

20th Tunisia Chemistry Conference



Organized by the

Tunisian Chemical Society



16-20 December 2018

Bel Azur Hotel, Hammamet - Tunisia

**Abstracts of Lectures and Communications
List of Participants**

Sunday 16 December 2018	
14.30	Welcoming participants, distribution of documents and check in
Monday 17 December 2018	
09.00 - 10.05	TCC 2018 Opening Ceremony
09.30 - 10.05	Plenary Lecture 1 <u>Philippe KAMALAPRIJA</u> <i>Chemical Abstracts Service</i>
10.10 - 10.45	Invited Lecture 2 <u>Mohamed M. CHEHIMI</u> & <u>Nabil KHELIFI</u>
10.45 - 11.30	Coffee break + Poster Session 1 (P1 - P47)
11.30 - 12.45	Oral Communications - Session 1 : OC01-OC05
13.00	Lunch
14.30 - 15.05	Plenary Lecture 3 <u>Noureddine JOUINI</u> <i>Université Paris 13, France</i>
15.15 - 16.30	Oral Communications - Session 2 : OC06-OC10
16.30 - 17.30	Coffee break + Poster Session 2 (P48 - P94)
17.30 - 18.45	Oral Communications - Session 3 : OC11-OC15
19.30	Dinner
Tuesday 18 December 2018	
09.00 - 09.35	Plenary Lecture 4 <u>Adel NEFZI</u> <i>Torrey Pines Institute, Florida, USA</i>
09.40 - 10.15	Plenary Lecture 5 <u>Antoine THILL</u> <i>University Paris-Saclay, France</i>
10.15 - 11.00	Coffee break + Poster Session 3 (P95 - P141)
11.00 - 12.30	Oral Communications - Session 4 : OC16-OC21
13.00	Lunch
14.30 - 15.05	Plenary Lecture 6 <u>Hédi MATTOUSSI</u> <i>Florida State University, USA</i>
15.15 - 16.30	Oral Communications - Session 5 : OC22-OC26
16.30 - 17.30	Coffee break + Poster Session 4 (P142 - P188)
17.30 - 19.00	Oral Communications - Session 6 : OC27-OC32
19.30	Dinner
Wednesday 19 December 2018	
09.00 - 09.35	Plenary Lecture 7 <u>Salim BARKALLAH</u> <i>Cambridge Isotope Laboratories, USA</i>
09.45 - 10.45	Oral Communications - Session 7 : OC33-OC36
10.45 - 11.30	Coffee break + Poster Session 5 (P189 - P235)
11.30 - 13.00	Oral Communications - Session 8 : OC37-OC42
13.00	Lunch
14.00 - 16.30	Ordinary General Assembly of the Tunisian Chemical Society
17.00	Election of the new National Bureau of the Tunisian Chemical Society Counting of votes and announcement of results
20.30	C o n f e r e n c e D i n n e r
Thursday 20 December 2018	
09.00 - 09.35	Plenary Lecture 8 <u>Anis TLILI</u> <i>Université Lyon1, France</i>
09.45 - 11.00	Oral Communications - Session 9 : OC43-OC47
11.00 - 11.45	Coffee break + Poster Session 6 (P236 - P280)
12.00	Awards Distribution and Closing Ceremony
13.00	Lunch and Check out

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

FOREWORD

It's a very exciting time for the Tunisian Chemical Society to celebrate its fortieth anniversary, which is another milestone in TCS's achievements that demonstrates that TCS has been able to maintain the coveted goals and objectives throughout this period of 40 years. Its commitment and perseverance allowed the Tunisian Chemical Society to approach one of the giants of scientific publisher - Springer - to take in charge the publication of its journal: Chemistry Africa - A Journal of the Tunisian Chemical Society.

Chemistry has grown significantly during the last two decades, and chemicals are a widespread social phenomenon. They have become significantly present in our daily life, whether for food, clothing, being, moving, etc. However, some of them are the origin of some health and environment problems. This fact does not affect their importance in society, since each product corresponds to a need. New compounds and new materials with new properties have always laid the foundation of new technologies that were limited.

It is indeed essential to work to improve the image of chemistry, sometimes altered by some special cases. The chemical industry is of great importance in the world, it has turned to new technologies, using less non-renewable resources to offer cleaner and safe products. It is also a source of innovation in most technologies, including health, communications, energy savings and the fight against climate change.

Here comes the role of research and researchers by designing and developing new molecules and new products or by improving existing ones; hence the importance of holding conferences to allow to those researchers to present their latest and most innovative work in various fields of chemistry.

Tunisia Chemistry Conference - TCC2018 - is open to young chemists, physicists and technologists who will be offered opportunities for oral and poster contributions. So, we really appreciate your participation in this conference. Renowned Invited Guests will deliver lectures on hot topics, whilst specific themed sessions will be organized to bring focus attention on the latest developments in different fields and topics of chemistry. Finally, we welcome industrials and Scientific Equipments Exponents to participate and share knowledge in different chemistry technologies.

So I wish all our guests a very pleasant stay in this very lovely resort, in Hammamet.

Pr. Adel MEGRICHE

Chairman of TCC 2018

Scientific Committee

Adel MEGRICHE (Chairman)	University of Tunis El Manar, FST-Tunis
Rym ABIDI	University of Carthage - FSB-Bizerte
Salim BARKALLAH	Cambridge Isotope Laboratories, Andover, USA
Taïcir BEN AYED	University of Carthage, INSAT-Tunis
Hatem BEN ROMDHANE	University of Tunis El Manar, FST-Tunis
Ridha BEN SALEM	University of Sfax, FSS-Sfax
Latifa BERGAOU	University of Carthage, INSAT-Tunis
Faiza BERGAYA	University of Orleans, Orleans, France
Taoufik BOUBAKER	University of Monastir, FSM-Monastir
Béchrir CHAOUACHI	University of Gabès, ENIG-Gabès
Samia CHERIF	University of Tunis El Manar, ISSBAT-Tunis
Safia DJEBBAR	Houari Boumediene University, USTHB, Algiers, Algeria
Mohamed Lotfi EFRIT	University of Tunis El Manar, FST-Tunis
Mama EL RHAZI	University of Hassan II of Casablanca, Morocco
Mahmoud FARHAT	University of Tripoli, Libya
Noureddine JOUINI	University of Paris 13 Nord, Galilee Institute, Villetaneuse, France
Mohamed KHITOUNI	University of Sfax, FSS-Sfax
Latifa LATROUS	University of Tunis El Manar, IPEIM-El Manar
Kamel MABROUK	University of Aix-Marseille, Marseille, France
Hatem MAJDOUB	University of Monastir, FSM-Monastir
Hedi MATTOUSSI	Florida State University, Florida, USA
Younes MOUSSAOUI	University of Gafsa, FSG-Gafsa

Scientific Committee (Continuation)

Hédi M'RABET	University of Tunis El Manar, FST-Tunis
Adel NEFZI	Institute for Molecular Studies, Port Saint Lucie, Florida, USA
Noureddine RAOUAFI	University of Tunis El Manar, FST-Tunis
Farhat REZGUI	University of Tunis El Manar, FST-Tunis
Mehrez ROMDHANE	University of Gabès, Enig-Gabès
Med Abderrahmène SANHOURY	University of Nouakchott, Mauritania
Wajda SMIRANI STA	University of Carthage - FSB-Bizerte
Ezzeddine SRASRA	Technopole Borj Cédria, CNRSM
Kamel TAIBI	Houari Boumediene University, USTHB, Algiers, Algeria
Anis TLILI	Claude Bernard University, Lyon 1, France
Hassib TOUNSI	University of Sfax, FSS-Sfax
Khaled WALHA	University of Sfax, FSS-Sfax

Organizing Committee

Halim HAMMI (Chairman)	Technopole Borj Cédria, CNRSM
Mohamed BELHOUCHE	University of Sfax, FSS-Sfax
Nizar BELLAKHAL	University of Carthage, INSAT-Tunis
Mahmoud CHEMINGUI	University of Gafsa, FSG-Gafsa
Latifa LATROUS	University of Tunis El Manar, IPEIM-El Manar
Amine MNIF	University of Tunis El Manar, FST-Tunis
Mehdi RAMMAH	University of Monastir, FSM-Monastir
Riadh TERNANE	University of Carthage - FSB-Bizerte
Abdelaziz TOUATI	University of Gabès, Enig-Gabès
Imed LAAJIMI	Tunisian Chemical Society

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<i>Sunday 16 December 2018</i>	
14.30	Welcoming participants, distribution of documents and check in
19.30	<i>Dinner</i>

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Monday 17 December 2018 (Morning)				
09.00 - 09.30	Opening Ceremony			
09.30 - 10.05	Plenary Lecture 1 <u>Philippe KAMALAPRIJA</u> <i>Chemical Abstracts Service representative for academic and commercial in Switzerland, Liechtenstein, Algeria, Morocco and Tunisia</i> CAS: The solutions behind the science Solve scientific information challenges			Chair: Mohamed Lotfi EFRIT
10.10 - 10.45	Invited Lecture 2 - Chemistry Africa: A Journal of the Tunisian Chemical Society <u>Mohamed M. CHEHIMI</u> : <i>Executive Editor-in-Chief, ICMPE, CNRS, Université Paris-Est, Marne-la-Vallée, France</i> <u>Nabil KHELIFI</u> : <i>Springer Senior Editor, MENA Program, Springer, Heidelberg, Germany</i> Where are we and where do we stand with ChAf ?			Chair: Halim HAMMI
10.45 - 11.30	Coffee break + Poster Session 1 (P 1 - P 47)			
Oral Communications - Session 1				
	Room A - Chair: Mohamed Toumi		Room B - Chair: Mohamed Khitouni	
	<i>Com.</i>	<i>communicating</i>	<i>Com.</i>	<i>communicating</i>
11.30 - 11.45	OC-01 A	ABID DERBEL Marwa	OC-01 B	ABIDI Raouia
11.45 - 12.00	OC-02 A	AJMI Jihen	OC-02 B	AOUAY Rachida
12.00 - 12.15	OC-03 A	AMMAR Hager	OC-03 B	ARIBI Jihene
12.15 - 12.30	OC-04 A	ASKRI Amira	OC-04 B	BEN SMIDA Youssef
12.30 - 12.45			OC-05 B	FLISS Outaf
Oral Communications - Session 1				
	Room C - Chair: Taicir Mzid Ben Ayed		Room D - Chair: Nizar Bellakhal	
	<i>Com.</i>	<i>communicating</i>	<i>Com.</i>	<i>communicating</i>
11.30 - 11.45	OC-01 C	ABDELLI Abderrahmen	OC-01 D	HIDOURI Mustapha
11.45 - 12.00	OC-02 C	ATOUI Dhieb	OC-02 D	ISSAOUI Chokri
12.00 - 12.15	OC-03 C	AYACHI Hajer	OC-03 D	JABBARI Imen
12.15 - 12.30	OC-04 C	AYADI Sameh	OC-04 D	JALEL Boutheina
12.30 - 12.45	OC-05 C	AZAZIEZ Kamilia	OC-05 D	JENDOUBI Imen
13.00	Lunch			

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Monday 17 December 2018 (Afternoon)				
14.30 - 15.05	Plenary Lecture 3 <u>Noureddine JOUINI</u> <i>Université Paris 13, Sorbonne Paris Cité, Laboratoire des Sciences des Procédés et des Matériaux, CNRS-UPR 3407, Villetaneuse, France</i> Bottom-up strategy combining polyol process and Spark Plasma Sintering process: A novel route to elaborate Dense Nanostructured Materials			Chair: Adel MEGRICHE
Oral Communications - Session 2				
	Room A - Chair: Zakaria El Aoud		Room B - Chair: Abderrahman Sanhoury	
	<i>Com.</i>	<i>communicating</i>	<i>Com.</i>	<i>communicating</i>
15.15 - 15.30	OC-06 A	BAHROUNI Yahya	OC-06 B	GHARSALLAH Mouna
15.30 - 15.45	OC-07 A	BAIZIG Jawaher	OC-07 B	GHRISS Ons
15.45 - 16.00	OC-08 A	BAYAR Imen	OC-08 B	MHALLA Jalel
16.00 - 16.15	OC-09 A	BDEY Seifeddine	OC-09 B	SAIDI Marwa
16.15 - 16.30	OC-10 A	BEJAOUI Abir	OC-10 B	LABIDI Malika
Oral Communications - Session 2				
	Room C - Chair: Farhat Rezgui		Room D - Chair: Mohamed Taieb Ben Dhia	
	<i>Com.</i>	<i>communicating</i>	<i>Com.</i>	<i>communicating</i>
15.15 - 15.30	OC-06 C	BEN HAMOUDA Kaouther	OC-06 D	JRABA Abderraouf
15.30 - 15.45	OC-07 C	SAOUDI Med Marouane		
15.45 - 16.00	OC-08 C	CHIRA Moemen	OC-08 D	KADRI Ines
16.00 - 16.15	OC-09 C	CHNITI Ines	OC-09 D	KAROUIA Amal
16.15 - 16.30	OC-10 C	ELHLELI Hanedi	OC-10 D	KHABBOUCHI Mohamed
16.30 - 17.30	Coffee break + Poster Session 2 (P 48 - P 94)			
Oral Communications - Session 3				
	Room A - Chair: Béchir Chaouachi		Room B - Chair: Taoufik Boubaker	
	<i>Com.</i>	<i>communicating</i>	<i>Com.</i>	<i>communicating</i>
17.30 - 17.45	OC-11 A	BEJAOUI Mehdi	OC-11 B	ZGHAL Imen
17.45 - 18.00	OC-12 A	BELAM Wahid	OC-12 B	ZOUAGHI Med Oussama
18.00 - 18.15	OC-13 A	BEN BARAKET Faiza	OC-13 B	NOUIRA Asma
18.15 - 18.30	OC-14 A	BEN JOMAA Mariem	OC-14 B	SAIDANI Nesrine
18.30 - 18.45	OC-15 A	BEN MBAREK Wael	OC-15 B	ZIDANI Chafika
Oral Communications - Session 3				
	Room C - Chair: Hichem Ben Jannet		Room D - Chair: Fathi TOUATI	
	<i>Com.</i>	<i>communicating</i>	<i>Com.</i>	<i>communicating</i>
17.30 - 17.45	OC-11 C	ESSID Kamel	OC-11 D	KHELFA Tarek
17.45 - 18.00	OC-12 C	FRAY Marwa	OC-12 D	KHITOUNI Nawel
18.00 - 18.15	OC-13 C	GHRAIRI Sondes	OC-13 D	KOUASS Salah
18.15 - 18.30	OC-14 C	HAJLAOUI Amel	OC-14 D	KSIKSI Regaya
18.30 - 18.45			OC-15 D	KAHLOUL Latifa
19.30	Dinner			

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Tuesday 18 December 2018 (Morning)				
09.00 - 09.35	Plenary Lecture 4 <u>Adel NEFZI</u> Torrey Pines Institute for Molecular Studies, Village Parkway, Port Saint Lucie, Florida, USA Combinatorial Chemistry: Concepts, Strategies and Applications			Chair: Mohamed Lotfi EFRIT
09.40 - 10.15	Plenary Lecture 5 <u>Antoine THILL</u> CEA Saclay, UMR 3685 CEA/CNRS, University Paris-Saclay, 91191 Gif-sur-Yvette, France Chemistry of Nanosized Tubular Clay Minerals			Chair: Hatem Ben ROMDHANE
10.15 - 11.00	Coffee break + Poster Session 3 (P 95 - P 141)			
Oral Communications - Session 4				
	Room A - Chair: Ahlem Kabadou		Room B - Chair: Sourour Chaabane	
	Com.	communicating	Com.	communicating
11.00 - 11.15	OC-16 A	BEN MOUSSA Oumaima	OC-16 B	ABIDLI Imen
11.15 - 11.30	OC-17 A	BEN YOUSSEF TRIKI Rym		
11.30 - 11.45	OC-18 A	BOUALLEGUI Thamer	OC-18 B	CHAABANE Laroussi
11.45 - 12.00	OC-19 A	BOUCHOUICHA Hamed	OC-19 B	EL KATEB Marwa
12.00 - 12.15	OC-20 A	BOUGHANMI Sonia	OC-20 B	BOUCHAOUR Mama
12.15 - 12.30	OC-21 A	BOUGUERRA Manel	OC-21 B	ETORKI Abdunnaser
Oral Communications - Session 4				
	Room C - Chair: Ridha Ben Salem		Room D - Chair: Salah Kouas	
	Com.	communicating	Com.	communicating
11.00 - 11.15	OC-16 C	JAMEL EDDINE Naourès	OC-16 D	LABIDI Islem
11.15 - 11.30	OC-17 C	JMAÏ Momtez		
11.30 - 11.45	OC-18 C	MKADMINI Khaoula	OC-18 D	LARBI Tarek
11.45 - 12.00	OC-19 C	KHDHIRI Emna	OC-19 D	LTAIEF Hasna
12.00 - 12.15	OC-20 C	KANZARI MNALLAH Dorra	OC-20 D	MARZOUGUI Basma
12.15 - 12.30	OC-21 C	MAALAOUÏ Ahlem	OC-21 D	MRAD Maroua
13.00	Lunch			

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Tuesday 18 December 2018 (Afternoon)				
14.30 - 15.05	Plenary Lecture 6 Hédi MATTOUSSI Department of Chemistry and Biochemistry, Florida State University, 95 Chieftan Way, Tallahassee, Florida 32306, USA Inorganic Nanocrystals Interfaced with Biological Systems			Chair: Nizar BELLAKHEL
Oral Communications - Session 5				
	Room A - Chair: Mohamed Abdelhedi		Room B - Chair: Younes Moussaoui	
	Com.	communicating	Com.	communicating
15.15 - 15.30	OC-22 A	BOUKETAYA Sabrine	OC-22 B	FAJRAOUI Afef
15.30 - 15.45			OC-23 B	HACHICHA Rahma
15.45 - 16.00	OC-24 A	DABBEBI Rawia	OC-24 B	JAHOUGH RABAI Wafa
16.00 - 16.15	OC-25 A	DAMMAK Khouloud	OC-25 B	HADJ-ZIANE ZAFOR Amel
16.15 - 16.30	OC-26 A	DGACHI Souad	OC-26 B	JARRAY Samira
	Room C- Chair: Houcine Ammar		Room D - Chair: Brahim Ayed	
	Com.	communicating	Com.	communicating
15.15 - 15.30	OC-22 C	MAAZAOUI Abir	OC-22 D	MSETRA Zohra
15.30 - 15.45	OC-23 C	MALEK Rim	OC-23 D	NASRI Rawia
15.45 - 16.00	OC-24 C	MECHI Hanen	OC-24 D	NBILI Wijdene
16.00 - 16.15	OC-25 C	MESSAOUDI Chayma	OC-25 D	NOURI Faten
16.15 - 16.30	OC-26 C	M'HAHAM Mohamed	OC-26 D	OUERGHI Zeineb
16.30 - 17.30	Coffee break + Poster Session 4 (P 142 - P 188)			
Oral Communications - Session 6				
	Room A - Chair: Mehrez Romdhane		Room B - Chair: Wahid Belam	
	Com.	communicating	Com.	communicating
17.30 - 17.45	OC-27 A	DHAHRI Ahmed	OC-27 B	JEBALI Sami
17.45 - 18.00	OC-28 A	DHAOU Mariem	OC-28 B	JEMILI Nouha
18.00 - 18.15	OC-29 A	DHIFI Marwa	OC-29 B	KHADHRI Nisrine
18.15 - 18.30	OC-30 A	DRIDI Wassim		
18.30 - 18.45	OC-31 A	ELFERJANI Atef	OC-31 B	HAZOURLI Sabir
	Room C - Chair: Nouredine Allouche		Room D - Chair: Mohamed Belhouchet	
	Com.	communicating	Com.	communicating
17.30 - 17.45			OC-27 D	REZGUI Eya
17.45 - 18.00	OC-28 C	RAISSI Hanen	OC-28 D	RHOUMA Salam
18.00 - 18.15	OC-29 C	TOUJ Nedra	OC-29 D	SAAD Yosra
18.15 - 18.30	OC-30 C	SGHAIRI Dhouha	OC-30 D	SAIDANI Mohamed Ali
18.30 - 18.45	OC-31 C	SIDHOM Ameni		
19.30	Dinner			

