoury, M. Romdhani Younes *FST - Tunis* Synthesis of new phosphorochloridates and phosphoramidates	**PC 30**
A. Siai, C.D. Brand, M. Ströbele, D. Enseling, T. Jüstel, H.J. Meyer *CRTEn - Borj Cédria* Optical properties of carbodiimide bridged network structure of $[RE_6O(NCN)_6]$ clusters in the structure of $RE_8O(CN_2)_{10}Br_2$, RE=La, Ce, Pr, Nd	**PC 31**
I. Souii, M.A. Sanhoury, M.L. Efrit, H. Mrabet *FST - Tunis* Synthesis and characterization of an unexpected mixture of two complexes obtained from reaction between tin(IV) chloride and bis-(acrylic α-aminophosphonates)	**PC 32**
M. Tahenti, N. Issaoui, T. Roisnel, H. Marouani, O. Al-Dossary, A.S. Kazachenko *FSB - Bizerte* Self-assembly of a new cobalt complex, $(C_6H_{14}N_2)_3\ [CoCl_4]Cl$: Synthesis, empirical and DFT calculations	**PC 33**
T. Taleb Amar, A. Maalaoui, M. Rzaigui, S. Akriche *FSB - Bizerte* Synthesis, crystal structure, Hirshfeld surface analysis and characterization of a new decavanadate complex with 2-amino-4-methyl-thiazol	**PC 34**
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R. Zarroug, B. Ayed *FSM - Monastir* New phosphotetradecavanadate with 2-picolinium: crystal structure, stability and binding interactions with bio-macromolecules	**PC 36**

Posters Communications' Abstracts

Crystal structure, Hirshfeld surfaces, computational study and physicochemical characterization of 2,5-di-tert-butylanilinuim chloride: $[C_{14}H_{24}N]Cl$

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The new organic salt 2,5-di-tert-butylanilinuim chloride $[C_{14}H_{24}N]Cl$ was obtained from an aqueous solution by slow evaporation at room temperature and characterized by various techniques, mainly crystal X-ray diffraction. This title compound crystallized in the monoclinic system with space group $P2_{1/}c$. The atomic arrangement can be described by hybrid pillars running along the *c*-axis. The crystal packing is stabilized by N-H…Cl and C-H…Cl hydrogen bonds to form a three-dimensional network. The intermolecular interactions were investigated by Hirshfeld surfaces and the associated 2D fingerprint plots. Furthermore, the vibrational absorption bands were identified by IR spectroscopy and were also calculated by Density Functional Theory (DFT). The optical property of the crystal was studied using solid-state UV-visible and photoluminescence spectroscopy. The **study** also presents the results of the ***DTA thermal*** analysis.

Key words: X-ray diffraction, Spectroscopy, Optical study, Hirshfeld surface, DFT, DTA.

Green synthesis and characterization of disubstituted imidazoles derivatives by an ecofriendly and efficient heterogenous nano-catalytic: nanocellulose based magnetic nanocomposite

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In the present work, a nanocellulose based magnetic nanocomposite was synthesized by an ecofriendly and a simple procedure and characterized by Fourier transform infrared spectroscopy (FTIR), X-Ray diffraction (XRD), thermogravimetric analysis (TGA), Scanning Electron microscopy (SEM), Energy dispersive X-Ray spectroscopy (EDX) and vibrating Sample electron (VSM). Then, it was used in a green and efficient procedure for one-pot multicomponent synthesis of imidazole derivatives by the condensation of diketone, benzaldehyde derivatives and ammonium acetate in ethanol. This procedure has advantages compared to the conventional method as the high yields, short reaction times and easy separation from the reaction mixture by using a magnet and reusability of the catalyst.

Key words: Fe_3O_4NPs, Nanocellulose, heterogeneous green Nano-catalyst, imidazole, recyclable.

Crystalline structure and physico-chemical stady of a new Co(II) transition-Metal complex with the countercation ligand 4-amino-2,6-dimetylpyrimidium

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A new complexe, $(Hamdimpy)_2[CoCl_4].H_2O$, with the countercation 4-amino-2,6-dimetylpyrimidium (Hamdimpy), is prepared and characterized by single crystal X-ray diffraction, elemental analysis and IR spectroscopy.. In this new compund, the central atom Co(II) is four-coordinated in a distorted tetrahedral fashion by four Cl^- ions. The [CoCl4]2− tetrahedra are arranged parallel to the plane $(\bar{1}10)$ at $x = (2n + 1)/2$ and the organic cations are grafted between them by establishing with them hydrogen bonds of CH…Cl and NH…Cl types. The vibrational absorption bands were identified by infrared and Raman spectroscopy. Intermolecular interactions were investigated via Hirshfeld surfaces. The compund is characterized by thermal analysis to determine their thermal behavior with respect to temperature.

Key words: coordination compound, X-ray structure, Hirshfeld surface, DTA-TGA.

Micellization and aggregation in aqueous amphiphilic ionic liquid and anionic polymer

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Because of their distinct properties, room temperature ionic liquids (RTILs) as a new solvent used in chemical processes and have been the target of many scientific investigations. For this application many ILs have been described as having advantageous properties over the "*traditional*" molecular solvents. Imidazolium-*based* ILs hold great interest in solvent, phase transfer catalyst and electrochemical applications. Many of these applications need the mixing of ILs with polyelectrolyte (PE) or salt. Inspired by the physicochemical characteristics of the ILs/ PE systems, large amount of works to mimic the interaction behavior between IL/ PE have been developed.That is an idea to study systems of polyelectrolyte/ ILs oppositely charged is not completely new. We employed UV-visible absorption spectroscopy, steady-state fluorescence spectroscopy, thermal fluorescence spectroscopy, viscosity (η) and dynamic light scattering (DLS) techniques to investigate the influence of [Amim][Br] on aggregation of PNIPAM polymer. [1-4]. In the present work, 1-allyl-3-methylimidazolium bromide (AmimBr) is synthesized.The aggregation behavior of IL in aqueous polymer solutions and their corresponding physicochemical properties have been investigated employing conductivity, volume, UV-visible spectroscopy.

Key words: Ionic liquid; critical micellization concentration (CMC); aggregation; molar volume.

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Synthesis of the Pyrazole Magnesium(II) *Meso*-tetrakis-(4-chlorophenyl) porphyrin) complex. Spectroscopic, Cyclic Voltammetry Investigations and X-ray Molecular structure

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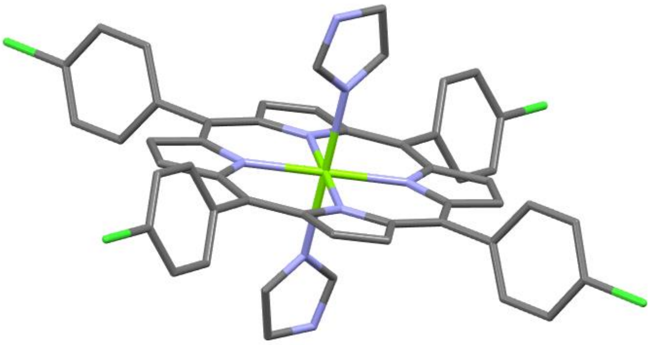
Synthetic magnesium porphyrins have attracted significant interest recently due to their application in different fields such as sensors [1], catalyst [2], antibacterial properties [3], organic catalysis [4], besides the relevance with chlorophyll molecules in photosynthesis.