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Wednesday 19 December 2018 (Morning)				
09.00 - 09.35	Plenary Lecture 7 Salim BARKALLAH Group Leader at Cambridge Isotope Laboratories, Andover (Greater Boston area), Massachusetts -USA Stable Isotope Compounds. Support for Technological Advances in Medical Research			Chair: Farhat REZGUI
Oral Communications - Session 7				
	Room A - Chair: Wajda Smirani Sta		Room B - Chair: Olfa Amri	
	Com.	communicating	Com.	communicating
9.45 - 10.00	OC-33 A	ELLEUCHI Sawssen	OC-33 B	KLIDI Nizar
10.00 - 10.15	OC-34 A	FEZAI Ramzi	OC-34 B	MAAOUI Mariem
10.15 - 10.30	OC-35 A	GDAIEM Med Amara	OC-35 B	MAHMOUD Imen
10.30 - 10.45	OC-36 A	GHARSALLAH Sana	OC-36 B	TANDJAOUI Nassima
	Room C - Chair: Mohamed Dammak		Room D - Chair: Walid Rekik	
	Com.	communicating	Com.	communicating
9.45 - 10.00	OC-33 C	TALBI Wassima		
10.00 - 10.15	OC-34 C	RAOUAFI Sondes	OC-34 D	WEDERNI Asma
10.15 - 10.30	OC-35 C	BEJAOUI Marouene	OC-35 D	ZINE ELABIDINE Mohamed
10.30 - 10.45				
10.45 - 11.30	Coffee break + Poster Session 5 (P 189 - P 235)			
Oral Communications - Session 8				
	Room A - Chair: Sami Guiza		Room B - Chair: Mohamed Trabelsi	
	Com.	communicating	Com.	communicating
11.30 - 11.45	OC-37 A	GOUTI Imen	OC-37 B	SAIDI Malek
11.45 - 12.00	OC-38 A	GUESMI Afef	OC-38 B	YAHIA Asma
12.00 - 12.15	OC-39 A	GUESMI Oussama	OC-39 B	HASSEN Sabri
12.15 - 12.30	OC-40 A	HADHRI Mariam	OC-40 B	BOUCHAOUR Tewfik
12.30 - 12.45	OC-41 A	HAJJI Hanen	OC-41 B	BOUSSEHEL Hamida
12.45 - 13.00	OC-42 A	HAMDI Nabil	OC-42 B	HAMMA Amel
	Room C - Chair: Lilia Ktari Dammak		Room D - Chair: Mourad Ben Sik Ali	
	Com.	communicating	Com.	communicating
11.30 - 11.45	OC-37 C	FAKHFAKH Jawhar	OC-37 D	ACHECH Amel
11.45 - 12.00	OC-38 C	ITAIMI DAMMAK Mariem	OC-38 D	JABLI Mahjoub
12.00 - 12.15	OC-39 C	MEDDEB Nadia	OC-39 D	JADLI Imen
12.15 - 12.30			OC-40 D	LOULEB Marwa
12.30 - 12.45	OC-41 C	REJAB Asma	OC-41 D	ALI RACHEDI Mahieddine
12.45 - 13.00	OC-42 C	SADIKI Fatma Zahra	OC-42 D	NAOUS Mohamed
13.00	Lunch			

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<i>Wednesday 19 December 2018 (Afternoon)</i>	
14.00 - 16.30	Ordinary General Assembly of the Tunisian Chemical Society
17.00	Election of the new National Bureau of the Tunisian Chemical Society Counting of votes and announcement of results
20.00	C o n f e r e n c e D i n n e r

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Thursday 20 December 2018 (Morning)				
09.00 - 09.35	Plenary Lecture 8 Anis TLILI Institut de Chimie et de Biochimie Moléculaires et Supramoléculaires, CNRS, Université Lyon1, France Late Stage Fluoroalkylselenolation			Chair: Hatem MAJDOUB
Oral Communications - Session 9				
	Room A - Chair: Latifa Latrous		Room B - Chair: Azaiez Ben Akacha	
	Com.	communicating	Com.	communicating
9.45 - 10.00	OC-43 A	HAMDI Sondes	OC-43 B	BOUAGGA Takwa
10.00 - 10.15	OC-44 A	HAMMAMI Saoussen	OC-44 B	BOUZIDI Souhir
10.15 - 10.30	OC-45 A	HARBAOUI Dhouha		
10.30 - 10.45	OC-46 A	HAMDADOU Nasr-Eddine		
	Room C - Chair: Ikram Chehidi			
	Com.	communicating		
09.45 - 10.00	OC-43 C	HKIRI Shaima		
10.00 - 10.15	OC-44 C	LARIBI Fahima		
10.15 - 10.30	OC-45 C	MANNAI Faten		
10.30 - 10.45	OC-46 C	ALKSKAS Ismail		
11.00 - 11.45	Coffee break + Poster Session 6 (P 236 - P 280)			
12.00	Awards distribution and Closing Ceremony			
13.00	Lunch and Check out			



Philippe **KAMALAPRIJA**



Chemical Abstracts Service representative for academic and commercial in Switzerland, Liechtenstein, Algeria, Morocco and Tunisia

Dr. Philippe Kamalaprija is the Chemical Abstracts Service representative for academic and commercial in Switzerland, Liechtenstein, Algeria, Morocco and Tunisia.

He holds a PhD degree in Organic Chemistry from the University of Geneva. His research was focused on determination of organic structures by NMR. Dr. Philippe Kamalaprija joined CAS in 2011. He has a high computer literacy and a deep knowledge in IT, which allows him to be a high level user of the tools that are used in his activities. He is also certified in Project Management, IT governance and Services Management.

CAS: the Solutions Behind the Science Solve Scientific Information Challenges

Dr. Philippe Kamalaprija

Account Manager, ACS International, Ltd. representing CAS

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TOGETHER WE WILL DO GREAT THINGS

Mohamed M. **CHEHIMI**



*Executive Editor-in-Chief
of Chemistry Africa
ICMPE - CNRS, Thiais, France*

Mohamed M. CHEHIMI is Senior Researcher at the French CNRS. He obtained his PhD degree in physical organic chemistry at the University Paris Diderot in 1988 and joined CNRS in 1989 for a permanent research position. His main research topics involve the design of reactive and functional polymer and nanocomposite coatings. He has spent time and efforts developing aryldiazonium salts as new coupling agents in materials science. The applications encompass adsorbents, electrochemical sensors, reactive fillers, antibacterial surfaces, and electronic devices. He is expert of X-ray photoelectron spectroscopy analysis for a broad range of materials including polymer composites. Dr. Chehimi has supervised over 22 PhD theses and collaborated with academic researchers from 20 countries. He is a reviewer for many international journals from reputable publishers. He has over 270 research papers, 23 book chapters and 3 patents to his credit. He is the editor of three books and guest-edited three themed issues. In 2017 Dr. Chehimi has been appointed Executive Editor-in-Chief of Chemistry Africa by the Tunisian Chemical Society and Springer.

Nabil KHELIFI



*Senior Editor
Earth Sciences & MENA Program
Springer, Heidelberg, Germany*

Nabil KHELIFI received fellowships from START in 2005 and the DAAD from 2006 to 2010 to continue with his Ph.D. studies in marine geosciences at the University of Kiel in Germany. After completing his Ph.D. in 2010, he received two postdoctoral research grants from the DFG to pursue his self-designed research projects at the GEOMAR Ocean Research Centre in Kiel, which involved reconstructing past changes in oceanography and climate in the North Atlantic and the Mediterranean Sea using marine sediment samples retrieved by the International Ocean Drilling Program. He subsequently published his research findings in prominent scientific journals. He also received funding from the ESF to co-organize two workshops on Pliocene climate in Bordeaux, France (2009) and Bristol, UK (2013). In early 2014, he received the Swiss Government Excellence Scholarship to continue with his research projects at the ETH in Zurich, Switzerland. Although his interest in scientific research remained strong, in March 2014 he decided to pursue his career as a Senior Publishing Editor with Springer, Germany. He is mainly responsible for developing Springer's publishing program in the Middle East & North Africa (MENA). He also helps researchers in MENA countries publish their work by delivering educational seminars for authors, reviewers, and journal editors to help improve their publication output and quality. He is also a Visiting Lecturer at the University of Carthage, Tunisia and King Saud University, KSA, where he offers M.Sc./Ph.D. courses on geo-communication/presentations and techniques for publishing papers, and career professional development workshops. Most recently, Dr. KHELIFI was awarded the 2016 Africa Green Future Leadership Award in recognition of work contributing to sustainable development by advancing science and promoting publications in Africa and the Middle East. In 2017 he has launched Chemistry Africa together with the Tunisian Chemical Society. The journal is part of Springer MENA program which currently consists of publishing and developing 18 academic journals from the Arab World.

Nouredine JOUINI



Université Paris 13, Sorbonne Paris Cité,

Laboratoire des Sciences des Procédés et des Matériaux,

Education: PhD Inorganic Chemistry and material science, University Nantes, France, 1984

Title: University Professor Class Exp.2

Professional address: LSPM-CNRS-UPR 3407, Institut Galilée, 99 av. J. B. Clément, 93430 Villetaneuse, France

Teaching subjects: Inorganic chemistry, Crystallography, material durability and corrosion, pollution, chemical hazard

Collective responsibility within Paris University 13: Sustainable development project manager, Scientific Integrity Referent

Research Interests: Ternary system A-B-I: phase diagram and characterisation, ternary system ($A_2O - M_2O_5 - M'_2O_5$ (A = alcalin or pseudo alcalin, M = Sb, Nb, Ta, M' = P, As): structure and conductivity, nanomaterials (oxides, layered double hydroxide, metal): elaboration by chimie douce routes, Nanostructured materials (metal, ceramic, oxides).

Current Research Projects:

- Lead free material for power module
- Bulk nanostructured materials: elaboration by bottom-up strategy combining chimie douce and non-conventional consolidation methods (Spark Plasma sintering)
- Magnetic nanoparticles: morphology and size control

Professional Activities: Editorial Board, Metals; Reviewer for various scientific journals, member of CNU section 33.

Bottom-up strategy combining polyol process and Spark Plasma Sintering process: A novel route to elaborate Dense Nanostructured Materials

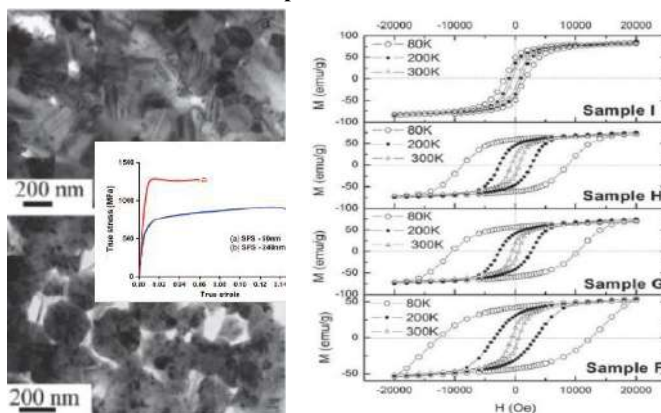
Noureddine Jouini

Université Paris 13, Sorbonne Paris Cité, Laboratoire des Sciences des Procédés et des Matériaux, CNRS-UPR 3407, 99 avenue J.-B. Clément, 93430 Villetaneuse, France

The nanostructured materials, an emerging class of materials, present superior and sometimes new mechanical and functional properties in comparison with corresponding coarsened-grain materials. This mainly originated from the small grain size which leads to a large amount of atoms located in or near the grain boundary. In this context we have developed a novel bottom-up strategy to elaborate such materials. First, nanoparticles with controlled morphology and size are prepared by the polyol process. In a second step, these nanopowders are consolidated by Spark Plasma Sintering process which appears to be the most promising process to limit the grain growth during consolidation. This leads to full dense nanostructured materials presenting nanoscaled properties. To illustrate this new bottom-up strategy, four classes of material have been chosen: Ferrite oxide CoFe_2O_4 , alloys based on cobalt and/or nickel, hydroxyapatite and the intermetallic compound Ag_3Sn . In in each case, a special attention will be payed to the influence of the SPS process parameters (temperature, pressure, and sintering time) on the as-obtained microstructures. Controlling the size and also the morphology of the grains constitutes the driving force which governs the properties of dense nanostructure materials.

Key words: Polyol, SPS, nanostructured materials, ferrite, nickel, cobalt, hydroxyapatite, nanoparticle

Graphical abstract



Dense nanostructured materials: Influence of SPS process on mechanical behavior of Co and on CoFe_2O_4 ferromagnetism

Adel **NEFZI**



*Director of Chemistry
Torrey Pines Institute for Molecular Studies
Village Parkway, Port Saint Lucie, Florida, USA*

Dr. Nefzi obtained his Ph.D. in Chemistry in 1995 from the University of Lausanne in Switzerland. Dr. Nefzi is currently an associate member and director of chemistry at Torrey Pines Institute for Molecular Studies (TPIMS) in Port Saint Lucie, Florida, working in the design and the synthesis of small molecules and heterocyclic combinatorial libraries and their application in drug discovery (www.tpims.org). He has more than 125 publications in many outstanding journals, numerous lectures at scientific symposia and nine issued US patents. Dr. Nefzi obtained many grant rewards from NIH and NSF for his research in Combinatorial Chemistry and Drug Discovery.

He is also, an adjunct professor at Florida Atlantic University. Between 2002 and 2008, Dr. Nefzi taught organic chemistry at the upper division of Organic Chemistry at the University of California San Diego (UCSD). Dr. Nefzi is a member of American Chemical Society, member of American Peptide Society, member of American Association of Pharmaceutical Scientists and member of Fluorine Chemistry Society. In addition, Dr. Nefzi is an executive member of The Society for the Advancement of Science and Technology in the Arab World (SASTA) (<http://www.sastaworld.com/>).

COMBINATORIAL CHEMISTRY: CONCEPTS, STRATEGIES AND APPLICATIONS

Adel NEFZI

*Torrey Pines Institute for Molecular Studies
Village Parkway, Port Saint Lucie, Florida, USA*

It has been estimated there are 30,000-50,000 genes in the human genome, with the vast majority of these currently having no known function. As these genes become more clearly defined and available for study, their use as therapeutic targets will be driven in part by the availability of chemical approaches to identify compounds which either activate or inhibit such “orphan” targets. Our laboratory has been actively involved in combinatorial chemistry methods since their inception. The steady improvement and expansion of combinatorial chemistry techniques over the past three decades have been our primary research focus. These approaches are truly revolutionary in their impact on the drug discovery process. Such diversity oriented synthesis and screening approaches are now utilized worldwide by virtually all pharmaceutical companies and, when possible, academic and non-profit research organizations as well. Thus, combinatorial synthetic systems are poised to enable the function of the many novel gene targets identified as potential targets to be addressed. This would have been prohibitively slow and/or expensive with methods previously available. Combinatorial chemistry is an important component of medicinal chemistry in the generation of leads and the subsequent generation of drug candidates. Our research group is interested in the design, synthesis, analysis, conformations, dynamics and structure-biological activity relationships of diverse nitrogen heterocycles of different ring sizes. Diaza- and triaza-cyclic compounds with different substitution patterns and embedded in various molecular frameworks constitute important structure classes in the search for bioactivity. Examples of the design and the identification of highly active compounds will be presented.

On behalf of



Pr. Faïza BERGAYA

Antoine
THILL

*Senior Scientist at CNRS
CRMD-CNRS-University of Orleans
Orleans, France*

Research Director Emeritus at CNRS
ICMN (Interfaces, Confinement, Matériaux et Nanostructures)
Editor-in-Chief of 'Applied Clay Science'
Series Editor of 'Developments in Clay Science' Elsevier

- * Member of the AIPEA Nomenclature Committee
- * Honorary member of the GFA (French Clay Group), France
- * Member of the Clay Minerals Society, USA
- * President of GFA (Groupe Français des Argiles) 2003 – 2007
- * Secretary of ECGA (European Clay Group Association) 1999 – 2003

Academic background

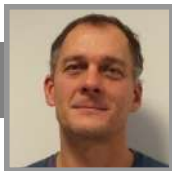
- Doctorat d'Etat Es-Sciences Physiques, 1978, University of Orleans
- Doctorat 3^{ème} cycle in Inorganic Chemistry 1971, University of Paris-La-Sorbonne
- Licence Es-Sciences in Chemical-Physics 1966, University of Tunis
(avec obtention du Prix Bourguiba)

Research Interest in Clay Science (Materials Science and Colloidal Science)

- Physical-chemistry of Clay Minerals (CM) such as Smectites, Kaolinite, Sepiolite, etc...
- Surface Properties: adsorption of molecules in gaseous and liquid phases on CM
- Interfacial Reactivity: intercalation - pillaring, organoclay, clay-polymer nanocomposites
- Structural and Textural modifications of CM by thermal, chemical and physical ways
- Rheological properties of clay colloids.

Research and Teaching Activities

- National and International collaborations with industrial partners and different academic researchers from Europe, Asia, Australia, Maghreb, USA...
- Direction of ~ 40 researchers: 20 PhD and more than 20 training students and post doc
- Teaching activity at different levels (University, Third Cycle...), at ERASMUS shoools.
- > 200 communications, including ~ 50 invited oral presentations (plenary lectures...)
- Six patents; more than 150 publications, including several book chapters
- Co-editor of several multi-authors books:
 1. 2006, "Handbook of Clay Science", First Edition, Vol 1, 1224 p, Elsevier.
 2. 2007, "Clay-based Polymer Nanocomposites (CPN)" Vol 15, 278 p, CMS Workshop Lectures. The Clay Minerals Society (publisher)
 3. 2013, "Handbook of Clay Science" Second Edition, Vol 5
Part A: Fundamentals, 874 p;
Part B: Techniques and Applications, 813 p, Elsevier
 4. The following published Volumes are:
Vol 6 (2015), Vol 7 (2016), Vol 8 (2017) and last Vol 9 published in November 2018



CHEMISTRY OF NANOSIZED TUBULAR CLAY MINERALS

Faïza ANNABI-BERGAYA

*CNRS - ICMN (Interfaces, Confinement, Matériaux et Nanostructures) 45071
Orléans, France*

Peng YUAN

*Chinese Academy of Sciences, Laboratory of Mineral Physics and Materials, Guangzhou
Institute of Geochemistry, Guangzhou 510640, China*

Antoine THILL

CEA Saclay, UMR 3685 CEA/CNRS, University Paris-Saclay, 91191 Gif-sur-Yvette, France

Natural and synthetic clays and clay minerals are a very big family with different structures, morphologies and properties. Clays, usually kaolins containing mainly kaolinite with laths morphology, are the oldest known pottery materials used in prehistory. As early as 1930, based on observation of the structure of asbestos-related minerals, Pauling proposed the existence of cylindrical structures formed by minerals in nature.