In this work, we have focused on the synthesis, the crystal structure, UV-visible, IR, NMR, fluorescence, cyclic voltammetry characterizations of the new magnsium(II) complex namely the (pyrazole){*meso*-tetrakis[4-(chloro)phenyl]porphyrinato}magnesium(II) with the formula [Mg(TClPP)($C_3H_4N_2$)$_2$] (**I**). The title compound crystallizes in the monoclinic crystal system (C_2/c space group). The cell parameters are: a = 23.994(1) Å, b =9.521(1) Å, c = 22.8777(1), β = 117.231(3)°, with V = 4647.2(9) Å^3 , Z = 4, R_1 = 0.0470, wR_2 = 0.1334, S = 1.037.

Key words: Magnesium(II) porphyrin complex; X-ray molecular structure; Photophysical properties;Cyclic voltammetry.



Structure of the [Mg(TClPP)($C_3H_4N_2$)$_2$] complex.

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Single crystal investigations, Hirshfeld surface analysis, DFT studies, molecular docking, physico-chemical characterization and biological activity of a Novel Non-Centrosymmetric Compound with Copper transition metal precursor

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A new non-centrosymmetric hybrid organic-inorganic material (2-ethylpiperazine tetrachlorocuprate(II)), has been prepared and analyzed using single-crystal X-ray diffraction, spectroscopic studies, optical absorption, photoluminescence properties, DFT studies, Hirshfeld, surface analyses and thermal studies. The title material $(C_6H_{16}N_2)[CuCl_4]$ crystallizes in orthorhombic system with unit cell dimensions of a = 7.4489 (8) Å, b = 9.9144 (10) Å, c = 17.4977(16) Å, $\alpha = \beta = \gamma = 90°$. The N-H···Cl and C-H···Cl hydrogen bonds are alternately connected by organic cations $[C_6H_{16}N_2]^{2+}$ and inorganic moieties $[CuCl_4]^{2-}$. The Hirshfeld surfaces investigated the nature and quantity of different interactions and their role in crystal packing. In addition, the energies of the frontier orbitals (LUMO and HOMO), the RDG and AIM analyses, and the natural bonding orbital are studied. TD/DFT computations were used to investigate the UV-Vis absorption photoluminescence and optical properties. The antioxidant activity of the newly isolated complex was tested using the DPPH and ABTS radical scavenging methods. In addition, an in silico investigation using molecular docking of the title material against SARS-CoV-2 variation (B.1.1.529) was also conducted to better understand the non-covalent interaction of cuprate (II) complexes with active amino acids in the SARS-CoV-2 spike protein.

Keywords: Organic-inorganic hybrid material, X-ray single-crystal structure, TD-DFT calculations, Spectroscopic studies, Anti-oxidant activity.

Synthesis of new S, N-Heterobidentate Ligands : *N*-(carbamothioyl)benzimidate

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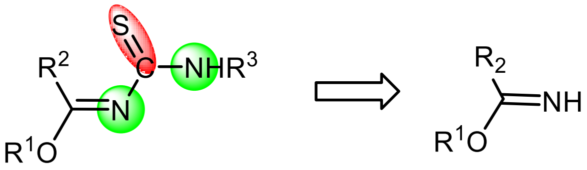
A great deal of work has been devoted to the study of thiourea because of their flexible coordination capacity. It is interesting to note that thiourea and substituted thioureas have coordinating capacity through both sulphur and nitrogen, although they are considered amongst the ligands having extremely low basicity.[1] Particularly, there has been considerable discussion with regard to the assignment of C=S stretching frequencies in such ligands.[2] As part of the synthesis of new ligand from imidate, this communication deals with the synthesis of new ligand from thiourea-imidates.



R^1 = Me, Et.
R^2 = Ph, Bn, i-Pr, *mMe*-Ph.
R^3 = Ph, $CH_2CH=CH_2$, Cyclohexyl.

Figure 1. Synthesis of new ligand from imidates.

Key words : Ligand, thiourea, imidate, *N*-(carbamothioyl)benzimidate.

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Elaboration and characterization of ecofriendly keratin/cellulose-based composites for oil/organic solvent absorption

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The recovery of oil spilled on water has become an important issue due to the environmental regulations [1]. This research provides the ecological development of a new environmental biomaterial keratin/cellulose using chicken feathers (CF) and cardboard (C) from environmental waste for the first time, to be exploited in oil/solvent absorption. The keratin/cellulose-based composites were obtained by combining the dissolution of CF and C waste in 1-butyl-3-methylimidazolium chloride ($Bmim^-Cl^+$) ionic liquid green solvent via regeneration, simply by the freeze-drying method. The characterization analysis of the synthesized keratin/cellulose-based composites was performed using FTIR, XRD, ATD/ATG and MEB microscopy. The as-prepared cryogel can absorb various oils and organic solvents. Moreover, its sorption capacity can reach up to 6.9–17.7 times the weight of the initial cryogel. This kind of CF/C cryogel revealed good and fast absorption efficiency. Through the kinetic analysis, it was found that the pseudo-second-order model was more appropriate for the keratin/cellulose cryogel oil absorption process [2]. Besides, owing to its low cost, good absorption capacity, and excellent reusability, this cryogel has potential for spill cleanup of oils and organic solvents.

Key words: Keratin, Cellulose, Composite, Cryogel, Oil absorption.

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Nitrile grafted [7] Helicenes through a photocyclization pathway of di-bromo-phenanthrene: Synthesis and photophysical properties

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Helicenes represent a class of polyaromatic hydrocarbons consisting of *ortho*-annellated benzene nuclei with a non-planar topology [1-2]. The helical structure of such molecules results from the repulsive interaction between terminal aromatic rings [3] making them inherently chiral despite the absence chiral centers. They have attracted much interest due to their unrivalled structural features [4-5]. These organic molecules present *left*- and *right*-handed chiral helical structures of *M* and *P* configuration, respectively [6]. In our work, new helically chiral heptacyclic compounds bearing suitable functional groups have been prepared, in a good overall yield, through a four-step sequence involving mild experimental conditions. The target polyfunctional [7]Helicenes showed a good solubility in common solvents and interesting optoelectronic properties. Their photophysical and electrochemical properties have been examined experimentally, and their HOMO and LUMO energy levels were found at 2.47eV- 2.62 eV.

Key words: Helicenes, Photooxidation, Coupling reactions, photophysical properties.

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Synthesis, characterization and chiroptical properties of a new thiahexhelicene

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Helicenes are polycyclic aromatic hydrocarbons made up of ortho-fused aromatic or heteroaromatic nuclei, presenting a non-planar π electron system [1], which results from a steric hindrance between the terminal aromatic rings. These organic molecules have exceptionally intense chiroptic properties, such as high optical rotation and very powerful electronic circular dichroism (ECD). The inherent chirality of helicenes combined with their high optical stability and their rigid structure, allowed them to gain an interest in transverse disciplines such as liquid crystal [2] sensors [3], chiral catalysts [4] and ligands for asymmetric synthesis and synthesis of polymers and motors molecules. A new helically chiral thia[6]helicene, bearing suitable functional groups has been prepared, in a good overall yield, through a four-step sequence involving mild experimental conditions. Optical resolution of the racemic helicene has been accomplished affording enantiomers (+)-**1** and (-)-**1** in high optical purity, and their chiroptical properties were experimentally examined. Other optical properties such as absorption and photoluminescence in solutions have been also examined experimentally and an emission in the visible region was noted.

Key words: Helicene, Photolysis, Cyclization, Photooxidation, Optical properties

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Photochemical evaluation of nitrile α, β-insaturated through a photooxidation pathway in benzo[c]phenanthrenic

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Polycyclic aromatic molecules present a class important nowadays. These aromatic molecules have attracted special attention due to their stability of the π-conjugated skeleton and the presence of inherent helical chirality. Recent developments in helicene chemistry have focused on the synthesis and optical resolution of new helicene derivatives [1] as well as on asymmetric catalysts [2], molecular recognition [3], and chiroptical functionalities. This work is about a design and synthesis of phenanthrene derivatives which is carried out by incorporating nitrile groups. [4]Helicenes was obtained in good overall yields involving mild experimental conditions and easy purification. Photophysical properties of these tetracyclic systems have been evaluated through UV–visible absorption and fluorescence spectroscopies.

Key words: Photolysis, Cyclization, Photooxidation, Optical properties

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Study of functional theories of the density of non-covalent interactions in [1-(2-aminoethyl) pipezinium] tetrabromidomercurate(II) monohydrate : analyzes of molecular structure, ELF, RDG, AIM, MEP, HUMO-LUMO and molecular docking studies»

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The molecular structure of $(C_6H_{17}N_3)[HgBr_4].H_2O$ was reported using the density functional theory method (DFT)/B3LYP and 6-311++G(d,p) as a basis set. The inter and intramolecular interactions of the non-covalent interactions in the compound were analyzed by RDG approaches with reduced density gradient, ELF electron localization function, topological AIM and molecular electrostatic potential MEP. Thus the HOMO and LUMO analyzes make it possible to explain the load transfer within the structure. The geometrical optimization, electronic, topological and biological activities were theoretically studied using DFT and the potential biological activities were investigated by using molecular docking analysis. These analyzes were used to determine the structural properties in order to assess the stability of the molecule.

Key words: DFT calculations, ELF, AIM, MEP, RDG, HOMO–LUMO and molecular docking analysis.

Elaboration, crystal structure, physico-chemical characterization and theoretical investigation of a new non-centrosymmetric Sn(IV) complex $(C_4H_{12}N_2)[SnCl_6]\cdot 3H_2O$

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The X-ray structure of a new hybrid organic-inorganic compound, piperazine-1,4-diium hexachlorostannate(IV) trihydrate $(C_4H_{12}N_2)[SnCl_6]\cdot 3H_2O$ has been determined. The title compound crystallizes in the chiral orthorhombic space group $P2_12_12_1$ with a = 9.6006(3) Å, b = 11.4705(5) Å, c = 14.3876(4) Å and with Flack parameter equal to 0.44(6). The atomic arrangement can be described by alternation of organic chains and inorganic ribbons. The crystal packing is stabilized by hydrogen bonds and van der Waals interactions. The 3D Hirshfeld surfaces and the associated 2D fingerprint plots were investigated for intermolecular interactions. The powder XRD pattern was in good agreement with the results of single crystal structure analysis. Scanning electronic microscopy (SEM) and energy-dispersive X-ray (EDX) were carried out. The vibrational absorption bands were identified by IR spectroscopy and were also calculated by Density Functional Theory (DFT). A good consistency was found between the calculated and experimental data. The optical property of the crystal was studied using optical absorption UV–visible and exhibited one large band at 250 nm, and photoluminescence measurements showed emission at 409 nm. Finally, the thermal analysis shows that this compound is stable below 380 K.

Keywords: Sn(IV) complex, Hirshfeld surface, X-ray diffraction, DFT calculation, Luminescence, property.

PREPARATION, SPECTROSCOPIC CHARACTERIZATION AND MOLECULAR STRUCTURE OF THE (3,5-LUTIDINE) (*MESO*-TETRATOLYLPORPHYRINATO) MAGNESIUM(II) COMPLEX

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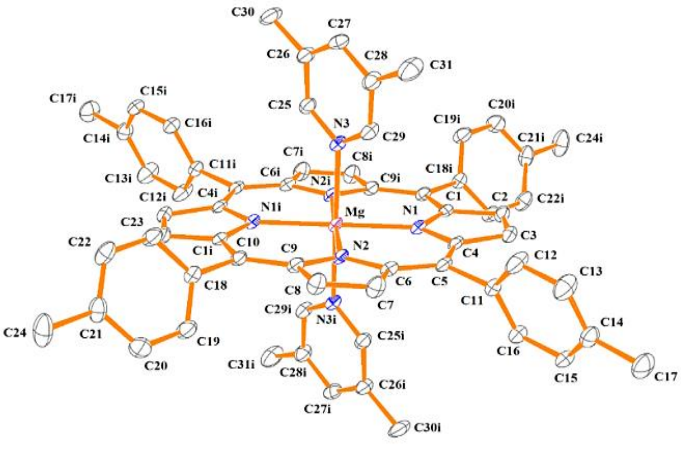
Porphyrins and metalloporphyrins have been studied in several research areas, especially because porphyrins species are involved in numerous biological systems such as the synthetic process of chlorophylls, energy transfer and as prosthetic groups on hemoproteins, such as the hemoglobin and cytochromes. In this communication we describe the synthesis and the spectroscopic characterization of a new porphyrin magnesium(II) with the 3,5-lutidineaxial ligand with a formula [Mg(TTP)(Lut)$_2$] (**I**).This Mg(II) metalloporphyrin was characterized by UV-Vis, fluorescence, IR and mass spectrometry. The cyclic voltammetry data was also investigated. Crystals of the title complex were obtained by slow diffusion of hexanes through the dichloromethane solution containing complex (**I**). Single crystal X-ray study of the [Mg^{II}(TTP)(Lut)$_2$] complex has been performed on a D8 VENTURE Bruker AXS. This coordination compound crystallizes in the monoclinic system (space group *P-1*) with the cell parameters: a = 9.373(7) Å; b = 11.5314(6)Å; c = 12.1821(8) Å; α = 88.316(2)°; β = 76.909(2)°, and γ = 74.756(2)°.