This presentation will focus on two examples of such less known rolled clay minerals with tubular nanostructures. These nanosized tubular clay minerals have at least one dimension in the nano range (between 1 and 100 nm) and a hollow tubular structure. Halloysite (**Figure 1**) which is mainly used after extraction from soils has an internal aluminol surface. Imogolite (**Figure 2**) can be also extracted from soils derived from weathered volcanic rocks, has an external aluminol surface. This opposite structural arrangement of the two nanoclay minerals leads to completely different properties. Moreover, halloysite appears very difficult to synthesise but it is easy to prepare synthetic imogolite nanotubes which are monodisperse in diameter (from 2 to 4 nm depending on composition) and polydisperse in length from several tens of nanometers up to several microns.

Thanks to microscopic and spectroscopic methods, the structures of some nanosized tubular clay minerals, such as halloysite and imogolite have been identified since the 50's. However, there was very little research on nanosized

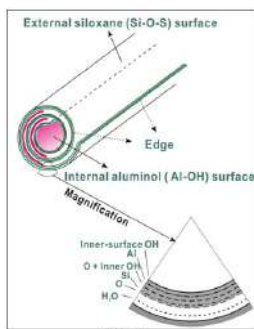


Figure 1

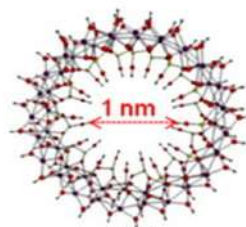


Figure 2

tubular clay minerals, and relevant papers were published only occasionally. The renewed interest since the 90's in nanosized tubular clay minerals can be partially attributed to the boom in studies on nanostructured materials and related applications, with the first synthesis of carbon nanotubes and several other nanotube materials (e.g., MoS₂ and BN). In the context of environmental science and technology, interest has been focused on using these low-cost and environmentally friendly natural materials as adsorbents for remediating pollution. This application is made possible by the high surface activity and amenability to surface modifications for versatile types of pollution treatment.

Reference:

P. Yuan, A. Thill and F. Bergaya (Eds) Nanosized tubular clay minerals, 754pp, 2016 Developments in Clay Science, Volume 7, Elsevier

Hédi **MATTOUSSI**



*Florida State University - Department of Chemistry and
Biochemistry & Integrated Nanoscience Institute
Tallahassee, FL 32306
Email: mattoussi@chem.fsu.edu*

Hedi Mattoussi is a Distinguished Research Professor at the Florida State University, Department of Chemistry and Biochemistry. Prior to joining FSU in 2009, he spent 12 years working as a senior Research Scientist at the US Naval Research Laboratory (Washington, DC). He earned a Ph.D. in Condensed Matter Physics in 1987 and a Habilitation to direct Research in Materials Physics in 1994, both from the University of Pierre & Marie Curie (Paris VI). He presently focuses on the development of inorganic nanoparticles and clusters and interfacing them with biological receptors.

Homepage: <http://www.chem.fsu.edu/~mattoussi/>

Inorganic Nanocrystals Interfaced with Biological Systems

Hedi Mattoussi

*Department of Chemistry and Biochemistry, Florida State University,
95 Chieftan Way, Tallahassee, Florida 32306*

Colloidal nanocrystals made of inorganic cores, grown via solution phase reactions, have dimensions of ~1-100 nm, a size regime that is comparable to those of biomolecules. Nanocrystals made of semiconductor, metal and metal oxide cores exhibit unique photo-physical properties. These materials offer great promises for use as platforms in biomedical applications. They have attracted much attention in the past three decades.

We have developed a new set of multifunctional, metal-coordinating polymers that are optimized for surface functionalizing a variety of inorganic nanocrystals. The ligand design exploits the effectiveness of the one-step nucleophilic addition reaction to install several anchoring groups, hydrophilic blocks and reactive functionalities into a single polymer chain. In particular, we have shown that, in addition to luminescent quantum dots, these ligands can be applied to functionalize iron oxide nanocrystals, Au nanoparticles, Au nanorods, and Au nano-shells alike. This surface-functionalization strategy yields reactive platforms that exhibit long-term colloidal stability over a broad range of biological conditions, while preventing corona formation. We have used the resulting hydrophilic platforms to develop a range of applications, which include biosensor design and imaging of live cells.

Salim BARKALLAH



*Group Leader at Cambridge Isotope Laboratories,
Andover (Greater Boston area), Massachusetts - USA*

A- EDUCATION:

- **1990 Maitrise de chimie** : Faculte des Sciences de Tunis
- **1992 DEA de chimie Organique**: Faculte des Sciences de Tunis

Supervisor: Prof. Belgacem Baccar

Title: "Synthese et caracterization d'hydrazones a-phosphonatees: voie de synthese de monoacylhydrazides et de la diethylphosphite.

• **93/94: Teaching Assistant at l'ENIG** : *teaching general and Introductory organic chemistry*

• **94/95 Fulbright Scholarship** : University of North Carolina at Chapel Hill-USA

Worked on Spiroxyphosphane in olefination chemistry. Studied the mechanism of first olefination reaction using spiroxyphosphoranes.

Supervisor: Prof. Slayton Evans Jr

• **96-2000: Teaching Assistant** at Faculte des Sciences de Tunis et Bizerte : *teaching general and organic chemistry- Research towards PhD*

• **Janvier 2000: Doctorat en Chimie organique** : Faculte des sciences de Tunis,
Supervisor: Prof. Hedi Zantour (Allah Yarhmou) **Title: Synthese et Reactivite de 2-phosphorylcyclanones et de Spirooxyphosphoranes.**

B-POSTDOCTORAL EXPERIENCE

• **September 2000- December 2001, Postdoctoral Fellow**

Department of Chemistry, University of Pennsylvania-Philadelphia-USA

Research advisor: Professor Marisa C. Kozlowski.

Asymmetric synthesis of amino-acid derivatives via Pd-catalyzed amidocarbonylation reaction.

Asymmetric synthesis of α -carboline derivatives using Pictet-Spengler reaction.

Asymmetric catalysis in Strecker reaction.

• **January 2002 - October 2003, Postdoctoral Fellow**

Department of Biochemistry and Biophysics, Medicine school -University of Pennsylvania

Research Adviser: Professor Dewey G. McCafferty

- Synthesis of unnatural amino acids

- Peptide synthesis on solid support

- Studies towards the total synthesis of glycopeptide Antibiotic Ramoplanin analogues on solid support. -Mechanism of action of Ramoplanin.

C- INDUSTRIAL EXPERIENCE 2003 - Present

Cambridge Isotope Laboratories- Andover (Greater Boston) , MA –USA

• **Position: Senior Chemist: 2003 - 2008**

• **Position: Senior Chemist II 2008 - 2014**

Development and synthesis of stable isotopes labeled organic compounds: steroid metabolites, environmental standards, amino acids, biologically active intermediates etc...

• **Managerial position: Group Leader 2014 - to present**

Supervises a group of 4 chemists (Bachelor, Masters and PhD holders)

D- PUBLICATIONS

• **Publications 15** in the following Journals:

(Nature Protocols, J. Proteome Research, J. Soc. Chim. Tunisie; J. Am. Chem. Soc.;

Tetrahedron Letters; Bioorg. Med. Chem.; Biopolymers; Peptide Science;

J. Soc. Alg. Chim; Phosphorus, Sulfur and Silicon, Acta Cryst.)

• **Patent 1:** "LYSINE ISOTOPOLOGUES, COMPOSITIONS COMPRISING THE SAME AND METHODS OF SYNTHESIS" WO 2014/150909 A1; 25 September 2014 (25.09.2014)

• **Text Book 1: L'essentiel de l'isomérisation et des mécanismes réactionnels**

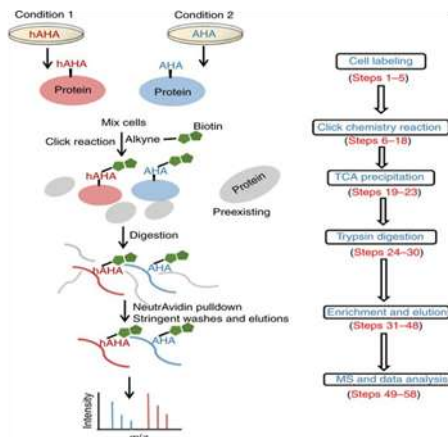
Published by CNUD 2001, Coauthor with Prof.. Hedi Mrabet, faculte des Sciences de Tunis- Tunisia

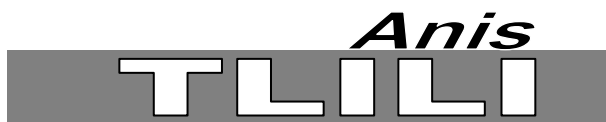
Stable Isotope Compounds Support for Technological Advances in Medical Research

Salim BARKALLAH

*Group Leader at Cambridge Isotope Laboratories,
Andover (Greater Boston area), Massachusetts -USA*

Cascades of new technologies are being made available to biotech communities to tackle complicated disease-related problems. Incorporation of non-canonical isotopically labeled amino acid into cell machinery through bio-orthogonal tagging together with advancements in mass spectrometry are paving the way to better understand disease at the cellular level. Heavy azidohomoalanine ($^{13}\text{C}_4$, $^{15}\text{N}_2$, hAHA), first synthesized at Cambridge Isotope Labs, is a key component in the novel technology HILAQ (Heavy Isotope Labeled Azidohomoalanine Quantitation).





*Institut de Chimie et de Biochimie Moléculaires et
Supramoléculaires, CNRS
Université Lyon1, Lyon, France
anis.tlili@univ-lyon1.fr*

Dr Anis Tlili is CNRS Research Fellow. After gaining a master's thesis with Pr. S. Jugé (Dijon), he completed his PhD in the group of Dr. M. Taillefer. (Montpellier, France) in the late 2011. Subsequently, he joined the group of Pr. M. Beller (LIKAT, Rostock, Germany) for postdoctoral stay. Anis undertook a second collaborative postdoctoral position (Commissariat de l'énergie atomique/ICSN, Paris). In 2014 he accepted a CNRS position. His current research interests lie in the area of homogeneous catalysis/ photocatalysis with particular focus on fluorine chemistry. Anis is author of more than 50 publications and patents and has been selected in 2018 to take part in the young investigator workshop of raising star in chemistry, Oxford (UK).

Late Stage Fluoroalkylselenolation

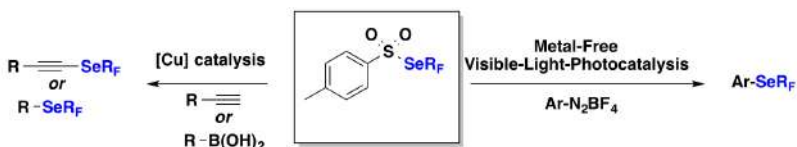
Anis Tlili

*Institut de Chimie et de Biochimie Moléculaires et Supramoléculaires, CNRS
Université Lyon1, Lyon, France
anis.tlili@univ-lyon1.fr*

Over the last decades, fluorinated molecules have significantly emerged due to the increasing interest in life science and materials. Among those compounds, trifluoromethyl group in combination with a heteroatom have shown appealing electronic and physico-chemical properties especially with chalcogen as sulfur and oxygen.

However, the selenylated analog SeCF₃ 3 was scarcely studied. This could be explained by the lack of efficient strategies to access trifluoromethylselenolated compounds. Noteworthy, our group have established the Hansch parameter of the SeCF₃ moiety (π SeCF₃ = 1.29) thus conferring one of the best lipophilic character for this motif.^[1]

Early this year, we successfully designed a new family of shelf-stable electrophilic reagent, namely the fluoroalkyltolueneselenosulfonates.^[1] We demonstrated that such electrophilic reagent allow for the first time the direct formation of C(sp)-R_F C(sp²)-R_F under copper catalysis under mild reaction conditions.^[2] Furthermore the use of such reagent allows the access to trifluoromethylselenolated arenes under metal-free visible light-photocatalysis.^[3]



References

- [1] *Chem. Eur. J.* **2018**, *24*, 3659-3670.
- [2] a) *Chem. Eur. J.* **2017**, *23*, 10013-10016 (HOT PAPER); b) *Adv. Synth. Catal.* **2017**, *359*, 3414-3420; c) *Chem. Eur. J.* **2018**, *24*, 97-100 (HOT PAPER).
- [3] a) *ChemComm* **2018**, *54*, 9909-9912 b) *Angew. Chem. Int. Ed.* **2018**, *57*, 11781-11785. (VIP).

Oral Communications' List

**(alphabetically
authors' name)**



Communicatings' Names	Ref
A. Abdelli , M. Jmaï, M.L. Efrit, H. M'rabet, D. Prim <i>FST - Tunis</i> Synthesis of new phosphorus heterocycles from functionalized allylphosphonates	OC1C
M. Abid Derbel , H. Naïli, W. Rekik <i>FSS - Sfax</i> Crystal structure, thermal behavior and magnetic properties of (C ₄ H ₁₄ N ₂)[CuBr _{2.19} Cl _{1.81}]	OC1A
R. Abidi , M. Hichri, C. Lafuente, I. Khattech <i>FST - Tunis</i> Thermophysical properties of the binary mixtures of Methyl levulinate + C1-C4 n-Alkanol and Ethyl levulinate + C1-C4 n-Alkanol at 298.15 K	OC1B
I. Abidli , N. Souissi, K. Essalah, X.R. Novoa <i>FST - Tunis</i> Anticorrosive effects of curcuma extract against the corrosion of iron: An electrochemical and computational study	OC16B
A. Achech , A. Haj Said <i>FSM - Monastir</i> Elaboration and characterization of Metal -Organic frameworks thin film obtained through layer by layer deposition	OC37D
J. Ajmi , I. Nagazi, A. Haddad <i>FSM - Monastir</i> Synthesis, structure of a new soduim selenomolybdate compound Na ₄ [Se ₂ Mo ₅ O ₂₁].5H ₂ O	OC2A
M. Ali Rachedi , S. Arroussi <i>ESTI, Annaba, Algeria</i> Effect of synthesis parameters on particle size of nanocrystalline NiAl intermetallic compound	OC41D
I. Alkskas <i>University of Misurata, Libua</i> Thermotropic liquid crystalline poly(azomethine-ether)s based on 1-phenethyl-4-piperidone	OC46C
H. Ammar , S. Nasr, E. Ben Salem <i>IPEIM - Monastir</i> Synthesis and characterization of sodium and carbonate co-substituted hydroxyfluorapatite	OC3A
R. Aouay , S. Jebri, I. Khattech <i>FST - Tunis</i> Poorly crystalline hydroxyapatite for cadmium removal in aqueous medium	OC2B
J. Aribi , W. Jahouach-Rabai, Z. Azzouz-Berriche, B. Hamrouni <i>CERTE - Borj Cédria</i> Radiolysis of Ibuprofen and Krtoprofen in aqueous solutions by irradiation process	OC3B

Communicatings' Names	Ref
A. Askri , K. Nahdi, A. Martínez-Arias <i>FSB - Bizerte</i> Study of supported La ₂ CuO ₄ perovskites for reverse water gas shift reaction	OC4A
D. Atoui , K. Said, R. Ben Salem <i>FSS - Sfax</i> Reactivity and selectivity study of the Heck coupling reaction activated by ultrasonic activation	OC2C
H. Ayachi , T. Boubaker <i>FSM - Monastir</i> Free energy relationships for s-complexation reactions of 7-X-4-nitrobenzofurazan	OC3C
S. Ayadi , - <i>INSTM, Port La Goulette - Tunis</i> Theoretical study of epoxide molecules reactivity with amines and alcohols	OC4C
K. Azaiez , T. Boubaker <i>FSM - Monastir</i> Electrophilicities of benzyldenecyanoacetates	OC5C
Y. Bahrouni , L. Benhamada <i>FSM - Monastir</i> Structural, physico-chemical properties and theoretical study of a new organic nitrate crystal (C ₉ H ₁₁ N ₂ O ₅) ₂ (NO ₃) ₂	OC6A
J. Baizig , A. Haj Abdallah, A. Haddad <i>FSM - Monastir</i> A novel member of MO36-polyoxoanion's family based on ammonium cations: Synthesis and physico-chemical characterization	OC7A
I. Bayar , L. Khedhiri, S. Soudani, C. Ben Nasr <i>FSB - Bizerte</i> Crystal structure, quantum mechanical investigation, IR and NMR spectroscopy of new Perchlorate : (2-(1-C ₄ H ₉ N ₂)C ₄ H ₅ N ₂).(ClO ₄) ₂	OC8A
S. Bdey , N. Fakhar Bourguiba, S.N. Savvin, M.F. Zid, P. Nunez <i>FST - Tunis</i> Synthesis, crystal structure and ionic conduction of Na _{5.22} Cu _{1.89} Al(AsO ₄) ₄	OC9A
A. Bejaoui , A. Souamti, D. Ben Hassen Chehimi <i>FSB - Bizerte</i> Synthesis and Electrical properties of Na ₆ Mg _{1-x} Co _x (SO ₄) ₄ Vanthoffite ceramics	OC10A
M. Bejaoui , H. Galai, A. Ben Haj Amara, H. Ben Rhaïem <i>FSB - Bizerte</i> Solubility enhancement of poorly soluble drugs by solid dispersion technique	OC35C