Key words: Magnesium(II) porphyrin complex; X-ray molecular structure; Photophysical properties;Cyclic voltammetry.



Ortep Diagram the [Mg^{II}(TTP)(Lut)$_2$] complex

Enhanced Dye Removal by Diatomite/Cationic Nanoholocellulose Nanocomposite: Modeling, Kinetics, Equilibrium, Thermodynamics, and Reusability Studies.

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Large amounts of dye wastewater are produced in many industries, such as textiles, paper and pulp, petroleum, clothing, printing, painting, etc [1]. This industrial wastewater resulting from the indiscriminate discharge of toxic dyes has caused environmental concerns over the past decades In this context, a novel diatomite/Cationic Holocellulose Nanofibers composite (DT/C-NFH) was synthesized successfully to remove IC from aqueous media. Analysis of pH zero point charge (pHpzc), scanning electron microscopy (SEM), and Fourier transform infrared spectroscopy (FTIR) were performed. The effects of solution pH (2-11), temperature (10-50°C), initial concentration (50-200 mg/L) and contact time were studied. The adsorption processes agreed well with the pseudo-second-order kinetic model and the Freundlich isotherm model. Thermodynamic studies have shown the exothermic nature of the overall adsorption process. Desorption tests showed that the IC removal efficiency decreased after six regeneration cycles.

Key words: Nanoholocellulose, Diatomite, nanocomposite, Indigo Carmine.

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The coordination behavior of a new hybrid compound $(C_6H_{14}N)_2[CdCl_4]$: Structural features, physicochemical characterization and theoretical study

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This paper deals with the crystal structure of the new non-centrosymmetric organic-inorganic hybrid material, $(C_6H_{14}N)_2[CdCl_4]$. Single crystal X-ray diffraction analysis shows that this compound crystallizes in the orthorhombic system, with the space group $Cmc2_1$ and the following parameters a = 27.257 (2) Å, b = 8.3560 (6) Å, c = 7.8872 (5) Å, V = 1796.4 (2) Å^3 and Z = 4. The structure provides a new interesting example of infinite inorganic chains of $[CdCl5]_n$ following the c crystallographic direction. The monoprotonated cyclohexyl-ammonium cations are linked to the anions via electrostatic, multiple bifurcated N—H…Cl hydrogen bonds and van der Waals interactions. To support experimental results, DFT calculations have been accomplished via the B3LYP method with 6–311++ G (d,p) and LANL2DZ basis set on molecular geometry, vibrational and electronic properties. The non-covalent interactions were studied through AIM and RDG analysis and quantitatively using the Hirshfeld surfaces (HS) associated with 2D fingerprint plots. The NLO properties have been also investigated by DFT and compared to the urea reference.

Keywords: Cd(II) complex, X-ray diffraction, DFT calculations, AIM, RDG, NLO.

SYNTHESIS, SPECTROSCOPIC AND STRUCTURAL CHARACTERIZATION OF THE BIS(FORMATE) CHROMIUM(III) PORPHYRIN COORDINATION COMPOUND

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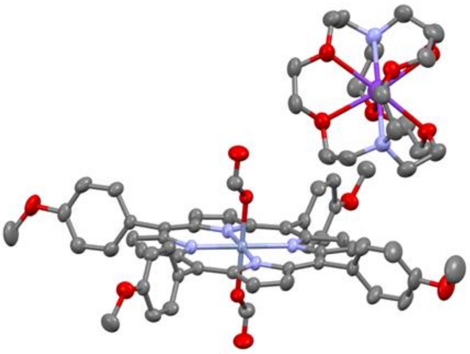
Although chromium (III) porphyrins are not naturally occurring substrates in biological systems, their chemical and photochemical properties have attracted the attention of scientists since the end of the sixties. **[1-3]** In the present study, we describe the synthesis and substitution reactions of the chloride chromium(III) porphyrins [Cr^{III}(TMPP)Cl] with the anionic potassium formate ligands. According to X-ray analysis, this is a rare example of metalloporphyrins bearing two axial format ligands with a formula [K(crypt-2.2.2)][$Cr^{III}(TMPP)(OCHO)_2]\cdot CH_2Cl_2$ (complex **I**). This compound crystallizes in the monoclinic crystal system with the non-centrosymmetric space group *P 21/n* with the cell parameters a = 15,389(3) Å, b = 26,922(5) Å, c = 15,619(3) A°, α = 90, β = 91,76(3), γ = 90, and V = 6468(2) $Å^3$, Z = 4. Further information on weak intermolecular contacts is provided by Hirshfeld surface analysis. The complex was also characterized in solution by IR, UV–vis, fluorescence, IR, ESI-HRMS mass spectrum and electrochemical studies.



Molecular structure of [$Cr^{III}(TMPP)(OCHO)_2]^-$ ion complex.

Key words: Chromium(III) porphyrin complex; X-ray molecular structure; Photophysical properties; Cyclic voltammetry.

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Structural, electronic properties and molecular docking investigations of the Leukopoiesis stimulating activity of 4,6-dimethyl-1,6-dihydropyridin-2-amino nitrate

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A new hybrid organic-inorganic material: 4,6-dimethyl-1,6-dihydropyridin-2-amino nitrate has been synthesized and characterized by X-ray diffraction technique and Fourier transform infrared (FT-IR) spectroscopy. The structural, electronic and topological properties were investigated by a theoretical approach along with a validation of vibrational properties using the dispersion-corrected density functional theory (DFT-D3) method (PWPB95 D3(BJ)) along with the meta-generalized gradient approximation (Meta-GGA) functional of the Minnesota family (M06-2x). All computations were conducted with the 6-311++G(2df,2pd) and def2-TZVP basis set. A visual study of weak interactions was achieved via Bader's Quantum theory of atoms in molecules (QTAIM), non-covalent interaction (NCI) using the promolecular electron density approach, Electron localization function and molecular electrostatic potential. Natural orbital analysis and charge delocalization were equally considered to comprehend and appraise the various intermolecular stabilization mechanisms in the studied system. Molecular electronic properties (quantum descriptors) were also investigated to assess the reactive nature and stability index of the synthesized structure. Due to the ionic nature and structural similarity of the studied compound with methyluracil, molecular docking investigations of the Leukopoiesis stimulating activity of were assessed and compared with a series of Krebs 'regulating enzymes. These studies divulged that the synthesized compound has the potential to stimulate the synthesis of nucleic acids, proteins, cell division and leukopoiesis.

Keywords: X-ray diffraction study; Natural Bond Orbital, Molecular docking; Molecular electronic properties; leukopoiesis stimulant

Molecular docking and DFT calculations of bis(2-amino-4-methoxy-6-methylpyrimidinium) bis(μ_2-chloro)-tetrachloro-di-copper(II)

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Due to biological importance and industrial applications of aminopyrimidines [1,2], we report the synthesis, the single crystal X-ray diffraction analysis, the Density Functional Theory (DFT) calculations and the spectroscopic study of the new hybrid compound (2-amino-4-methoxy-6-methylpyrimidinium) bis(μ_2-chloro)-tetrachloro-di-copper(II). DFT is a quantum-mechanical approach for calculating the electronic structure of atoms, molecules, and solids in chemistry and physics and it is very important for organic and inorganic molecules. The DFT calculations which perform in this study include the calculation of Mulliken loads, Frontier Orbitals, Molecular Electrostatic Potential (MEP) surfaces and determination of the optimized structure. The AutoDock Vina program was used to perform molecular docking between complex ligand and HSP90/PDB: 5LRZ. The title molecule was the most promising hit chemical, and the receptor PDB: 5LRZ (2.00 Å) proved to be a better receptor for this study, maybe due to its higher resolution value. We can say that it is very effective in inhibition PDB: 5LRZ. Drug-likeness profile and *in silico* ADME features of the compound were examined. The investigated compound exhibits a strong pharmacokinetic property, with oral bioavailability and good absorption, according to drug-likeness and ADME properties and no violation of Lipinski rules occurred or results satisfied the Lipinski's rule of five

Keywords: Molecular docking ; Drug-likeness ; ADME properties ; DFT calculations

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Coordination Behavior and Biological Activity of Some Transition Metal Complexes with Potassium sorbate and Sodium benzoate Ligands

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The aim of this work is to synthesize, characterize and evaluate the biological activity of two food preservatives : Potassium sorbate and Sodium benzoate and their metal-Co(II), Ni(II) Cu(II) and Zn(II) chelates. The newly chelates were characterized by elemental analysis, IR, mass and ^{1}HNMR spectra, thermogravimetric analysis (TGA) and biological activity. The antibacterial and antifungal activities of the ligands and its metal complexes were screened against bacterial species (Staphylococcus aureus, Bacillus subtilis and Escherichia coli) and fungi (Candida albicans). Ampicillin and amphotericin were used as references for antibacterial and antifungal studies. The activity data show that the metal complexes have a promising biological activity comparable with parent free ligand against bacterial and fungal species.

Keywords : Potassium sorbate, Sodium benzoate, Transition Metal Complex, Antibacterial Activity.

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Synthesis of new fluorescent pyrazolines via the NITEC reaction

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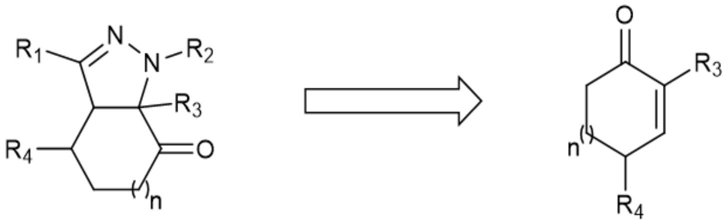
In this work we have focused on the synthesis of a series of pyrazoles via the NITEC[1] (nitrile imine-mediated tetrazole-ene cycloaddition) reaction between tetrazoles and functionalized cyclenones. The latter were subjected to absorbance and fluorescence measurements in order to use them as ligands for heavy metal complexation reactions and for the evaluation of their biological activity[2].



NITEC Reaction

Key words: NITEC, Cycloaddition, Pyrazole, Cyclénones.

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Synthesis, caractérisation, and optical properties of the novel organic-inorganic hybrid material bis (4-fluorobenzylammonium) tetrachloridozincate(II): $[C_7H_9NF]_2ZnCl_4$

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A novel organic-inorganic hybrid material $[C_7H_9NF]_2ZnCl_4$ has been obtained by slow evaporation at room temperature and characterised by single –crystal X-ray diffraction. The structure of the title bis (4-fluorobenzylammonium) tetrachloridozincate (II) crystallizes in the monoclinic space group $P2_1/n$ with the following cell parameters: a = 15.1956(10) Å, b=7.2108(3), c = 36.103(2) Å, β=93.100(6) V = 3950.1 Å3 and Z = 8. The crystal structure was solved and refined to R=0.0514 with 3688 independent reflections. The atomic arrangement can be described by a tetrahedral $[ZnCl_4]^{2-}$ anions and 4-fluorobenzylammonuim $[C_7H_9NF]^+$ cations which are interconnected by hydrogen bonding contact N-H...Cl and Van Der Waals interactions, in which they may be effective in the stabilization of the crystal structure, so as to build layers developing parallel to (b,c) planes.The infrared (IR) and Raman spectra of the title compound were recorded at room temperature and then analyzed. The optical study was also investigated by UV–vis absorption.

Keywords: Organic-inorganic hybrid material; chemical synthesis; Single crystal X-ray diffraction; Crystal structure; optical absorption; vibrational study.

Growth, single crystal investigation and Physico-chemical Properties of Thiocyanate Coordination Compounds based on Cadmium transition metal precursor

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A novel hybrid organic-inorganic compound based on 1,4-Dimethylpiperazinium $[(C_6H_{16}N_2)Cd(SCN)_4]$, was prepared by evaporation crystal growth method at room temperature. This complexe was characterized by X-ray crystal structure, spectroscopic methods such as the FTIR analysis supported for the presence of surface ligands groups of thiocyanates and to identify the vibrational absorption bands. Optical studies such as the UV-visible spectroscopy showed the optical transparency of the complexe to have the cutoff wavelength at the range of 346 to 579 nm. Thermal analyses were also occurred in the range of [273–600 K] and showed the decomposition of the complexe.

Based on the results of these techniques, the formation of the desired complexe was confirmed. Hence, the piperazinium ring adopts a slightly distorted chair conformation which is more stable because it does not have any steric hindrance or steric repulsion between the hydrogen bonds and which favors the entity coordination. Intermolecular interactions were investigated by Hirshfeld surfaces and contact enrichment tools. In the crystals, Extensive intermolecular interactions have been used in the self-assembly of motifs, ranging from strong H-bonds, the components are linked mainly by N-H…S hydrogen-bonding interactions, resulting in a three-dimensional network.

The arrangements of the anions and cations in the solids are governed not only by the size and symmetry of the cations, but also by the non-covalent bonds in the crystal structures.

Key words: Inorganic chemistry, Materials chemistry, DRX, crystal structure, heterocyclic aromatic bases, anti-oxidant behavior.