Communicatings' Names	Ref
M. Bejaoui , A. Elmhamdi, K. Nahdi, A. Martínez-Arias <i>FSB - Bizerte</i> Effect of addition of different promoter on the performance of CoFe ₂ O ₄ catalyst in CO-PROX	OC11A
W. Belam , - <i>FSB - Bizerte</i> Sol-gel Chemistry Autocombustion Synthesis and DTA-TGA, XRPD, SIC, ⁷ Li, ⁶³ Cu MAS-NMR and magnetic studies of the Li-Cu substituted cobalt ferrite nanoparticles LiCu _{0.5} Co _{0.75} Fe _{1.5} O ₄	OC12A
F. Ben Baraket , B. Pedras, E. Torres, M. João Brites, M. Dammak, M.N. Berberan-Santos <i>FSS - Sfax</i> Optical, photophysical and electrochemical properties of phenoxazine and phenothiazine derivatives for OLED applications	OC13A
K. Ben Hamouda , R. Omrani, M.L. Efrat, A. Ben Akacha <i>FST - Tunis</i> Synthesis of thiazolines and thiazolidinones derivatives from benzylphosphonates	OC6C
M. Ben Jomaa , N. Fakhar Bourguiba, H. Chebbi, M.F. Zid <i>FST - Tunis</i> Crystal structure, Hirshfeld surface analysis and energy framework calculations of a new organic perchlorate, (C ₉ H ₁₀ N ₃)[ClO ₄]	OC14A
W. Ben Mbarek , E. Pineda, L. Escoda, J.J. Suñol, M. Khitouni <i>FSS - Sfax</i> Influence of minor additions of Fe and Co on the azo dye degradation ability of Mn-Al particles	OC15A
O. Ben Moussa , H. Chebbi, L.R. Falvello, T. Milagros, M.F. Zid <i>FST - Tunis</i> Crystal structure, physico-chemical studies, Hirshfeld surface analysis and theoretical calculations of a novel hybrid material, bis(2,6-diaminopyridinium) hexachloridostannate(IV)	OC16A
Y. Ben Smida , K. Horchani-Naifer, M. Férid <i>CNRSM - Borj Cédria</i> Transport pathways simulation of cations in crystal materials	OC4B
R. Ben Youssef Triki , N. Sdiri, K. Horchani-Naifer, M. Férid <i>CNRSM - Borj Cédria</i> Structural properties of Ho _{1-x} Ba _x CrO ₃ ceramics	OC17A
T. Bouagga , T. Harizi, F. Sakli <i>ENIM - Monastir</i> Surface treatment of Tunisian wool by chlorination using sodium hypochlorite for industrial applications of textiles	OC43B
T. Bouallegui , B. Ayed, A. Haddad <i>FSM - Monastir</i> A novel inorganic-organic hybrid material based on β-Anderson polyoxomolybdate: Synthesis and physico-chemical characterization	OC18A

Communicatings' Names	Ref
M. Bouchaour , L. Merad, R. Bensaha, S A. Benyelles, D. Guettaia, A. Ouldabbas, N-E. Chabanesari, N. Maloufi <i>University of Tlemcen, Algeria</i> Degradation of methylene blue using ZNO photocatalyst in water purification	OC20B
T. Bouchaour , M. Mihoub, Y.H. Bendahma. Hamri, U. Maschke <i>University Abou Bakr Belkaïd, Tlemcen, Algeria</i> Elaboration and characterization of a poly (HEMA) network and an interpenetrated polymer network based on cellulose and HEMA application to wastewater remediation by colorant retention	OC40B
H. Bouchouicha , G. Panczer, Y. Guyot, D. De Ligny, R. Ternane <i>FSB - Bizerte</i> Luminescent properties of co-doped Eu ³⁺ / Eu ²⁺ calcium aluminosilicate glass-ceramics: a potential tunable luminophore	OC19A
S. Boughanmi , I. labidi, A. Megriche, M. El Maaoui, A. Nonat <i>FST - Tunis</i> Integration of natural fluorapatite as a raw material for cement production	OC20A
M. Bouguerra , M. Belhouchet <i>FSS - Sfax</i> Synthesis and characterization of two organic-inorganic salts: Sulfates of diphenyl sulfone derivatives	OC21A
S. Bouketaya , M.S.M. Abdelbaky, S. Garcia-Granda , M. Dammak <i>FSS - Sfax</i> Hydrothermal synthesis, crystal structure, thermal behavior and vibrational studies of the novel hybrid iron fluoride (III), FeF ₆ (C ₂ N ₅ H ₆) ₃ FH	OC22A
H. Boussehel , H. Debchi <i>University of Biskra, Algeria</i> Influence of potassium permanganate treatment on the mechanical properties and thermal behavior of palm fibers reinforced polyvinyl chloride composites	OC41B
S. Bouzidi , M. Amara Gdaïem, J. Dhahri, E.K. Hlil <i>FSM - Monastir</i> Large magnetocaloric entropy change at room temperature in soft ferromagnetic manganite La _{0.75} Ca _{0.05} Na _{0.20} MnO ₃	OC44B

Communicatings' Names	Ref
L. Chaabane , E. Beyou, P. Alcouffe, M.H.V Baouab <i>FSM - Monastir</i> Removal of nickel (II) using a novel synthetic bis(2-pyridylmethyl)amino-chloroacetyl chloride- ethylenediamine-grafted GO sheets	OC18B
M. Chira , G. Rigane, C. Calas-Blanchard, R. Rouillon, R. Ben Salem <i>FSS - Sfax</i> Variation of the antioxidant properties of olive oil according to the methods of preparation (<i>Olea europaea</i> L. cv. <i>Chemlali</i> Sfax)	OC8C
I. Chniti , M.A. Sanhoury, M.T. Ben Dhia <i>FST - Tunis</i> Synthesis and characterization of new mixed bis(thio)carbamate-phosphoramidate derivatives	OC9C
R. Dabbabi , J. Barroso De Aguiar, S. Baklouti <i>FSS - Sfax</i> Alkali-activated mortar based on phosphate washing waste	OC24A
K. Dammak , M. Porchia, F. Tisato, H. Naïli <i>FSS - Sfax</i> Synthesis of new copper(I) complexes with hydrophilic aminomethylphosphines	OC25A
S. Dgachi , H. Naïli, M.M. Turnbull <i>FSS - Sfax</i> A study on organic templated metal halides: Structure, thermal analysis and magnetic properties	OC26A
A. Dhahri , E. Dhahri, E.K. Hlil <i>FSM - Monastir</i> Electrical conductivity and dielectric behaviour of nanocrystalline $\text{La}_{0.6}\text{Gd}_{0.1}\text{Sr}_{0.3}\text{Mn}_{0.75}\text{Si}_{0.25}\text{O}_3$	OC27A
M. Dhaou , S. Guerhazi, E. Elaloui <i>FSS - Sfax</i> Synthesis and Characterization of Zn-doped mesoporous TiO_2 nanoparticles as efficient materiel for photocatalyticapplications	OC28A
M. Dhifi , A. Haddad <i>FSM - Monastir</i> Hydrothermal synthesis, characterization and crystal structure of new inorganic-organic hybrid materials based on metatungstate type units	OC29A
W. Dridi , M.F. Zid <i>FST - Tunis</i> Electrical and vibrational properties studies of $\text{Na}_{0.45}\text{K}_{1.55}\text{Cu}_3(\text{MoO}_4)_4$	OC30A

Communicatings' Names	Ref
M. El Kateb , C. Trelu, A. Darwich, M. Rivallin, M. Bechelany, S. Lacour, G. Lesage, M. Cretin, N. Bellakhal <i>FST - Tunis</i> Mineralization of nanofiltration concentrate of Landfill Leachate by electrochemical advanced oxidation processes	OC19B
A. Elferjani , S. Garcia-Granda, M. Dammak <i>FSS - Sfax</i> Synthesis, structural study and phase transitions characterization of a new inorganic compound: $\text{Tl}_{0.92}(\text{NH}_4)_{0.08}(\text{SO}_4)_{0.65}(\text{SeO}_4)_{0.35}.\text{Te}(\text{OH})_6$	OC31A
H. Elhleli , F. Mannai, Y. Moussaoui <i>FSG - Gafsa</i> Extraction and physicochemical characterization of mucilage extracted from <i>Opuntia ficus indica</i>	OC10C
S. Elleuchi , K. Jarraya, A. Gil, M.J. Calhorda <i>FSS - Sfax</i> Theoretical study of the interaction of $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ with DNA : A way to fight against cancer	OC33A
K. Essid , M.H. Frikha <i>FSS - Sfax</i> Reactivity of mixed carboxylic-fatty anhydrides as acylating agents using heterogeneous acid catalysts	OC11C
A. Etorki , M.A. Kammashi, M.S. Elhabbat, I.S. Shaban <i>University of Tripoli, Libya</i> Application of polyaniline nanoparticles modified screen printed carbon electrode as a sensor for determination of Hg(II) in groundwater samples	OC21B
A. Fajraoui , J. Ben Nasr, C. Lacoste, M. Ben Amar <i>ENIS - Sfax</i> Casting of PLA mixed with natural dye	OC22B
J. Fakhfakh , M. Affes, I. Daoud, V. Brieudes, M. Halabalaki, A. El Feki, N. Allouche <i>FSS - Sfax</i> Extensive study of Tunisian <i>Lycium arabicum</i> Boiss. by UHPLC/ HR-ESI-MS/MS and evaluation of its antioxidant and anti-lipase activities	OC37C
R. Fezai , M. Rzaigui <i>FSB - Bizerte</i> Biophysicochemical study of a hybrid cyclohexaphosphate	OC34A
O. Fliss , K. Essaleh, A. Ben Fredj <i>IPEIM - El Manar</i> Theoretical study on the conformations and the tautomerization processes of glyphosate in aqueous solution	OC5B
M. Fray , R. Abidi, M. Bennazza, T. Barhoumi-Slimi <i>FST - Tunis</i> Synthesis and characterisation of 2,5-disubstituted 1,3,4-oxadiazoles through oxidative cyclization of <i>N</i> -acylhydrazones	OC12C

Communicatings' Names	Ref
M.A. Gdaïem , C. Rayssi, N. Hamdaoui, J. Dhahri <i>FSM - Monastir</i> Bias dependent dielectric properties study of $\text{La}_{0.8}\text{Ba}_{0.1}\text{Ca}_{0.1}\text{Mn}_{0.85}\text{Co}_{0.15}\text{O}_3$ at room temperature	OC35A
M. Gharsallah , J. Gainza , F. Serrano-Sanchez , M. Funes, F. Carrascoso , N.M. Nemes, O.J. Dura , J.A. Alonso <i>FSS - Sfax</i> Thermoelectric properties of new chalcogenide layered compounds	OC6B
S. Gharsallah , M. Chemingui, C. Charnay, M. Khitouni <i>FSS - Sfax</i> Synthesis and characterization of composite material based on magnesium phosphate cement for cesium retention	OC36A
S. Ghraïri , M.A.K. Sanhoury , B. Crousse, T. Barhoumi-Slimi <i>FST - Tunis</i> Synthesis and characterization of new tin tetrachloride complexes with β -chlorovinyl aldehydes	OC13C
O. Ghriss , H. Benamor, M. Razak Jeday, D. Thomas <i>ENIG - Gabès</i> Scrubbing of gaseous nitrogen oxides in cables-bundle contactor	OC7B
I. Gouti , H. Litaïem, M. Dammak <i>FSS - Sfax</i> Order-disorder phase transition in the Cesium SelenateTellurate material at high temperature	OC37A
A. Guesmi , H. Marouani <i>FSB - Bizerte</i> Synthesis, structure and physico-chemical studies of a novel oxalate material $\text{C}_8\text{H}_{14}\text{N}_2(\text{C}_2\text{O}_4)$	OC38A
O. Guesmi , L. Ktari, S. Garcia-Granda, M. Dammak <i>FSS - Sfax</i> Structure, thermal decomposition and spectroscopic characterization of a new hybrid iron fluoride $\text{Fe}_4\text{F}_{18} \cdot (8\text{-Hydroxyquinoline})_6$	OC39A
R. Hachicha , R. Zarrougui, S. Messaoudi, S. Le Vot, O. Fontaine, F. Favier, O. Ghodbane <i>INRAP - Sidi Thabet</i> Physical properties, electrochemical stabilities and molecular dynamics study of novel ionic liquids based on N-allyl-N,N-dimethylethylammonium cation	OC23B
M. Hadhri , A. Haddad, B. Ayed <i>FSM - Monastir</i> Crystal structure, vibrational spectroscopy, optical properties and Hirshfeld surface analysis of adeninium dichromate and trichromate	OC40A
A. Hadj-Ziane Zafour , A. Ben Yacoub, A. Skender, K. Boutemak <i>University Saad Dahlab, Blida, Algeria</i> Biocidal effect of <i>Melia azedarach</i> seed oil encapsulated on devastating insect species and environmental protection	OC25B

Communicatings' Names	Ref
H. Hajji , E. Ben Salem <i>IPEIM - Monastir</i> Study of the influence of synthesis parameters on the physico-chemical properties of hydroxyfluoroapatite via the Taguchi method	OC41A
A. Hajlaoui , H. Ben Jannet, A. Romdhane <i>FSM - Monastir</i> Design and synthesis of novel pyranotriazolopyrimidine derivatives	OC14C
N. Hamdadou , E. Ouadah, M.A. Ouaguel <i>Ecole Nationale Polytechnique d'Oran, Algeria</i> Preparation and characterisation of tungsten oxide WO ₃ thin films	OC46A
N. Hamdi , L. Bessais, A. Ben Haj Amara, W. Belam <i>FSB - Bizerte</i> Synthesis by the Sol-Gel autocombustion method and physicochemical characterizations of ferrimagnetic nanoferrites of Ni _{0.2} Cu _{0.4} Co _{0.4} Fe ₂ O ₄	OC42A
S. Hamdi , K. Nahdi, L. Favergeon <i>FSB - Bizerte</i> The influence of water vapor in magnesium oxide carbonation	OC43A
A. Hamma , S. Bouhelal <i>University Ferhat Abbas</i> UV accelerated aging of biobased/kenaf fibres composite: Viscoelastic behaviour in molten state & thermal properties	OC42B
S. Hammami , A. Megriche <i>FST - Tunis</i> Spectroscopic studies, optical properties and structural characterization by Rietveld refinements of nano crystal lithium rare earth polyphosphates [LiGd _(1-x) Eu _x (PO ₃) ₄]	OC44A
D. Harbaoui , D. Harbaoui, M.M.S. Sanada, C. Rossignol, E.K. Hlil, K. Zaidat, S. Obbade, N. Amdouni <i>FST - Tunis</i> Structural, magnetic, electrical and electrochemical properties of O3-Type layered materials: NaNi _{1/3} Mn _{1/3} Co _(1/3-x) Fe _x O ₂	OC45A
S. Hassen , H. Chebbi, M.F.Zid, Y. Arfaoui <i>FST - Tunis</i> spectroscopic and thermal studies, theoretical investigation and photocatalysis application of 2-aminobenzimidazolium tetrachlorocobaltate(II)	OC39B
S. Hazourli , M. Ziati, M. Bendaia, R. Abrane <i>University of Annaba, Algeria</i> Removal of arsenic (III) from an aqueous solution by adsorption on coal raw and treated resulting from date pits	OC31B
M. Hidouri <i>ISSAT - Gabès</i> Ionic conduction of a strontium britholite doped with lanthanum and neodymium	OC1D

Communicatings' Names	Ref
S. Hkiri , A. Hafidh, S. Touil, A. Samarat <i>FSB - Bizerte</i> Synthesis and antimicrobial evaluation of Novel 1,3,4-oxadiazole derivatives	OC43C
C. Issaoui , A. Guesmi <i>FST - Tunis</i> Synthesis and structural study of the-monoclinic phase $\text{Na}_4\text{Co}_{7-x}\text{Al}_{0.67x}(\text{As}_{1-y}\text{P}_y\text{O}_4)_6$. ($x = 1.60$; $y = 0.116$)	OC2D
M. Itaimi Dammak , Z. Mzoughi, I. Chakroun, H. Ben Mansour, D. Le Cerf, H. Majdoub <i>FSM - Monastir</i> Optimization of polysaccharides extraction from Quince peels: Partial characterization, antioxidant and antiproliferative properties	OC38C
I. Jabbari , M. Baira, H. Maaref , R. Mghaieth <i>FSM - Monastir</i> C-DLTS interface defects in $\text{Al}_{0.22}\text{Ga}_{0.78}\text{N}/\text{GaN}$ HEMTs on SiC: Spatial location of E2 traps	OC3D
M. Jabli , N. Sebeia, A. Ghith <i>ENIM - Monastir</i> Green synthesis of copper nanoparticles using biological <i>Cynomorium</i> <i>Coccineum</i> L. and Nerium Oleander extracts and study of their interaction with organic pollutants	OC38D
I. Jadli , M. Aouassa, S. Johnston, H. Maaref, L. Favre, A. Ronda, I. Berbezier, A. Bandyopadhyay, Sung Kyu Kim, I. Karaman, J. Yong Lee, R.M'ghaieth <i>FSM - Monastir</i> Elaboration and characterization of Germanium nanocrystals for next generation of nonvolatile memory and GeMn nanocrystals for spintronics	OC39D
W. Jahouach Rabai , W. Jahouach-Rabai, Z. Azzouz-Berriche, R. Lahsni, B. Tuccio-Lauricella <i>CERTE - Borj Cédria</i> Degradation efficiency and toxicity evolution of emerging contaminants in water solutions	OC24B
B. Jalel , N. Ennaceur, R. Henchiri <i>FSG - Gabès</i> Synthesis, structure and characterization of a hybrid centrosymmetric material (4-Dimethylaminopyridinium nitrate gallic acid monohydrate)	OC4D
N. Jamel Eddine , Yekdhan Kacem, J. Kraiem <i>FSM - Monastir</i> Iron-Catalyzed the solventless etherification under green conditions	OC16C
S. Jarray , N. Etteyeb, J. Bouajila, A. Romane, M. Romdhane <i>INSAT - Tunis</i> Tunisian Palm (<i>Phoenix dactylifera</i> L.) leaves: Anti-corrosive activity against the corrosion of steel in acidic media	OC26B

Communicatings' Names	Ref
S. Jebali , L. Latrous <i>FST - Tunis</i> Chemometric optimization and validation of a novel method for the simultaneous separation of five antihistaminic in pharmaceutical formulations by UPLC-UV.	OC27B
N. Jemili , W. Essafi <i>INRAP - Sidi Thabet</i> Electrostatic complexation of polyelectrolytes in aqueous solution	OC28B
I. Jendoubi , M. Ptak, A. Pikul, J. Chmielowiec, A. Ciupa, M. Maczka, M.F. Zid <i>FST - Tunis</i> Synthesis, crystal structure, phonon, magnetic and electrical properties of new molybdate $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$	OC5D
M. Jmaï , V. Blot, M.L. Efrit, J. Lebreton, H. M'rabet <i>FST - Tunis</i> Synthesis of some novel Pyrazolines derivatives trough 1,3-Dipolar cycloaddition between Dialkyl (allyloxymethyl)phosphonate and nitrile imines	OC17C
A. Jraba , A. Zohra, E. El Aloui <i>FSG - Gabès</i> Sol-gel synthesis and characterization of monolith and transparent Sr, Fe and Al doped TiO_2	OC6D
I. Kadri , H. Naïli, W. Rekik <i>FSS - Sfax</i> Elaboration, structure, spectroscopy study and thermal behavior of piperzinediium triaquatrchloro iron(III) chloride	OC8D
L. Kahloul , H. Chadli, A. Hebbaz, S. Meddah <i>University of Annaba, Algeria</i> Electrochemical behavior of a porous TiNiCu biomaterial	OC15D
D. Kanzari Mnallah , M.L. Efrit, A. Ben Akacha <i>FST - Tunis</i> Synthesis, conformational analysis of new diastereomeric cyclophosphamides	OC20C
A. Karouia , C. Slama, F. Schoenstein , M. Abdellaoui , N. Jouini <i>INRAP - Sidi Thabet</i> Spark plasma sintering of $\text{Ti}_{0.7}\text{W}_{0.3}\text{C}$ powders prepared by mechanical alloying	OC9D