Rheological and physicochemical properties of polysaccharides extracted from *Opuntia* (Cactaceae)

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The extraction of polysaccharides was carried out from *Opuntia* (Cactaceae) cladodes with characteristics adapted to be applied in different fields such as cosmetic and pharmaceutical industry, the packaging sector, etc. In this work, the extraction and precipitation of polysaccharides from *Opuntia* (Cactaceae) cladodes were done using green solvent of precipitation. After depolymerization (by acid hydrolysis) and sugar analysis using ionic chromatography, the polysaccharide extracts have four main monomers: L-arabinose, D-galactose, D-glucose and D-xylose. The rheological behavior of the mucilage solutions greatly depends with the concentration, molecular weight and particle size of the dispersed particles. Based on these results, the polysaccharide extracts obtained from *Opuntia* (Cactaceae) could be used as polymer filler for many applications.

Key words: polysaccharides, cladodes, rheological behavior, particle distribution

Synthesis, spectroscopic and structural of manganese(III) porphyrin complex: $[Mn^{III}(TTP)(DMAP)_2](SO_3CF_3)\cdot 3/2(CHCl_3)$

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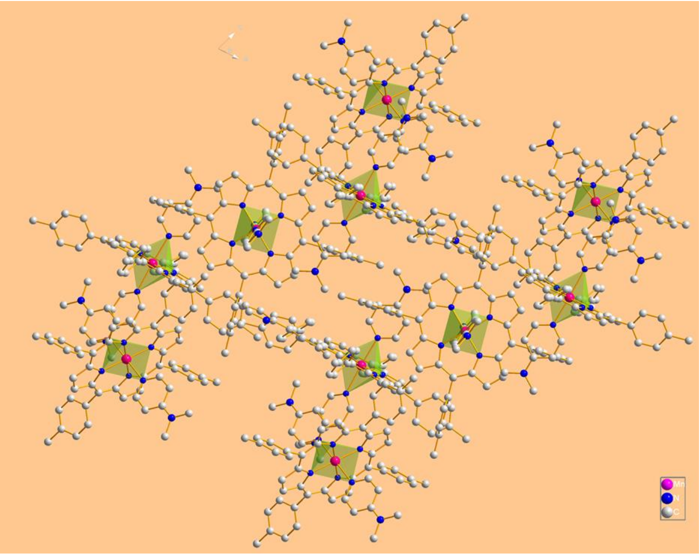
Catalysis has been a topic of interest since its discovery in chemistry centuries ago. Porphyrins and metalloporphyrins occupy an important role in this field specifically manganese(III) porphyrin complex[**1–3**].

This work aims at synthesizing a novel metalloporphyrin of manganese(III). with the formula: $[Mn^{III}(TTP)(DMAP)_2](SO_3CF_3)\cdot 3/2(CHCl_3)$ (**I**), where TTP is the *meso-tetra(para-methylphenyl)porphyrin* and DMAP is 4-dimethylaminopyridin.

Compound (**I**) was prepared by the reaction of the $[Mn^{III}(TTP)(SO_3CF_3)]$ with an excess of 4-dimethylaminopyridin in chloroform. This complex was characterized by UV-visible, IR, mass spectrum, cyclic voltammetry, and X ray crystallography techniques.

The data collection was made at low temperature (150 K) and complex (**I**) crystalizes in the triclinic crystal system with the *P-1* space group. The cell parameters are : a = 16.622Å, b = 16.792Å, c = 26.460Å and α = 86.54Å, β = 72,24Å, γ = 63.80 Å, V = 6287Å^3 and Z = 4 with R_1 = 0.0814 and wR_2 = 0.1989.



View showing the manganese polyhedral in complex **I**.

Key words: Manganese(III) porphyrin; Single crystal X-ray molecular structure; UV-visible; IR; cyclic voltammetry.

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Synthesis, X-ray structure, DFT investigation and molecular docking of novel ligand: A cyclic polyamide with anti HIV-1 (RT), antiplatelet and anticoagulant activities

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1,3,5-tricyclohexyl-1,3,5-triazinane-2,4,6-trione was obtained with high chemoselectivity and excellent yield, through an efficient and simple cyclotrimerization of isocyanatocyclohexane performed at room temperature and under mild reaction condition. Single crystal X-ray diffraction was used to investigate its molecular structure. DFT calculations, intrinsic reaction coordinate (IRC), Wiberg bond index and FOMs computational studies were performed to get more insights into the stability and the reaction mechanism. Furthermore, the molecular docking was successfully employed to suggest that the ligand selected showed antiplatelet and anticoagulant activities. Further, the molecular interactions of test T*Cy*-TAZTO were investigated by molecular docking studies against selected targets of blood aggregation and coagulation pathways. Test compounds possessed high affinity for COX-1, GPIIb/IIIa, GP-VI, PG-I2 and F-X receptors. Molecular docking was performed to suggest the best HIV-1 resistance against HIV-1 reverse transcriptase (RT) might be responsible for anti-tyrosinase property. [1]

Key words: Cyclotrimerization, DFT calculations, Wiberg bond indices, Molecular Docking

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Reference

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Growth, Single crystal investigation, Hirshfeld surface analysis, DFT studies, Molecular docking, Physico-chemical characterization and, in vitro, antioxidant activity of a novel hybrid complex

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Interaction of the diphosphoric acid ($H_4P_2O_7$) and organic ligand (3.4-dimethylaniline) with transition metal ions, cobalt (II) chloride leads to the formation of novel stable Co(II)-diphosphate cluster with empirical formula $(C_8H_{12}N)_2[Co(H_2P_2O_7)_2(H_2O)_2].2H_2O$. The structure of the synthesized material was confirmed by single crystal XRD at 120 K. The crystal was plate and crystallized in the triclinic $P\bar{1}$ space group with a = 7.5340(4) Å, b = 7.5445(4) Å, c = 13.6896(8) Å, α = 84.215(5)°, β = 76.038(5)°, γ = 74.284(5)°, V = 726.38(7) Å^3 and Z = 1. Full-matrix least-squares refinement converged at R = 0.035 and Rw = 0.088 for 3636 independent observed reflections. Indeed, the purity phase was confirmed by the powder X-ray diffraction. A detailed analysis of the intermolecular close interactions and their percentage contribution has been performed based on the Hirshfeld surfaces and their associated two-dimensional fingerprint plots. In this context, spectroscopic studies were performed to distinguish the different chemical functional groups and their environments in this molecule. To determine the optical properties, the UV-Visible and luminescence behavior were investigated. The magnetic properties have been investigated in the temperature range 2-300 k. The geometry of the hybrid complex was optimized in the gas phase, using density functional theory (B3LYP) with the 6-31+G (d,p) basis sets, it is found that the calculated and the experimental results were in good consistency. Furthermore, the synthesized product was screened for its antioxidant activities. Molecular docking study was additionally carried.

Keywords: Transition metal; Co(II) diphosphate cluster; Optimized geometry; Magnetic properties; Molecular docking.