Communicatings' Names	Ref
M. Khabbouchi , K. Hosni, M. Mezni, E. Srasra <i>CNRSM - Borj Cédria</i> Structural characterizations and mechanical behavior of activated clay-based $\text{Si}_5(\text{PO}_4)_6\text{O}$ and SiP_2O_7 compounds	OC10D
N. Khadhri , M. El Khames Saad, Y. Moussaoui <i>FSG - Gafsa</i> Removal of amoxicillin in fixed-bed column packed with activated carbon derived from date palm	OC29B
E. Khdhiri , K. Mnafigui, H. Ammar, S. Abid <i>FSS - Sfax</i> 3-acetyl-coumarin <i>N</i> -benzoylhydrazone: synthesis and biological activity	OC19C
T. Khelfa , M.A. Rekik, J.M. Cabrera-Marrero, T. Baudin, A.L. Helbert, F. Brisset, M. Khitouni <i>FSS - Sfax</i> Thermal stability of AA6060 aluminum alloy after equal channel angular pressing	OC11D
N. Khitouni , R. Daly, L. Escoda, N. Llorca-Isern, J.J. Suñol, M. Dammak <i>FSS - Sfax</i> Structural, magnetic and the thermal stability characterizations of the nanostructured $\text{Fe}_{50}\text{Co}_{25}\text{Ni}_{15}\text{B}_{10}$ alloy prepared by mechanical alloying	OC12D
N. Klidi , D. Clematis, M.P. Carpanese, A. Gadri, S. Ammar, M. Panizza <i>FSG - Gabès</i> Electrochemical oxidation of crystal violet using a BDD anode with a solid polymer electrolyte	OC33B
S. Kouass , H. Dhaouadi, F. Touati <i>INRAP - Sidi Thabet</i> Synthesis, characterization and study physical properties of iron oxide Fe_3O_4	OC13D
R. Ksiksi , H. Chebbi, M. Graia <i>FST - Tunis</i> Preparation, crystal structure and Hirshfeld surface analysis of vanadium(V) complex, 4-isopropylpyridin-1-ium decavanadate hydrate $(\text{C}_8\text{H}_{12}\text{N})_6\text{V}_{10}\text{O}_{28} \cdot 16\text{H}_2\text{O}$	OC14D
I. Labidi , S. Boughanmi, A. Khelidj, A. Megriche <i>FST - Tunis</i> Does the limestone (CaCO_3) addition affect the hydration kinetics of resisting sulfate (RS) Portland cement?	OC16D
M. Labidi , S. Labidi <i>University Badji Mokhtar, Annaba, Algeria</i> First-principles study of rock-salt $\text{Ca}_{1-x}\text{Sr}_x\text{O}$ ternary alloys	OC10B

Communicatings' Names	Ref
T. Larbi , S. Abidi, K. Doll, M. Amlouk <i>FST - Tunis</i> Structural, elastic, vibrational and thermodynamic properties of Cerium oxide CeO ₂ . A combined experimental and ab initio investigation	OC18D
F. Laribi , M.A.K. Sanhoury, I. Chehidi <i>FST - Tunis</i> Tin(IV) chloride complexes with highly fluorinated phosphoramidates and phosphates: Synthesis and multinuclear (¹ H, ¹⁹ F, ³¹ P and ¹¹⁹ Sn) NMR characterization	OC44C
M. Louleb , M. Algarra, L. Latrous, M. Zougagh, A. Ríos <i>FST - Tunis</i> Sub-nanomolar detection of dopamine in human fluids by N-doped carbon dots	OC40D
H. Ltaief , S. Ben Ali, A. Mahroug, V. Fretti, M. Belhouchet <i>FSS - Sfax</i> Synthesis, structural determination and physicochemical properties of C ₂₄ H ₃₆ Cl ₆ CuN ₄ O ₈ S ₂	OC19D
A. Maalaoui , S. Akriche <i>FSB - Bizerte</i> Synthesis, characterization and antimicrobial activity of a novel fluorescent tetra-V- substituted keggin heteropolyoxotungstate decorated with imidazolium cations	OC21C
M. Maoui , A. Anton, R. Boukchina, N. Hajjaji <i>ISSTEG - Gabès</i> Toxicity assessment of pesticide use in tomato production : Case study of a Tunisian-Dutch soilless greenhouse	OC34B
A. Maazaoui , M. Romdhani Younes <i>FST - Tunis</i> An efficient synthesis of new allyloxy-β-hydroxy and bis(allyloxy)sulfides	OC22C
I. Mahmoud , C. Fersi, A. Alatrache <i>INRAP - Sidi Thabet</i> The optimization of wastewater treatment using ultrafiltration process	OC35B
R. Malek , V. Luzet, F. Chabchoub, L. Ismaili <i>University of Sfax, Tunisia</i> Synthesis of donepezil-chromone hybrids via the Passerini reaction	OC23C
F. Mannai , A. Dufresne, E. Elaloui, Younes Moussaoui <i>FSG - Gafsa</i> Thermal and viscoelastic behavior of green composite reinforced with fibrous networks obtained from <i>Opuntia</i> (Cactaceae)	OC45C
B. Marzougui , M.I.Houchati, N. Sdiri, A.H. Hamzaoui <i>FSB - Bizerte</i> +Electrical conductivity and dielectric properties of Ln _{1.8} Sr _{0.2} CuO ₄ (Ln=La, Pr and Nd)	OC20D

Communicatings' Names	Ref
H. Mechi , M.A.K. Sanhoury, M.T. Ben Dhia <i>FST - Tunis</i> Preparation and characterisation of tin(IV) complexes with biologically relevant organophosphates	OC24C
N. Meddeb , H. Galai, K. Nahdi <i>FSB - Bizerte</i> Effect of grinding on the thermal stability of a trihydrate atorvastatin: A CRTA study	OC39C
C. Messaoudi , A. Abdelli, M.L. Efrat, H. M'rabet <i>FST - Tunis</i> Reactivity of β -ethoxycarbonylated <i>N</i> -methylphosphonate allylamines with amines, thiols and dithiols	OC25C
M. M'hailham , K. Ebeid, F. Ebnou, M.T. Ben Dhia, M.A.K. Sanhoury <i>University Nouakchott Al Aasriya, Mauritania</i> Synthesis and characterisation of beryllium (II) complexes with phosphoramides bearing different cyclic amino groups	OC26C
J. Mhalla , S. Boughammoura, A. Ghazouani <i>FSM - Monastir</i> Prediction of polyion conformation and interpretation of some anomalies of polyelectrolytes in terms of superposition principle and dielectric friction	OC8B
K. Mkadmini , M. Hammami, C. Rihouey, D. Le Cerf, R. Ksouri, H. Majdoub <i>CBBC - Borj Cédria</i> Molecular weight degradation, rheological properties and antioxidants activities of polysaccharides from <i>Zizyphus lotus</i> fruit under ultrasonic treatment	OC18C
M. Mrad , T. Ben Chaabane, R. Schneider <i>FSB - Bizerte</i> Synthesis, characterization and optical properties of core/shell AgInS ₂ /ZnS quantum dots	OC21D
Z. Msetra , M. Chemingui, V. Optasanu, M. Khitouni <i>FSS - Sfax</i> Structural and microstructural studies of cobalt-based compounds and iron obtained by mechanical alloying	OC22D
M. Naous , F. Bouanani S, Rubio Bravo <i>University of Oran, Algeria</i> Application of hybrids magnetic nanoparticles for extraction of aromatic amines from environmental samples	OC42D

Communicatings' Names	Ref
R. Nasri , T. Larbi, M.F. Zid <i>FST - Tunis</i> Structural, Spectroscopic Analysis and Photocatalytic Activity of $K_2Co_2(MoO_4)_3$	OC23D
W. Nbili , C. Ben Nasr <i>FSB - Bizerte</i> A Hirshfeld surface analysis, crystal structure and physicochemical studies of a Cd (II) complex with the 4,4'-dimethyl-2,2'-dipyridyl ligand	OC24D
A. Nouria , S. Attia-Essaies, E. Srasra <i>CNRSM - Borj Cédria</i> Elaboration and thermal study of composites from used polystyrene	OC13B
F. Nouri , R. Ternane <i>FSB - Bizerte</i> Synthesis, electrical and dielectrical properties of phosphate-sulfate fluorapatites $Ca_{10-x}Na_x(PO_4)_{6-x}(SO_4)_xF_2$	OC25D
Z. Ouerghi , T. Roisnel, R. Fezai, R. Kefi <i>FSB - Bizerte</i> Physico-chemical characterization, Hirshfeld surface analysis and opto-electric properties of a new hybrid material: Tris (2-amino-5-chloropyridinium) hexachlorobismuthate(III)	OC26D
H. Raissi , T. Boubaker <i>FSM - Monastir</i> Electrophilicities of benzofurazans and correlations structure-reactivity	OC28C
S. Raouafi , F. Aloui, B. Ben Hassine <i>FSM - Monastir</i> Synthesis and optical properties of new pentacyclic helicenes	OC34C
A. Rejab , H. Ksibi, S. Rodriguez Rojo, M.J. Cocero <i>ENIS - Sfax</i> Study and valorization of the active principles of some plants of southern Tunisia	OC41C
E. Rezgui , C. Issaoui, N. Ouerfelli <i>FST - Tunis</i> Relationship between crystal structure and electric properties of $LiFePO_4$, and cations conduction pathways simulation is approved by the bond valence sum	OC27D
S. Rhouma , S. Saïd, C. Autret, A. Megriche <i>FST - Tunis</i> Dielectric properties of $Ca_{0.9}Sr_{0.1}Cu_{2.9}Mg_{0.1}Ti_4O_{12}$ (CSCMTO) – x $SrTiO_3$ (STO) composites prepared by solid-state reaction	OC28D
Y. Saad , I. Alvarez-Serrano, M.L. López, M. Hidouri <i>FSM - Monastir</i> Microstructural characterization and thermistor behavior of lead-free x $NaNbO_3$ - (1-x) $BiFeO_3$ electroceramics	OC29D

Communicatings' Names	Ref
<u>F.Z. Sadiki</u> , M. El Idrissi , A. Amchrouq, M. Sbity , L. Hritcu , P.A. Postu , O. Cioanca, A. Trifan <i>University Moulay Ismail, Meknès, Morocco</i> Chemical composition, antibacterial and antioxidant activities of essential oils of <i>Pinus halepensis</i> Mill. and <i>Tetraclinis articulata</i> (Vahl) Masters	OC42C
<u>M.A. Saidani</u> , A. Fkiri, L.S. Smiri <i>FSB - Bizerte</i> Facile synthesis of Ag/ZnO photocatalysts on the degradation of diuron herbicide under solar light and the investigation of its antibacterial activity for waste-water treatment	OC30D
<u>N. Saidani</u> <i>FSB - Bizerte</i> Electrochemical copolymerization of fluoro-functionalized conducting polymers	OC14B
<u>M. Saidi</u> , F. Fourcade, F. Geneste , A. Amrane, N. Bellakhal <i>INSAT - Tunis</i> Electrochemical oxidation of chlortetracycline antibiotic on a nickel foam electrode: Biodegradability improvement	OC37B
<u>M. Saidi</u> , S. Walha, A. Kabadou, M. Jemmali, L. Bessais <i>FSS - Sfax</i> Isothermal section of the Gd-Fe-Cr ternary system at 800°C	OC9B
<u>M.M. Saoudi</u> , A. Khaled, J. Bouajila <i>FST - Tunis</i> Phenolic composition and biological activities of <i>Rumex crispus</i> , <i>Rumex roseus</i> and <i>Diplotaxis Simplex</i>	OC7C
<u>M. Sellami</u> , M. Barre, M. Toumi <i>FSS - Sfax</i> Structural, thermal and dielectric properties of phosphoric acid-based geopolymer with Metakaolin	OC32D
<u>D. Sghairi</u> , M. Romdhani-Younes, J. Thibonnet <i>FST - Tunis</i> Synthesis and reactivity of 3-amino-propiolate derivatives	OC30C
<u>A. Sidhom</u> , J.F. Soulé, H. Doucet, F. Allouche <i>FSS - Sfax</i> The formation of 5- and 6-membered rings through Pd-catalyzed intramolecular direct arylations of 5-aminopyrazoles bearing 2-bromoaryl substituents on the amino group	OC31C

Communicatings' Names	Ref
S. Souissi , T. Boubaker <i>FSM - Monastir</i> Quantification of the electrophilic reactivities of substituted thiophenes and correlations structure-reactivity	OC32C
W. Talbi , Y. Kacem, J. Kraiem <i>FSM - Monastir</i> A simple and green synthesis of thiazolines and oxazolines	OC33C
N. Tandjaoui , M. Abouseoud, A. Couvert, A. Amrane <i>University Ibn Khaldoun, Tiaret, Algeria</i> Elimination of phenolic compounds from waste air by absorption and enzymatic biodegradation	OC36B
N. Touj , M. Sauthier, L. Mansour, N. Hamdi <i>FSB - Bizerte</i> Efficient N-heterocyclic carbene palladium (II) catalysts formed in situ for carbonylative SUZUKI coupling reaction of arylboronic acids with 2-bromopyridine under co pressure leading to unsymmetrical arylpyridine ketones: Synthesis, characterization and cytotoxic activities	OC29C
A. Wederni , E. Pineda, L. Escoda, J.J. Suñol, M. Khitouni <i>FSS - Sfax</i> Magnetic properties, martensitic and magneto-structural transformations of ferromagnetic Ni-Mn-Sn-Cu shape memory alloys	OC34D
A. Yahia , C. Fersi, F. Touati <i>INRAP - Sidi Thabet</i> Substitution of chemical coagulants by biopolymers for the treatment of tannery wastewater	OC38B
I. Zghal , J. Farjas, J. Camps, P. Roura, M. Dammak <i>FSS - Sfax</i> Thermogravimetric measurement of the equilibrium vapour: Application to water and triethanolamine	OC11B
C. Zidani , B. Benyoucef <i>University of Tlemcen, Algeria</i> Analysis of a novel design of conical solar furnace supplied by optical fibers	OC15B
M. Zine Elabidine , A. Bechrifa, A. Contreras, D.S. Brauer, I. Khattech <i>FST - Tunis</i> Optimization of composite synthesis by sintering process	OC35D
M.O. Zouaghi , B. Champagne, Y. Arfaoui <i>FST - Tunis</i> Theoretical study of physical and optical properties of metallo-phthalocyanine derivatives	OC12B

Oral Communications' Abstracts



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CRYSTAL STRUCTURE, THERMAL BEHAVIOR AND MAGNETIC PROPERTIES OF $(C_4H_{14}N_2)[CuBr_{2.19}Cl_{1.81}]$

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A new bromide-chloride copper (II) templated by 1,4-diaminobutane was synthesized and crystallographically characterized by single-crystal X-ray diffraction. The title compound crystallizes in the monoclinic space group $P2_1/c$ with two formula unit per cell and the following parameters: $a = 9.3580(10)$ Å; $b = 7.7360(10)$ Å; $c = 7.7590(10)$ Å, $\beta = 102.833(9)^\circ$ and $V = 102.833(9)$ Å³.

The 2D structure is formed of a metallic layer parallel to the (b,c) plane obtained by corner sharing between octahedra built of copper(II) cation surrounded by six bromide/chloride anions. The protonated diamine is linked in the space between two anionic layers. The thermal decomposition of the precursor proceeds through three stages giving rise to the copper oxide as a final product. The optical study reveals that the title compound undergoes three optical absorption bands at 318, 460 and 774 nm, respectively. The gap energy value is 3.21 eV which confirms that the new hybrid compound is a semiconductor material. The magnetic measurements show that the title compound present interesting ferromagnetic interactions.

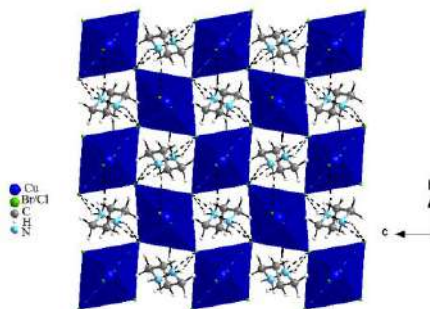


Figure: Projection of the structure along the a -axis.

Key words: Hybrid material, 2D structure, IR spectroscopy, thermogravimetric measurement, Magnetic properties.

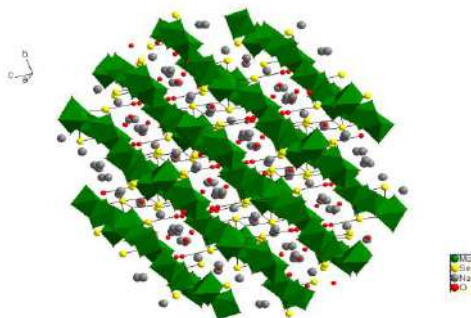
Synthesis, Structure of a New Sodium Selenomolybdate Compound $\text{Na}_4 [\text{Se}_2\text{Mo}_5\text{O}_{21}]\cdot 5\text{H}_2\text{O}$

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Polyoxometalates (POMs) as early-transition-metal oxide clusters have received much attention in various fields such as catalysis, ion exchange, electrochemistry, magnetism and medicine for their enormous variety of structures and unique properties [1-4]. Because of this importance, it was of interest to synthesize a new member of pentamolybdates $\text{Na}_4 [\text{Se}_2\text{Mo}_5\text{O}_{21}]\cdot 5\text{H}_2\text{O}$ and to investigate. The title compound was crystallized in the triclinic system, space group P-1 with $a = 11.1600 \text{ \AA}$, $b = 14.3948 \text{ \AA}$, $c = 14.9613 \text{ \AA}$, $\alpha = 89.963^\circ$, $\beta = 76.072^\circ$, $\gamma = 86.640^\circ$, $Z = 8$.

The structure is characterized by the presence of clusters $[\text{Se}_2\text{Mo}_5\text{O}_{21}]^{4-}$ type Strandberg. The association of these units with Na^+ ions as well as water molecules by means of hydrogen bonds and electrostatic interactions, leads to a complex three-dimensional structure. The crystal structure of compound is stabilized by an extensive network of hydrogen bonds. Theoretical and experimental studies were reported in this work; thermal, electrochemical and spectral analysis also Hirshfeld surface study



View perspective of the compound (1)

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Synthesis and characterization of sodium and carbonate co-substituted hydroxyfluorapatite

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Sodium and carbonate co-substituted hydroxyfluorapatite were prepared by double decomposition method. The obtained powders were investigated by X-ray diffraction, infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy. For $x \leq 3.5$, all the diagrams indicate that the prepared powders are single-phase apatite. Above this value the excess of CaCO_3 remained unreacted. The parameter a decreased progressively with the increase of content of CO_3^{2-} and Na^+ while the parameter c increased. The introduction of CO_3^{2-} and Na^+ in the apatite framework involved a decrease of the crystallinity of the as prepared powders due to the reduction of the particle size. The as prepared powders treated at 1000°C revealed a partial decomposition of the carbonate apatite phase with CO_2 releasing and CaO formation.

Study of supported La_2CuO_4 perovskites for reverse water gas shift reaction

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Recently, the global carbon dioxide atmospheric concentration reached the 400 ppm threshold and emissions are expected to increase to 45 Gt/year by 2040 due to population and economic growth [1]. Various strategies of carbon capture and sequestration (CCS) at large emission sources such as power plants are needed to decrease the level of accumulation of CO_2 in the atmosphere. CCS is considered a potential CO_2 mitigation technique, but this method will not be able to migrate more than 1% of the global CO_2 emissions. Here, an alternative to CCS is proposed, where CO_2 can be transformed to high-value chemicals needed to close a synthetic carbon cycle. The reverse water gas shift reaction (RWGS) is a promising route, where the reaction of CO_2 and hydrogen (H_2) produces carbon monoxide (CO) and water (H_2O): $\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ $\Delta H^\circ = 41.2 \text{ kJ.mol}^{-1}$. Furthermore, produced CO and H_2 can be used to produce long-chain hydrocarbons ($\text{CO} + (y/2x+1) \text{H}_2 \rightarrow (1/x) \text{C}_x\text{H}_y + \text{H}_2\text{O}$) and high value-added chemical raw materials ($n\text{CO} + (2m+n-1)/2\text{H}_2 \rightarrow \text{C}_n\text{H}_{m-1}\text{OH} + (n-1) \text{H}_2\text{O}$) via the Fischer-Tropsch reaction. The produced water can be separated by simple condensation and then water electrolysis is employed to produce H_2 . Thus, the carbon neutral cycle can be created with CO_2 as an energy carrier via the RWGS reaction to achieve zero emission of CO_2 . Much attention has been paid recently to perovskite-type oxides as catalysts due to their activity and thermal stability. As opposed to using bulk single-phase catalyst pellets, the inclusion of supporting materials is necessary to improve perovskite surface area and accelerate oxygen self-diffusion. Within this context, the aim of this work is the study of the catalytic performance of ceria supported on La_2CuO_4 in RWGS. Several characterization techniques were employed to gain information on the chemical structure and catalytic behavior of supported catalysts $x\%\text{CeO}_2/\text{La}_2\text{CuO}_4$, such as XRD (Fig1), S_{BET} and H_2 -TPR. Their catalytic activity has been tested under RWGS conditions in combination with *operando*-DRIFTS in order to establish main structural and catalytic properties for this type of materials.

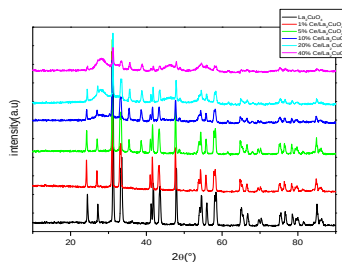


Figure 1. XRD profiles of $x\%\text{CeO}_2/\text{La}_2\text{CuO}_4$

Keywords: reverse water gas shift, CO_2 , CeO_2 , perovskite, La_2CuO_4 .

Reference

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Structural, Physico-chemical Properties and Theoretical Study of a new Organic Nitrate Crystal ($C_9H_{11}N_2O_5$)₂ (NO_3)₂

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Crystals of 3-nitrotyrosinium nitrate has been prepared and grown at room temperature. This compound crystallizes in the monoclinic system with non-centrosymmetric P2₁ space group. The unit cell dimensions are a = 13.8275 (10) Å, b= 5.7666 (4) Å, c= 15.5280 (12) Å with V= 1211.10 (16) Å³ and Z = 4. The structure has been solved using direct method and refined to a reliability R factor of 0.053.

The structure of this compound was determined by using X-ray data collection on single-crystal. The 3-nitrotyrosinium nitrate structure consists of 3-nitrotyrosinium cations ($C_9H_{11}N_2O_5^+$) and nitrate anions (NO_3^-) interconnected by a system of hydrogen bonds so as to build a three dimensional arrangement.

In the present work, we describe the crystal structure. The UV-visible, thermal behavior and the IR spectroscopic studies of this new compound are discussed. The optimized molecular structure, HOMO–LUMO energy gap and the optical properties have been performed, using the density functional theory (DFT) method, at B3LYP/6-31G (d,p).

Key words: Hybrid; X-ray diffraction; DFT calculus; infrared spectroscopy; Thermogravimetric analysis, optical properties.

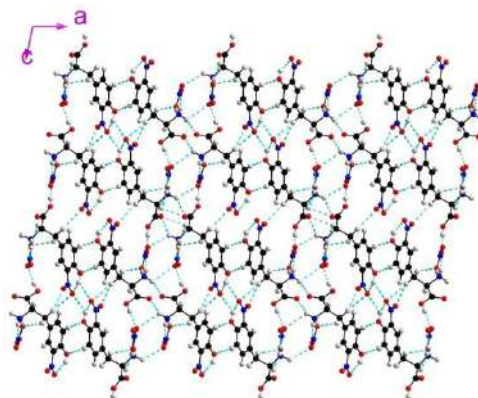


Fig.1. Projection along the b-axis of the atomic arrangement in ($C_9H_{11}N_2O_5$)₂ (NO_3)₂

A NOVEL MEMBER OF MO₃₆-POLYOXOANION'S FAMILY BASED ON AMMONIUM CATIONS: SYNTHESIS AND PHYSICO-CHEMICAL CHARACTERIZATION

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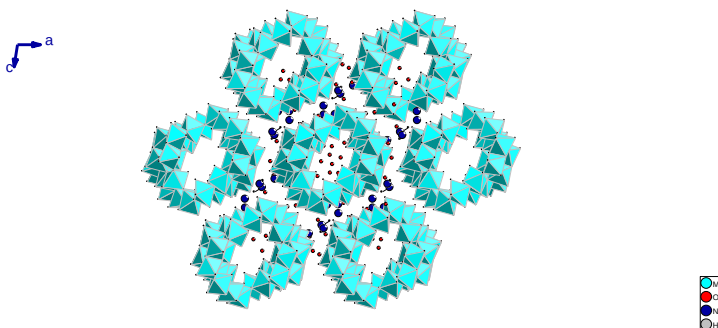
A new Mo₃₆-polyoxomolybdate with ammonium cations formulated as (NH₄)₁₀[Mo₃₆O₁₁₀(OH)₆(H₂O)₁₂].n H₂O was synthesized by conventional solution method at room temperature.

It was structurally characterized by single-crystal X-ray diffraction methods. The title compound crystallized in the monoclinic system, space group P2₁/n with unit a = 16.4782(2) Å, b = 18.6844(2) Å, c = 24.6484(3) Å, β = 90.945(1)°, V = 7496.58(2) Å³.

In fact, the clusters are connected to the ammonium cations via Hydrogen bonds to create a supramolecular structure.

The refinement of the structure led to a residual factor R = 0.034.

Key words: Giant polyoxomolybdates, synthesis and crystal structure, X-ray diffraction, infrared spectroscopy, UV-VIS, TG analysis.



The packing view of the compound (NH₄)₁₀[Mo₃₆O₁₁₀(OH)₆(H₂O)_n].n H₂O
along the b axis

Crystal structure, quantum mechanical investigation, IR and NMR spectroscopy of new Perchlorate : $(2-(1-C_4H_9N_2)C_4H_5N_2).(ClO_4)_2$

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Hydrogen bonds of hybrid compounds are of great interest because of their widespread biological occurrence [1, 2]. The supramolecular networks become especially interesting when the cation and anion can participate in hydrogen-bonding. In recent years, much attention has been devoted to the study of perchlorate salts containing organic cations owing to their interesting properties such as ferroelectric and dielectric behaviors [3].

In the present contribution, we report the synthesis and characterization of a new organic perchlorate 2-(1-piperazinyl)pyrimidinium bis(perchlorate). Molecular structure is determined by single crystal X-ray diffraction analysis. The unit formula of this compound, contains two inorganic perchlorate anions and one $[2-(1-C_4H_9N_2)C_4H_5N_2]^{2+}$ dication (Fig. 1). This compound crystallizes in the monoclinic space group $P2_1/c$ ($Z = 4$). In the atomic arrangement, the organic cations are inserted between the mineral anions via N-H...O and C-H...O interactions ensuring the cohesion and the stability of the crystalline edifice so as to generate a three dimensional structure (Fig. 2). The vibrational absorption bands were identified by infrared spectroscopy. This compound is also investigated by solid-state ^{13}C , ^{35}Cl and ^{15}N CP-MAS NMR spectroscopy. DFT calculations allowed the attribution of the IR and NMR bands.

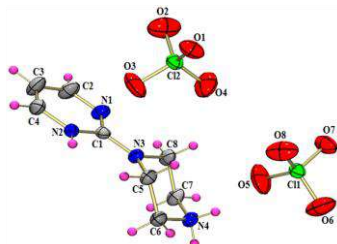


Fig. 1: Asymmetric unit of $(2-(1-C_4H_9N_2)C_4H_5N_2).(ClO_4)_2$

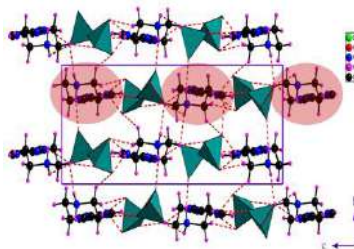


Fig. 2: The crystal packing of $(2-(1-C_4H_9N_2)C_4H_5N_2).(ClO_4)_2$ viewed along the a axis.

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Synthesis, crystal structure and ionic conduction of $\text{Na}_{5.22}\text{Cu}_{1.89}\text{Al}(\text{AsO}_4)_4$

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Blue single crystals of $\text{Na}_{5.22}\text{Cu}_{1.89}\text{Al}(\text{AsO}_4)_4$ have been prepared by solid state reaction and have been characterized by X-ray diffraction techniques, scanning electron microscopy and the electrochemical impedance spectroscopy. The structure (triclinic, P-1, $a=5.111$ (2) Å, $b=7.577$ (7) Å, $c=9.332$ (3) Å, $\alpha=88.73^\circ$ (2), $\beta=75.74^\circ$ (3), $\gamma=89.56^\circ$ (2)) can be described as a three-dimensional framework resulted from corner-connection between MO_5 ($M=\text{Cu}, \text{Al}$) square pyramids and AsO_4 polyhedra. This architecture gives rise to tunnels running along the [100] direction where the sodium ions are located. The ionic conductivity measurements are performed on pellet with relative density of 95 %. The highest overall conductivity of $1.5 \times 10^{-5} \text{ S.cm}^{-1}$ was found at 575°C with $E_a=1.14 \text{ eV}$.

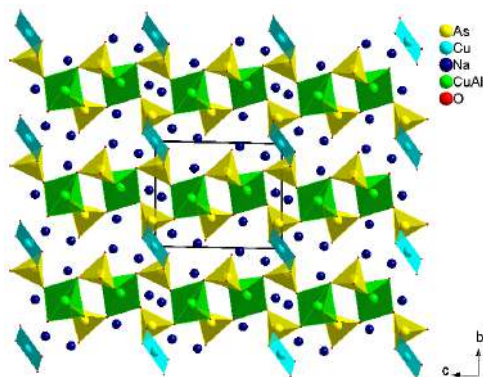


Figure: Projection of $\text{Na}_{5.22}\text{Cu}_{1.89}\text{Al}(\text{AsO}_4)_4$ structure along the a axis.

Keywords: XRD, Crystal structure, Impedance spectroscopy, Ionic conductivity.

Synthesis and Electrical properties of $\text{Na}_6\text{Mg}_{1-x}\text{Co}_x(\text{SO}_4)_4$ Vanthoffite ceramics

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$\text{Na}_6\text{Mg}_{1-x}\text{Co}_x(\text{SO}_4)_4$ ceramics denoted as NMCoSx ($x=0.1, 0.3, 0.5, 0.7$ and 1) were obtained via the solid state reaction method. Refinement of structural parameters confirmed that the Co^{2+} dopant can replace the magnesium in this structure with a slight increase of the lattice parameters. The spectroscopic studies by means of infrared (IR) and visible (Vis) spectroscopies revealed the vibrational mode of sulfate groups and verified the amount of cobalt inserted in the host lattice. Electrical conductivity was studied by impedance spectroscopy in the [553–733 K] temperature range and results show that the materials present a semiconductor ionic character and the conductivity increases when the Co^{2+} dopant content x increases. Results also show that at low temperatures, NMCoSx ($x = 0.5$) has the highest electrical conductivity representing a candidate that may be used as an electrode in sodium-ion batteries.

EFFECT OF ADDITION OF DIFFERENT PROMOTER ON THE PERFORMANCE OF CoFe_2O_4 CATALYST IN CO-PROX

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In general, the catalytic activity of a catalyst depends on several factors such as the nature of the support, the addition of the promoter, the particle size and the nature of the pretreatment. Various catalysts have shown good performance for preferential CO oxidation process (CO-PROX). Spinel based catalysts have been widely used in this process. It has been shown that their catalytic properties depend strongly to the characteristics of contact established between the promoter and the spinel support [1]. The objective of this work is to highlight the effect of the addition of different promoters, namely Ce, Cu and Zr to CoFe_2O_4 catalyst on its performance in CO-PROX. Therefore, the Ce/ CoFe_2O_4 , Zr/ CoFe_2O_4 and Cu/ CoFe_2O_4 catalysts were prepared by the impregnation method.

Comparing the CO conversion curves and selectivity of CO_2 of the three prepared catalysts during the CO-PROX oxidation reaction it is possible to conclude that CoFe_2O_4 catalyst gives the better catalytic activity. The differences in behavior of the prepared catalysts were explained based, firstly, on the type of contacts between the three promoters and the support and secondly on the analysis results of their catalytic activities complemented by operando-DRIFTS.

Keywords: CoFe_2O_4 ; CO-PROX; catalytic activity; DRIFTS.

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Sol-gel Chemistry Autocombustion Synthesis and DTA-TGA, XRPD, SIC, ^7Li , ^{63}Cu MAS-NMR and Magnetic Studies of the Li-Cu Substituted Cobalt Ferrite Nanoparticles $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

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The Li-Cu substituted CoFe_2O_4 nanoferrite: $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$, has been synthesized by sol-gel autocombustion method in order to obtain a pure nanosized powder and then characterized by the following physicochemical techniques: coupled DTA-TGA, XRPD, CIS, ^7Li - ^{63}Cu MAS-NMR and SQUID magnetometry measurements. The thermal behavior, before and after the autocombustion of the studied material, has been deduced from its DTA-TGA thermogram (Figure 1). Whereas, the recorded XRP diffractogram, (Figure 2), has been indexed in the spinel cubic system with Fd3m space group and the unit cell parameter, $a = 8.371 \text{ \AA}$, has been calculated by the least square fit refinement. Moreover, the CIS study has highlighted the best total electric conductivity, $\sigma_{\text{Tot}}(373\text{K}) = 8.96 \times 10^{-3} \text{ S.cm}^{-1}$, and as a result enhance the excellent lithium fast cation conductor behavior of the title nanoferrite (Figure 3-4). However, the ^7Li - ^{63}Cu MAS-NMR spectroscopy study permitted to conclude that both lithium and copper cations occupy only one crystallographic site each one (Figure 5-6). Furthermore, the magnetic measurements in the ZFC-FC and hysteresis modes have put in evidence the ferrimagnetic and superparamagnetic behavior of the studied nanoferrite below and above the blocking temperature, $T_b = 292.69 \text{ K}$, respectively (Figure 7-8), with intrinsic magnetic parameters: $M_s = 61.538 \text{ emu/g}$, $M_r = 27.500 \text{ emu/g}$, $H_c = 10.171 \text{ KOe}$.

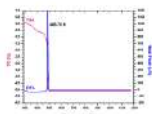


Figure 1: The Thermogram DTA-TGA of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

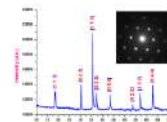


Figure 2: The X-Ray Powder Diffractogram of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

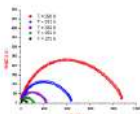


Figure 3 : The Impedance Diagram of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

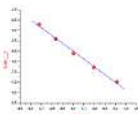


Figure 4 : Arrhenius Plot of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

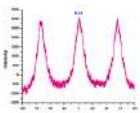


Figure 5 : ^7Li MAS NMR spectrum of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

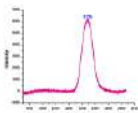


Figure 6: ^{63}Cu MAS NMR spectrum of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

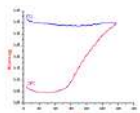


Figure 7 : The Recorded ZFC-FC Magnetization of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

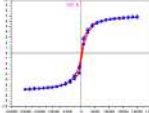


Figure 8 : The 300 K hysteresis loop of the Nanomaterial $\text{LiCu}_{0.5}\text{Co}_{0.75}\text{Fe}_{1.5}\text{O}_4$

Optical, Photophysical and Electrochemical properties of phenoxazine and phenothiazine derivatives for OLED applications

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Recently, organic fluorescence emitters with Thermally Activated Delayed Fluorescence (TADF) have attracted much attention in that these materials use thermally activated up-conversion of triplet (T1) into singlet (S1) state, giving stable fluorescence with very high singlet yields [1-3]. TADF materials, similar to the emitters for the high efficient Organic Light Emitting Diodes (OLEDs) by charge-transfer (CT) excited state, require a sufficiently small energy gap between the triplet and singlet (ΔE_{ST}) to enable up-conversion of the triplet excitons to singlet excitons and realize 100% internal quantum efficiency of the exciton formation generated by electric excitation at S1. Thus, enormous efforts have been endeavoured to minimize ΔE_{ST} and then enhance the reverse intersystem crossing (RISC) by molecular structure design, leading to the maximization of TADF. Nowadays, particularly designed organic materials with donor-acceptor structures are used to minimize the HOMO-LUMO overlap.

Four new phenoxazine and phenothiazine luminescent derivatives were synthesized and fully characterized. Their design had in mind their potential TADF properties, which were confirmed to different extents, depending on the molecular structure. Globally, the four derivatives can be applied in OLED devices with good efficiency.

Keywords

Organic Light Emitting Diodes, internal quantum efficiency, Thermally Activated Delayed Fluorescence

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Crystal structure, Hirshfeld surface analysis and energy framework calculations of a new organic perchlorate, (C₉H₁₀N₃)[ClO₄]

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A new 3-amino-5-phenylpyrazolium perchlorate, (C₉H₁₀N₃)[ClO₄] (**I**), has been synthesized by slow evaporation at room temperature and characterized by single crystal X-ray diffraction. Compound (**I**) crystallizes in the monoclinic system with the space group C2/c, Z=4, and unit cell parameters $a = 26.768$ (2) Å, $b = 5.444$ (2) Å, $c = 15.027$ (2) Å, $\beta = 96.148$ (2)°. The molecular aggregations are stabilized through intricate three dimensional hydrogen bonding network formed by the classical N-H...O hydrogen bonds. The three-dimensional Hirshfeld surface (3D-HS) [**1**] and the two-dimensional fingerprint plots (2D-FP) [**2**] reveal that the structure is dominated by H...O/O...H (38.2%) and H...H (25.9%) contacts (**Fig.1**). In addition, energy framework calculations were used to analyse and visualize the three dimensional topology of the crystal packing. The electrostatic energy framework is dominant over the dispersion energy framework.