Synthesis, crystallographic structure and Hirschfeld surface analysis of a new tetranuclear anionic bromobismuthate(III): $[C_{12}H_{20}N_2]_2Bi_4Br_{16}.2H_2O$

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This present research makes in attention the synthesis of an organic inorganic hybrid compound with new tetranuclear anionic bromobismuthates with formula: $[C_{12}H_{20}N_2]_2Bi_4Br_{16}•2H_2O$ by slow evaporation at room temperature. It is characterized by X-ray diffraction. Indeed, this compound crystallizes in the monoclinic space group $P2_1/c$ with the following parameters: a = 12.3534(6), b = 24.0296(9), c = 17.8715(8) Å, β = 92.302(5)°, V = 5300.8(4) $Å^3$ and Z = 4. The crystal structure consists of discrete $[Bi_4Br_{16}]^{4-}$ cluster and two kinds of the 2-phenylethylpiperazinium cations. The crystal structure is stabilized through intermolecular N–H…Br, C–H…Br and N–H…O hydrogen bonds and Br…Br interactions. The vibrational absorption bands were identified by infrared spectroscopy. Crystal structure analysis was supported with the Hirshfeld surface (HS) analysis and fingerprint plots enabled the identification of the significant intermolecular interactions. The Hirshfeld surface analysis of intermolecular interactions confirmed that the contacts: Br…H/H…Br and H…H make the largest contribution to the HS and play a dominant role in the crystal structure of the investigated compound.

Key words: X-ray diffraction, tetranuclear, bromobismuthates(III).

Fractionation, characterization and Biological Activities of Tunisian *Capparis spinosa* L.

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Several plants belonging to the genus *Capparis* are the focus of growing interest due to their medicinal properties and singular nutritional [1,2]. In the present study, leaves samples from *C. spinosa* L. were conducted to determine antioxidant and antifungal activities of divers fractions from *Capparis spinosa* L. [3]. The powdered leaves of this plant were extracted by ethanol (80%) solvent and then separated by liquid-liquid extraction. The results of this separation were n-hexane, ethyl acetate, butanol and water fractions. Total phenolic, flavonoid and tanins amounts, radical scavenging as well as reductive properties were determined by well-established chemical and analytical procedures. Furthermore, the fractions were characterized by Pyrolysis–gas chromatography–mass spectrometry (Py-GC-MS) and Fourier Transform Infrared Spectroscopy (FT-IR). The ethyl acetate fraction exhibited the strongest radical scavenging and reductive activities as compared to the other extracts, most probably due to the highest concentration of phenolics. Further analysis by Py-GC-MS showed the ethyl acetate fraction was more enriched in polyphenols (36 %) while the butanol purified fraction from proteins (62 %). The diethyl ether fraction presented significant fungal inhibition efficacy against *Aspergillus niger*. Present data confirm the multipurpose potential of *Capparis spinosa* L. for functional applications or designing bio-based drug formulations.

Key words: *Capparis spinosa* L., L-L extraction, natural products, Py-GC-MS, hydroxyl-aromatic

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Synthesis of new phosphorochloridates and phosphoramidates

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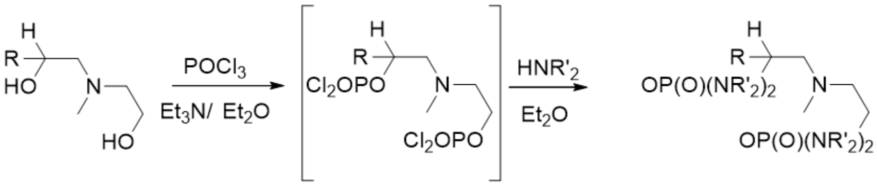
The β-amino alcohols have received much attention in the pharmaceutical industry, given their importance in the treatment of human diseases [1,2]. They can also be used as organophosphorus intermediates which have diverse agrochemical uses [3]. In this work, we describe the synthesis of new β,β'-aminodiols through epoxide opening reaction. The reactivity of these β-aminodiols towards phosphoryl chloride is investigated, which gives a number of corresponding phosphorochloridates and phosphoramidates. These new organophosphorus compounds were characterized by multinuclear (^{1}H, ^{13}C and ^{31}P) NMR and IR spectroscopy. In addition to their possible biological activity, the novel phosphoramidate derivatives could be also used as potential ligands towards different metal ions.



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

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

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Optical Properties of Carbodiimide Bridged Network Structure of $[RE_6O(NCN)_6]$ Clusters in the Structure of $RE_8O(CN_2)_{10}Br_2$, RE=La, Ce, Pr, Nd

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A great number of rare earth (RE) dinitridocarbonates, usually subdivided into carbodiimides $(N =C= N)^{2-}$ and cyanamides $(N\equiv C\text{-}N)^{2-}$ have been studied. The vast growth of this field originates from the development of a most useful synthesis route for this type of compounds, namely the solid-state metathesis reaction [1]. This work reports new rare earth (RE) carbodiimides having the formula $RE_8O(CN_2)_{10}Br_2$ which were synthesized by solid-state metathesis reactions. The structure determinations and refinements, based on single-crystal X-ray diffraction data, are performed with the space group $P\bar{3}c1$ [2]. Homologous compounds with RE=La, Ce, Pr, and Nd are assigned isotypically. The refined crystal structure appears most unusual for rare earth carbodiimide compounds. The most remarkable feature in the crystal structure is the centrosymmetric $[Re_6O]$ cluster core that is interconnected by carbodiimide (N=C=N) ions into a complex network structure, and contains additional RE^{3+} ions in the structure. Crystals of the compounds show characteristic colors of their corresponding RE^{3+} ions and behave stable in air. $Ce_8O(CN_2)_{10}Br_2$ is a photoluminescent material that is showing a broad and efficient emission band in the yellow region of the visible spectrum.

Key words: Solid-state metathesis, Carbodiimide, Rare earth, Luminescence, Structure elucidation, cluster.

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Synthesis and characterization of an unexpected mixture of two complexes obtained from reaction between tin(IV) chloride and bis-(acrylic α-aminophosphonates)

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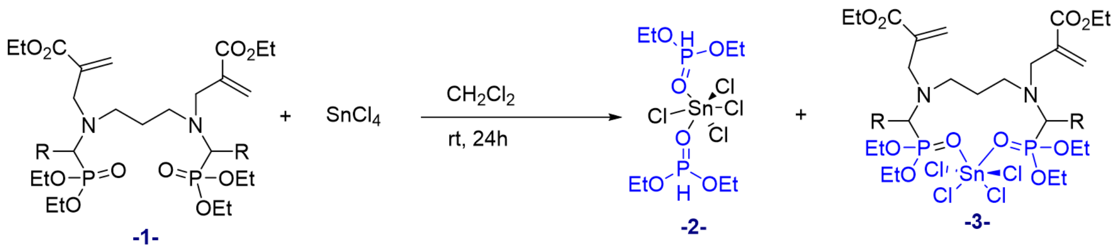
Phosphonates are known for their broad spectra of biological activities, they have been used as therapeutic agents for the treatment of bone disorders, hypocalcemia and osteoporosis. [1-3]. We have recently prepared a new series of bis-(acrylic α-aminophosphonates) (**1**) from a coupling reaction between bis-(aminophosphonates) and α-(bromo)methylacrylate. The coordination chemistry of these bisphophonates where explored through reaction of bis-(acrylic α-aminophosphonates) (L) and tin tetrachloride in anhydrous CH_2Cl_2. An unexpected mixture of two complexes: $[SnCl_4L]$ (**2**) and $[SnCl_4L'_2]$ (**3**) {L' = $(C_2H_5O)_2P(O)H$} was obtained. These adducts were characterized using multinuclear (^1H, ^{13}C, ^{31}P, ^{119}Sn) NMR spectroscopy.



Keywords: Bis-(acrylic α–aminophosphonates), tin(IV) chloride, NMR spectroscopy.

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Synthesis, empirical and DFT calculations of a new cobalt complex: $(C_6H_{14}N)_3[CoCl_4]Cl$

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The aim of this work is the preparation and the crystallization of new organic-inorganic hybrid compound including cyclohexylamine and $[CoCl_4]^{2-}$, $(C_6H_{14}N)_3[CoCl_4]Cl$. Our compound has been studied by single-crystal X-ray diffraction (XRD), IR and TG-DTA examination. The XRD investigation allows to structurally distinguish our material by its monoclinic system and $P2_1/n$ space group through the lattice parameters a = 15.2645 (12) Å, b = 10.0843 (7) Å, c = 17.4450 (13) Å, β = 95.957 (3)° and Z = 4. The crystal arrangement shows inorganic entities of $[CoCl_4]^{2-}$ and chloride spreading in $(10\bar{1})$ planewhich are connected to cyclohexylammonium cations via N(C)—H…Cl H-bonds. The experimental studies on the compound have been accompanied computationally by DFT calculations via the B3LYP functional. The intermolecular interactions using were quantitatively studied by 3D-HS coupled with two dimensional fingerprint (2D-FP) plots and analyzed by the RDG and AIM approaches. The electron localization function (ELF) investigation was performed to explain the chemical structure of $(C_6H_{14}N)_3[CoCl_4]Cl$.

Keywords: Hirshfeld surfaces; ELF; AIM; RDG; NCI.

Synthesis, crystal structure, Hirshfeld surface analysis and characterization of a new Decavanadate complex with 2-amino-4-methyl-thiazol

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A novel decavanadate cluster templated with organic cations, $(C_4H_6N_2S)_4[H_2V_{10}O_{28}].2H_2O$ (2A4MTV10) has been synthesized in aqueous solution and characterized by single crystal X-Ray diffraction, IR, and UV Vis spectroscopies. The X-ray structure determination revealed the discrete decavanadate cage-like clusters $[H_2V_{10}O_{28}]^{4-}$. The asymmetric unit is composed of decavanadate biprotonated $[H_2V_{10}O_{28}]^{4-}$ anions, two 2-amino-4-methylthiazol $(C_4H_6N_2S)^+$ cations and two water molecules. The cohesion is provided by multiple hydrogen bonds (O-H---N, O-H---O and N-H---O) involving water molecules, organic molecules, and Vander Waals bonds for the connection between the organic molecules. The IR spectra proved the presence of organic cations, decavanadate $[H_2V_{10}O_{28}]^{4-}$ groups and water molecules. Intermolecular interactions were investigated by Hirshfeld surfaces and contact enrichment tools. The optical study of 2A4MTV10 was performed to define the optical band gap and to determine the blue fluorescent behavior of the grown crystals. Thermal decomposition of the sample in the temperature range of 30-700°C revealed that it decomposes in three stages and results in a vanadium oxide residue from the progressive volatilization of decavanadate.

Key words: Decavanadate, Synthesis, Single-crystal XRD

Synthesis and characterization of ZnAl-layered double hydroxide as an efficient adsorbent for MO removal from aqueous solution

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In recent decades, dyes are used in different processes like textile industries. They are characterized by their toxicity and carcinogenic effects on human health and aquatic system [1]. The layered double hydroxide (HDL) also known as anionic clays are considered as an important class of ionic lamellar solids. The properties of LDH made them a candidate in various application such us adsorption of dyes [2]. In this context ZnAl-LDH was synthesized using the co-precipitation method at pH 10 and characterized by XRD, FTIR, XPS, TGA and N_2-adsorption-desorption then test its performance as an adsorbent to eliminate methyl orange (MO) from aqueous solution. The effect of pH, concentration of MO solution and equilibrium time was investigated. In addition, adsorption isotherms and mechanism are determined.

Key words: dyes, adsorption, layered double hydroxide, isotherms

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New phosphotetradecavanadate with 2-picolinium: crystal structure, stability and binding interactions with bio-macromolecules

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Polyoxdovanadates (POVs) are a relevant subfamily of POMs and have been attracting increasing attention. The various coordination geometries and cluster sizes demonstrated by vanadium oxide polyhedral shapes and the different oxidation states that vanadium can adopt give rise to a great variety of different architectures [**1**]. POVs show more structural flexibility featuring tetrahedral [VO_4], square pyramidal [VO_5], and octahedral [VO_6] units [**2**]. In addition, POVs are often described as being “less stable” than tungstates and molybdates, which is most likely due to a combination of their structural flexibility, complex protonation chemistry, possible hydrolysis and redox activity [**2**]. Namely vanadate is well known to be an inhibitor Na^+/K^+- ATPase **[3]** and POVs have been being discussed to have ion pumps such as Na^+/K^+-ATPase and Ca^{2+}-ATPase as one of the possible targets in their biological action [**4].**
New bicapped Keggin polyoxovanadates with organic cations, $(C_6H_8N)_6(NH_4)[H_2PV_{14}O_{42}].2H_2O$, ($PV_{14}O_{42}$ = PV14, C_6H_7N = 2-picoline) was synthesized. The compounds are isolated and characterized in the solid state and in solution by elemental analysis, powder X-Ray diffraction, FTIR, UV-Vis, ^{51}V NMR and fluorescence spectroscopies. Further confirmation of the PV14 structures was obtained by single-crystal X-ray diffraction studies. This compound crystallized in a Triclinic system, P-1 space group with the cell parameters: a = 9.8287(2) Å, b = 12.4089(3) Å, c = 13.1873(4) Å, α=91.552(3)° β = 96.429(2) ° and γ = 93.773(2)°. Upon addition of compound to solutions of DNA changes were observed in the UV-Vis absorption and circular dichroism spectra, and strong quenching was recorded by fluorescence spectroscopy upon adding compound to solutions of bovine serum albumin.

Key words: Phosphotetradecavanadate, X-Ray diffraction, DNA interaction, BSA binding

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