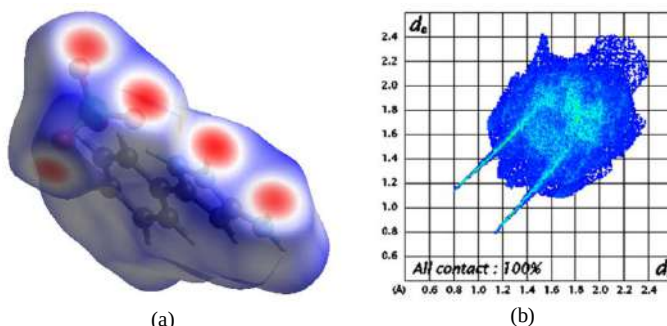


Fig.1: View of the 3D-HS mapped with d_{norm} (a) and the 2D-FP of (**I**) showing all contacts (b).

Key words: crystal structure, organic perchlorate, Hirshfeld surface.

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Influence of minor additions of Fe and Co on the azo dye degradation ability of Mn-Al particles.

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Azo compounds are one of the most common families of dyes used in textile and leather treatments. An important step during the treatment of water polluted by these compounds is the degradation of the compounds by breaking the N=N bonds, producing the de-colorization of the water. In this work, we present the decolorization of reactive black 5 solutions using Mn-Al-Co and Mn-Al-Fe nanostructured powders produced by ball milling. The morphology and the phase structure of the metallic powders were characterized by scanning electron microscopy coupled with EDS microanalysis and by X-Ray diffraction. The decolorization efficiency of reactive black 5 solutions were assessed by monitoring the dye degradation by ultraviolet/visible absorption spectrophotometry. Fe doped Mn-Al showed a fast kinetics and high efficiency. 40 mgL⁻¹ of dye solution was successfully decolorized in 5 min using 0.25 g / 100 mL of powders, even in neutral pH conditions. On the other hand, Mn-Al-Co powders were able to successfully decolorize the dyed solution in 10 min in the same conditions. The efficiency of the intermetallic particles is higher than those found with Mn particles. The efficiency was also checked in other azo dyes solutions. To summarize, nanocrystalline Fe-doped Mn-Al exhibits superior properties, such as high reactivity and efficiency, wide applicability and low corrosion loss, in comparison with Co-doped in the same alloys.

Keywords: Ball milling; Reactive Black 5; Decolorization; UV-visible spectrophotometry, LC-MS analyses.

**Thermophysical properties of the binary mixtures
of Methyl levulinate + C1-C4 n-Alkanol
and Ethyl levulinate + C1-C4 n-Alkanol at 298.15 K**

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The thermophysical behavior of eight binary mixtures formed by methyl levulinate or ethyl levulinate with methanol, ethanol, 1-propanol, or 1-butanol has been studied through the measurement of density, ρ , and speed of sound, u , over the whole composition range at $T = 298.15$ K and $p = 0.1$ MPa. From experimental results, excess volumes, V^E , and excess isentropic compressibilities, K_S^E , have been calculated. In addition excess molar enthalpies, H^E , has been also determined. All the binary systems analyzed present negative excess isentropic compressibilities and positive excess molar enthalpies over the whole composition range. The excess volumes are negative for the mixtures containing methanol or ethanol and turn to positive for those containing 1-propanol or 1-butanol. Finally, the excess properties obtained in this work have been discussed taking into consideration the associated character of components, methyl levulinate or ethyl levulinate and alkanols. The results obtained were discussed in terms of structural effects and specific molecular interactions. The influence of the alkanol chain length was considered.

Keywords: Alcohols ; Thermophysical properties ; Density ; Ethyl levulinate ; Excess properties ; Methyl levulinate ; Speed of sound.

Poorly crystalline hydroxyapatite for cadmium removal in aqueous medium

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Cadmium is a toxic, cumulative and classified as carcinogenic of category. It's the third most ubiquitous heavy metal in drinking water. Therefore, the development of effective remediation techniques becomes of a great interest. In this context, adsorption on apatites used to be a very interesting method to recover toxic metals from contaminated waters. Indeed, these materials are thermally stable, low soluble and non-harmful for the environment.

This study includes an optimisation of various parameters affecting the cadmium fixation on this material and particularly the heat treatment.

The synthesis of hydroxyapatite having the general formula $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ was carried out by the "double decomposition method". It consists in adding, drop by drop, a solution of diammonium hydrogen phosphate into a boiling solution of calcium nitrate with a molar ratio of reactants Ca/P equal to 1.67. The pH of precipitation has been maintained close to 11 by successive additions of ammonia solution. The dried precipitate was ignited at different temperatures ranging from 100°C to 800°C.

The identification of the functional groups of the hydroxyapatite was carried out by IR spectroscopy analysis, whereas the characterization of the mineral phase by X-ray diffraction allowed determining the lattice parameters of the apatite. The Brunauer, Emmett and Teller (BET) method was applied to study the effect of the heat treatment on the surface properties of the product.

The sorption study was carried by "batch" technique. The highest capacity of Cd retention was observed with the materials treated at low temperatures.

Keywords: cadmium; hydroxyapatite; adsorption; heat treatment.

RADIOLYSIS OF IBUPROFEN AND KETOPROFEN IN AQUEOUS SOLUTIONS BY IRRADIATION PROCESS

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Among processes responsible for pollutant removal in water systems, the last decade brought significant development of novel processes based on efficient reactions of free radicals, where of special importance are advanced oxidation processes based on the use of hydroxyl radical •OH. One of the most efficient ways of their production is water radiolysis by the use of ionizing radiation. In the present work, the degradation of ketoprofen (KET) and Ibuprofen (IBP) was investigated in aqueous solutions using gamma radiolysis. Due to its resistance to biodegradation and resistance against conventional wastewater treatments, these compounds were detected in the aquatic environment at trace concentrations.

In this study aqueous solutions having different concentrations 0.1-1 mmol/L, were irradiated with irradiation doses from 3 to 15 kGy, by a Cobalt-60 source with an absorbed dose rate of 6.1 kGy/h rate. This work is focusing on testing the efficiency of this process on pharmaceuticals removal. It involved testing the effect of the initial concentration of the target drug and the absorbed dose on the degradation of selected samples. A sophisticated analytical study was released to quantify the detected radio-induced radicals (EPR and HPLC). The findings showed that gamma irradiation is effective in removing of IBP and KET from aqueous solutions and tends to remove the chemical oxygen demand (COD) and concentration of radio-induced radicals confirming their synergistic effect to attempt total mineralization.

Key.words: pharmaceuticals- gamma irradiation- hydroxyl radical-HPLC- EPR.

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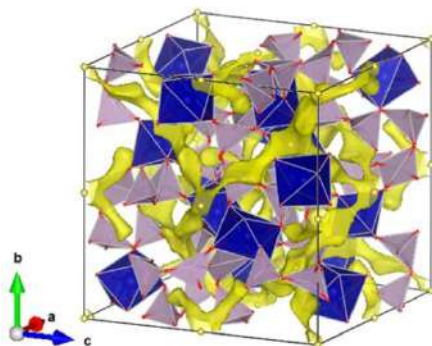
Transport pathways simulation of cations in crystal materials

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The simulation of transport pathways of cations, anions or protons in crystal structure is the best way to explain the electrical behavior of materials. The prediction of electrical and electro-chemical properties of materials based on theoretical study can be very useful to reduce time and fee of experiences. Thus, it is a new vision to take the good way of investigation. In this aim, the Density functional theory **DFT** and molecular dynamics **MD** are the two well know tools to study the crystal structure [1-2]. Unfortunately, calculation using this two theories take lot of time and need a workstation with excellent performance. Therefore, an alternative way take place in this aim, it is the use of new static calculation models such as **BVS (Bond Valence Sum)** [3], **BVSM (Bond Valence Sum Mapper)** [4] and **BVSE (Bond Valence Site Energy)** [4]. The advantage of these static models is: they can be used on personal computer with few calculation time. Nevertheless, the disadvantage of static models are not yet resolved.

Keywords: DFT, MD, BVS, BVSM, BVSE



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Theoretical Study on the Conformations and the Tautomerization Processes of Glyphosate In Aqueous Solution

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A theoretical investigation on the conformational analysis of the commercially most successful herbicide compound, **Glyphosate (N-(phosphonomethyl)glycine)**, have been made at various quantum chemical levels of theory RHF, B3LYP and MP2 with different basis sets in the gas phase and in solution. The effect of the inclusion of an empirical term to standard DFT (DFT-D) in the prediction of the conformational energies and in assessing the relative stabilities between the conformers has been analyzed. The results calculated at different levels of theory were compared. From this study, zwitterionic structures were found preferred over the neutral uncharged structures, in good accord with the experimentally determined X-ray structure of pure Glyphosate as well as with the observations of analogous bioactive molecules in solution. All the possible tautomerization processes (zwitterion→neutral form) of glyphosate were studied in aqueous solution. The activation barriers needed for the proton transfer to occur have been calculated. The results obtained allowed to elucidate the limiting step for the tautomerization of Glyphosate in aqueous solution.

Key words: Glyphosate; Quantum Chemical Calculations; Conformations; Tautomerization

Thermoelectric properties of new chalcogenide layered compounds

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Thermoelectric materials are outstanding to transform temperature differences directly and reversibly into electrical voltage. Exploiting waste heat recovery as a source of power generation could help towards energy sustainability. Recently, the SnSe semiconductor was identified, in single-crystal form, as a mid-temperature thermoelectric material with record high figure of merit, high power factor and surprisingly low thermal conductivity. We describe the preparation of polycrystals of alloys of SnSe obtained by arc-melting; a rapid synthesis that results in strongly nanostructured samples with low thermal conductivity, advantageous for thermoelectricity, approaching the amorphous limit, around 0.3–0.5 W/mK. An initial screening of novel samples $\text{Sn}_{1-x}\text{M}_x\text{Se}$, by alloying with 3d and 4d transition metals such as $\text{M} = \text{Mn}, \text{Y}, \text{Ag}, \text{Mo}, \text{Cd}$ or Au , provides for a means to optimize the power factor. $\text{M} = \text{Mo}, \text{Ag}$, with excellent values, are described in detail with characterization by x-ray powder diffraction (XRD), scanning electron microscopy (SEM), and electronic and thermal transport measurements. Rietveld analysis of XRD data demonstrates near-perfect stoichiometries of the above-mentioned alloys. SEM analysis shows stacking of nanosized sheets, with large surfaces parallel to layered slabs. An apparatus was developed for the simultaneous measurement of the Seebeck coefficient and electric conductivity at elevated temperatures.

Keywords : thermoelectrics, nanostructuration, lattice thermal conductivity, thermopower, SnSe alloying.

Scrubbing of gaseous nitrogen oxides in cables-bundle contactor

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In this work, the removal of dilute nitrogen oxides NO_x from the gaseous effluents by absorption into aqueous nitric acid solutions containing or not hydrogen peroxide, was studied. All continuous absorption tests were carried out at ambient conditions and at 50 Pa as NO_x partial pressure. The effects of the oxidation ratio, the presence of HNO₃ and the initial H₂O₂ concentration on the NO_x absorption efficiency (A_{NO_x}), were studied. The tests results revealed that A_{NO_x} increases with an increase in OR and in initial H₂O₂ concentration in the scrubbing liquid, but decreases with the presence of HNO₃ without H₂O₂.

Prediction of Polyion Conformation and Interpretation of some Anomalies of Polyelectrolytes in terms of Superposition principle and Dielectric friction.

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Contrarily to electrolytes, dilute polyelectrolyte solutions do not obey to Debye limiting law characterized by a linear decreases of their thermodynamic and transport properties with the square root of the ionic force.

This difference results from the high-density charge of the polyions, which leads to the ionic condensation process, and to the flexibility of the polyion chain and to its ability to change conformation.

However, despite the recent progress of polyelectrolyte theories based on the scaling concepts [1], and on the generalization of Manning's model, at different concentration regimes, the great interdependence between polyion conformation, counterion condensation process and frictional process remain incompletely explained.

On the other hand, experiments show in some conditions, that the degree of condensation of counterions remains constant in a large range of concentration. This anomaly not observed in computer simulations, seems to be in contradiction with the Ostwald's principle.

Moreover, translational dielectric friction on polyions is ignored by the present theories despite its important role for stretched polyion chains.

Finally, both hydrodynamic and ionic frictions on polyions cannot completely explain the abnormal behavior of the equivalent conductivity of some polyelectrolytes with the nature of the counter-ions in complete contradiction with Kohlraush law.

In this oral contribution, the flexible conformation of polyions is represented by an ellipsoid characterized by a variable eccentricity, a structural charge, a structural length, and a total counterion concentration. Starting from BBGKY equation, and Superposition Principle, in the case of Many fixed Central ions (or charged groups), we present an original approach, based on a generalization of the Debye-MSA model (with a matrix method [2]), in order to predict the more stable conformation, the degree of ionic condensation and the different frictional processes on the polyions.

Indeed, comparison between conductivity results and the calculated predictions according to this model, allows to analyze in the framework of equilibrium and non-equilibrium thermodynamics, the high interdependence between: conformation, condensation of counterions, and hydrodynamic, electrophoretic, ionic and dielectric frictions [3]; to interpret the apparent anomalies and to detect conformational second order transitions [4], [5].

Keywords: ellipsoidal polyion; ionic condensation; dielectric friction; conductivity

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Isothermal section of the Gd-Fe-Cr ternary system at 800°C

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Isothermal section of the Gd-Fe-Cr system have been investigated at 800°C by characterization of the equilibrated alloys with the help of scanning electron microscopy coupled with energy-dispersive spectrometry (SEM-EDS) and powder X-ray diffraction (PXRD) techniques. This isothermal section consists of seven single-phase regions, eight two-phase regions and five three-phase regions. The existence of four binary compounds (GdFe₂, GdFe₃, Gd₂Fe₁₇, α(FeCr)) and one ternary compound (GdFe₁₀Cr₂) was confirmed in this phase diagram. All measured compositions and unit-cell refinements were performed at room temperature from quenched samples annealed at 800°C for one week. The maximum solid solubilities of Cr in GdFe₂ and Gd₂Fe₁₇ are respectively about 11.66 and 13, 15 at.% Cr. The GdFe_{12-x}Cr_x solid solution with the ThMn₁₂-type structure (space group I4/mmm) has a broad solubility ranging from x = 2 to 3.

First-principles study of rock-salt $\text{Ca}_{1-x}\text{Sr}_x\text{O}$ ternary alloys

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The structural and electronic properties of $\text{Ca}_{1-x}\text{Sr}_x\text{O}$ ternary alloys in NaCl structures at various Sr concentrations are presented. The calculations are performed using the full potential linearized augmented plane wave (FP-LAPW) method within the density functional theory (DFT) the generalized gradient approximation (GGA) of Perdew et al., Deviation of the lattice constants from Vegard's law and bulk modulus from linear concentration dependence (LCD) were observed for the alloys. The microscopic origins of the gap bowing were explained by using the approach of Zunger and co-workers. In addition, total and partial densities of states and Charge densities were calculated.

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Thermogravimetric measurement of the equilibrium vapour: Application to water and triethanolamine.

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Thermogravimetry (TG) is especially suited to analyze vaporization and sublimation processes. The applicability of isoconversional methods to the evaporation kinetics is studied. Besides, it's shown that the degree of TEA decomposition depends on the surrounding atmosphere and on the conditions for gas evaporation; the easier the gas evaporation, the smaller the degree of decomposition. In view of the volatiles formed, a reaction pathway is proposed for the thermal decomposition of TEA.

Therefore, with the temperature evolution of P_s determined, we have simulated the evaporation of water for two different geometries: films deposited on a substrate, Eq (1), and water inside an open crucible, Eq (2).

The use of films to analyze the evaporation kinetics has several advantages: the determination of the vapor pressure from TG is straightforward, liquid cooling related to its evaporation is negligible and, allows exploring lower temperatures and a wider temperature interval than with crucibles.

In this work, we have developed a method to determine the equilibrium vapor pressure based on the TG analysis of films performed at different heating rates. The method has been successfully applied to water and TEA evaporation.

In the case of TEA we have been able to determine the equilibrium vapour pressure in a pressure range larger than four decades.

Keywords

Equilibrium vapor pressure, Triethanolamine vapor pressure, Water vapor pressure.

Equations

Eq (1)

$$-\frac{dm}{dt} = \phi \frac{M}{RT} Q P_s$$

Eq (2)

$$-\frac{dm}{dt} = \frac{DSM}{RT h_{ef} DS + \phi h_{ef} Q} P_s$$

THEORETICAL STUDY OF PHYSICAL AND OPTICAL PROPERTIES OF METALLO-PHTHALOCYANINE DERIVATIVES AND THEIR PERFORMANCES IN THE GRATZEL PHOTOVOLTAIC CELL

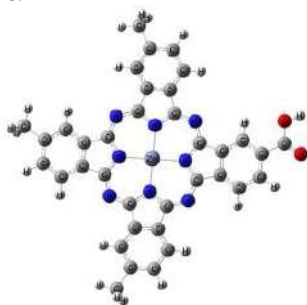
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In our presentation, we report on a theoretical study about the electronic and optical properties of metallo-phthalocyanine derivatives with the aim to discuss their performances in a Grätzel photovoltaic cell. First, we optimized the geometries of different structures using the B3LYP/6-311G(d) [1] method and then we calculated the excited states properties with the functional ω B97X-D [2]. This latter was found to be the best performer for excitation energy calculations. According to the LHE values, we found that Zn(II) gives the best efficiency in this series of phthalocyanines with respect to other transition metals (Mn, Fe, Co, Cu and Ni). The addition of an aromatic rings or multi-acid groups in the metallo-phthalocyanines leads to enhance the efficiency of the energy conversion and the collected electrons.



Structure of TT1Me

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Elaboration and Thermal study of composites from used polystyrene

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Recycling is a waste treatment process that consists of reusing all or part of a waste to make a new product; it allows reintroducing materials in another cycle of production.

Recycling has two major ecological consequences:

- Reduction of the volume of waste and the fight against environmental pollution.
- The preservation of natural resources, since the recycled product is used instead of the virgin material.

The objective of this work is in the context of the valorization of natural resources very abundant in Tunisia such as calcite which is used for the elaboration of polymer matrix composites with better physicochemical properties than their precursors. In addition, the search for a new mode of treatment and recovery of plastic waste and more specifically polystyrene (PS) which is fragile and has a low chemical resistance requires the use of reinforcements and additives in most applications. To improve their performance, the Tunisian calcite (CaCO_3) supplied from the Gabes region was used for the production of polystyrene-calcite (PS- CaCO_3) composites synthesized by introducing three different concentrations of calcite into the used PS matrix. The PS / calcite composites were prepared by the method (voie solvent). Composite (PS / calcite) series synthesized were characterized by X-ray diffraction (XRD), infrared absorption spectroscopy (IR), and photoluminescence (PL).

The results of the composites characterization suggests the existence of a possible interaction between the polymer matrix and the calcite

The results of the composites characterizations were supported by the thermal properties study, by DSC and TGA which indicates that the thermal stability of PS / CaCO_3 is better than that of the PS matrix.

The temperature onset is increasing for these composites to a percentage of 10% calcite ($T_{\text{onset}} = 385.01^\circ\text{C}$), and the decomposition temperature increases significantly with the percentage of calcite introduced and is greater than that of polystyrene PS ($T_d = 429.21^\circ\text{C}$).

Electrochemical copolymerization of fluoro-functionalized conducting polymers

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In the present work, we have synthesized a set of fluoro-functionalized polyaniline conducting polymers. Poly(aniline-co-2-fluoroaniline) was synthesized from aniline (ANI) and 2-fluoroaniline (2FA) dissolved in aqueous solution in acidic conditions with different molar ratio (feed ratio 2FA :ANI) ranging from 0 to 10. The polymers are formed by oxidative coupling of precursor comonomers and we used chemical and electrochemical methods for the synthesis.

We determined the composition of the synthesised copolymers using XPS spectroscopy and we checked their conductivity by four-point probe method.

The electrochemical synthesis was performed by potentiostatic and potentiodynamic methods on different working electrode such as platinum and transparent Indium Tin Oxide (ITO) electrodes. The chemical synthesis of the copolymer was performed by using ammonium peroxydisulfate as an oxidant.

In the electrochemical synthesis we checked the influence of the anodic potential limit (ranging from 1.1 to 1.2V) on the incorporation of fluoro-aniline monomer to the final copolymer. We were able to obtain copolymers with a maximum amount of 0.7 F atoms per nitrogen atom.

The conductivity of polyaniline and the copolymer synthesized was checked and polyaniline presents higher conductivity than the copolymer containing fluoro moieties.

Key words: Electrochemistry; Copolymerization; Fluoro-functionalized polyaniline.

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

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Optical fibers can add interesting possibilities in solar concentrator systems. The aims of this study are to optimize the coupling of a paraboloidal dish, which concentrates direct solar irradiance with dual axes tracking component, and the optical fiber, which transmits concentrated solar energy. We present review previous studies on the transmission of concentrated solar energy via optical fibers (TCSEvOF), and provide a mathematical model for coupling paraboloidal dish and the optical fiber. This paper reports on theoretical realization of a recently proposed solar optical fiber mini dish light concentrator connected to a conical solar furnace. The prototype dish is 21.8 cm in diameter. We present the daily power obtained at the output of the optical fiber, the power supply is estimated to be 25 W at the end. Then we show that the energy transported is diffused until the enclosure then disperse inside it, this energy is absorbed by the receiver. Temperatures higher than 800°K may be reached while maintaining very good efficiency.

Key words: Solar energy; Optical fiber; Paraboloidal dish; Conical solar furnace

Synthesis of new phosphorus heterocycles from functionalized allylphosphonates

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The wide panel of pharmaceutical and biological activities displayed by isoxazoline and pyrazoline derivatives focused the interest of the scientific community. Indeed, isoxazolines were reported as a novel class of parasiticides¹ and exhibit a broad range of biological effects, including anticancer and anti-inflammatory activities.² Recently, pyrazolines have also been successfully used as COX-2 inhibitors³ and anticonvulsant drugs.⁴ As part of our program aimed at the preparation of new phosphorus heterocycles from allylphosphonates **1**,⁵ we describe herein the synthesis of new isoxazolines and pyrazolines bearing a phosphonomethyl group. Our approach based on 1,3-dipolar cycloaddition reaction between allylphosphonates **1** and chlorooximes or nitrile imines under mild conditions.

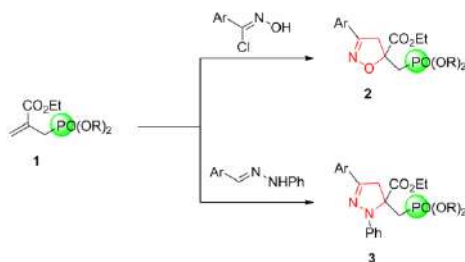


Fig. Access to isoxazolines **2** and pyrazolines **3**.

Key words: Allylphosphonates, 1,3-dipolar cycloaddition, isoxazolines, pyrazolines.

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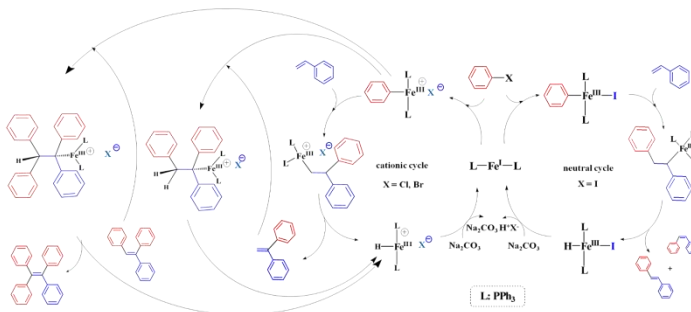
Reactivity and selectivity study of the Heck coupling reaction activated by ultrasonic activation

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The study of the sonochemical activation of the Heck reaction has shown excellent efficiency for a very short period of just a few minutes. In addition, it has also shown an improvement of some catalytic systems that are less active in the conventional mode. Moreover, it has been shown that the coupling reactivity and selectivity are affected by the experimental conditions. Indeed, in an aprotic polar medium, the arylation becomes more selective on styrene's external carbon, and the more important the M-X bond is, the more selective the arylation becomes on the β -carbon of styrene. It has also been found that, the evolution and selectivity of the reaction is affected by both electronic and steric effects of the ligand.



Scheme. Neutral and cationic mechanisms of the Heck coupling reaction

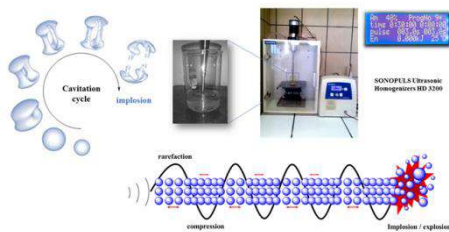


Fig. ultrasonic activation of the Heck coupling reactions

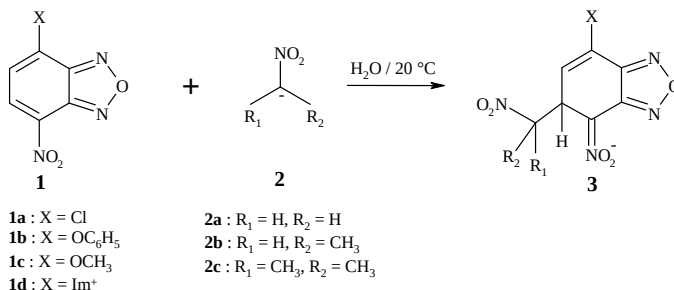
Key words: Catalyst, Heck Coupling reaction, Ultrasonic activation.

FREE ENERGY RELATIONSHIPS FOR σ -COMPLEXATION REACTIONS OF 7-X-4-NITROBENZOFURAZAN

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The kinetics of the reactions of 7-X-4-nitrobenzofurazan **1a-d** (X = Cl, OC₆H₅, OCH₃ and Im⁺) with a serie of nitroalkaly anions **2a-c** have been studied by UV-Visible spectroscopy in water at 20 °C (Scheme 1).



Scheme 1

The resulting second-order rate constants follow the linear free energy relationship (Eq. (1)), which allowed us to derive their electrophilicity parameters E. On the other hand, we will show that with the E parameters determined in this work, it is possible to predict rate constants for the reactions of these benzofurazans with a large varetty of nucleophiles. The structure-reactivity relationships of these electrophiles are also discussed.

$$\log k (20\text{ }^{\circ}\text{C}) = s_N (E + N) \quad (1)$$

Key words: Kinetics, Electrophilicity, Benzofurazan, Nitroalkaly Anions, Complexes- σ , Mary's Equation.

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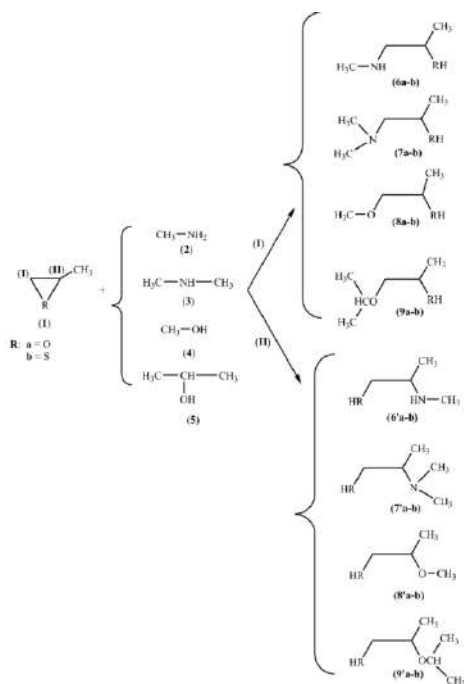
Theoretical study of epoxide molecules reactivity with amines and alcohols

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Several applications are involving thermal curing resins especially three-dimensional epoxy amine networks [1]. Due to its good mechanical and electrical proprieties besides an important resistance to a wide range of chemical reagents, they are used in aerospace and automotive industries[2,3]. In this work, we are interested to study the reactivity of epoxides molecules **1a-b** with alcohols and amines. Based on the DFT (density functional theory) calculation method with the standard basis set 6-311G** and the two functional such as BPW91 and B3LYP, we discuss, from thermodynamic and orbital points of view, the possibility and the stereoselectivity of these reactions.



Keywords : heterocyclic molecules, B3LYP, reactivity

References

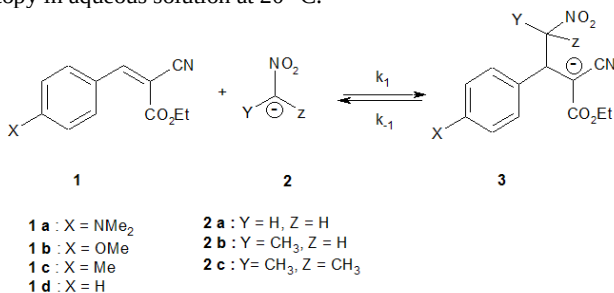
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ELECTROPHILICITIES OF BENZYLIDENECYANOACETATES

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The kinetics of the reactions of the benzylidenecyanoacetates **1** (X = H, Me, OMe, and NMe₂) with nitroalkyl anions **2** have been studied by uv-vis spectroscopy in aqueous solution at 20 °C.



The resulting second-order rate constants were used to evaluate the electrophilicity parameters *E* of these series of Michael acceptors **1** according to the linear free enthalpy relationship

$$\log k (20\text{ }^{\circ}\text{C}) = s_N (E + N).$$

Structure-reactivity relationships are discussed, and it is shown that the electrophilicity parameters *E* derived in this work are linearly related to the Hammett–Brown substituent constants (σ_p^+).

Key words: Kinetics, Electrophilicity Parameter, Hammett's Equation, Mayr's Approach, Substituent Effects, Michael Acceptors.

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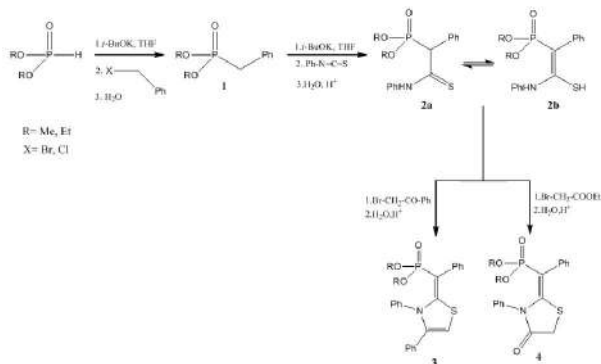
Synthesis of thiazolines and thiazolidinones derivatives from benzylphosphonates

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Heterocyclic compounds occupy an important class in the synthesis organic. Thiazolidinones derivatives are described in the literature as compounds with interesting pharmacological properties, namely antiviral¹, antibacterial², antidiabetic³. Various methods are used for the synthesis of thiazoles and thiazolidinones, e.g the reaction between isothiocyanates and phosphonoacetonitriles, in the presence of *t*-BuOK, with a brominated derivative⁴.

The condensation mole to mole of phenylisothiocyanate on benzylphosphonates **1** provides a thioamides **2** which reacts with a brominated derivative such as 2-bromoacetophenone and ethyl bromoacetate, leading so to the formation of thiazolines **3** and thiazolidinones **4**.



Key words: phenylisothiocyanate, benzylphosphonates, thioamides, thiazolines, thiazolidinones.

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Phenolic composition and biological activities of *Rumex crispus*, *Rumex roseus* and *Diplotaxis Simplex*

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Background: The scientific community and agro-industry are directed towards herbal extracts because of their availability, biodegradability and less toxicity¹⁻³. As a part of research of biocontrols, our study was invested by *Rumex crispus*, *Rumex roseus* and *D. simplex* as local bioresource. Therefore, the aim of this study is to determine the phenolic composition of methanolic extract obtained from their Aerial parts (stems, leaves and flowers) and test its biological activity.

Materials/Methods: The powdered of aerial parts of plants: *Rumex crispus*, *Rumex roseus* and *D. simplex* were extracted with different solvents of increasing polarity namely cyclohexane, dichloromethane and methanol^{4,5}. An assessment of the anti-oxidant properties of all extracts was performed using DPPH assay. We also investigated the anti-cholinesterase, anti-xanthine oxidase and cytotoxic (against MCF-7 and HCT-116) activities. The methanolic fraction was analyzed by HPLC-UV and GC-MS.

Results: Results revealed a phenolic fingerprint composed by emodin, chlorogenic, caffeic, syringic, *p*-coumaric, sinapic and trans-3-hydroxycinnamic acids, luteolin-7-glucoside, catechin hydrate, epicatechin-3-O-gallate, trans-resveratrol, apigenin-8-C-glucoside, isorhamnetin-3-O-glucoside, luteolin and kaempferol. Methanolic extract from *Rumex crispus* (Aerial part) provides the best results of activities anti-Alzheimer, anti-inflammatory, and cytotoxic⁶.

Conclusion: The results showed the interesting polyphenolic profile of the methanolic fraction from the *Rumex roseus* leaves, *Rumex crispus* and suggest it as an interesting source of health-promoting polyphenols.

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Variation of the antioxidant properties of olive oil according to the methods of preparation (*Olea europaea* L. cv. *Chemlali* Sfax)

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Régis Rouillon^{a,b}, Ridha Ben Salem^c

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Among the constituents present in olive oil, there are antioxidant substances such as phenolic compounds whose content may be influenced by the process of manufacturing the oil (treatment of microwave and ultrasonic treatment with different times as well as the addition of a co-adjuvant such as citrate sodium with two concentration (150 et 300 g/L)). Therefore, the objective of this work was to investigate and optimize various classical and original spectrophotometric methods in order to evaluate those which are the most appropriate for the quantification of phenolic compounds on the one hand and the antioxidant capacity of olive oil on the other hand. Actually, only the results obtained with two antioxidant compounds (AOX) are presented, namely tyrosol, one of the major compounds present in olive oil and gallic acid frequently used as a reference. The highest content of polyphenols in equivalence of tyrosol corresponds for olive oil obtained after 10 minutes of ultrasonic treatment presents 10.8 mg / kg of oil using Folin reagent's while 16.8 mg GAE / kg of oil using the method based on gold nanoparticles (AuNPs). On the other hand, the antioxydant activity, using ABTS assay, of *chemlali* olive oil obtained after ultrasound treatment (35 KHz) reach its maximum when olive paste was treated for 40 and 60 minutes.

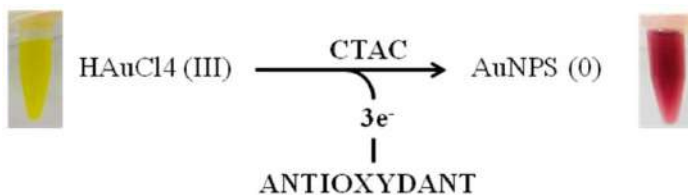


Fig. Formation of gold nanoparticles AuNPs

Key words: olive oil, antioxidant capacity, phenolic compounds.

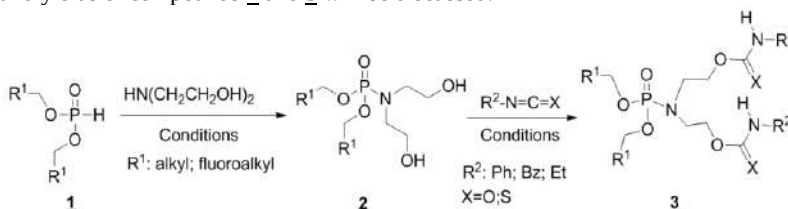
Synthesis and characterization of new mixed bis(thio)carbamate-phosphoramidate derivatives

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^a *Laboratory of Structural Organic Chemistry: Synthesis and Physico-chemical Studies, Department of Chemistry, Faculty of Sciences of Tunis, University of Tunis El-Manar 2092, El Manar I Tunis, Tunisia*

^b *Unité de Recherche en Chimie des Matériaux, Department of Chemistry, Faculty of Sciences and Techniques, UNA, Nouakchott, Mauritania*

Phosphoramidates and (thio)carbamates are abundant structural motifs widely present in natural and synthetic compounds of various applications in industrial, agricultural, biochemical, and medicinal areas [1-3]. They are also important precursors for the synthesis of various bioactive compounds serving as a motif for natural products, phosphonopeptides, amino acid analogs, prodrugs and pharmacological agents [4,5]. Combination of these two families paves the way to new molecules having combined properties of both molecules. In the present work, we describe the synthesis of a new series of fused thiocarbamate phosphoramidate compounds **3** from alkylphosphoramidates of type **2** and iso(thio)cyanates using the corresponding phosphites **1** as the starting products (Scheme 1). All these compounds were characterized with multinuclear (¹H, ¹³C, ¹⁹F and ³¹P) NMR and IR spectroscopic techniques. The effect of different substituents on the reactivity and yields of compounds **2** and **3** will be discussed.



Scheme 1

Keywords : alkylphosphoramidates; iso(thio)cyanates; (thio)carbamates.

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Extraction and physicochemical characterization of mucilage extracted from *Opuntia ficus indica*

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Mucilage was extracted from the cladodes of *Opuntia ficus indica* using optimized conditions: pad/water ratio = 1/1(w/w), temperature = 80°C, pH = 2, 4, 9 and 12, and extraction time = 2 h. Ethanol was used for the precipitation step. The obtained material was analyzed to determine the distribution of carbohydrates including rhamnose, arabinose, xylose, mannose, glucose, galactose, pectin, fructose and galacturonic acid. The residual material obtained after extraction of mucilage are intended for treatment of wastewater.

Key words: *Opuntia ficus indica*, extraction, mucilage, adsorption.

Reactivity of mixed carboxylic-fatty anhydrides as acylating agents using heterogeneous acid catalysts

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Mixed anhydrides constitute an important class of useful chemical intermediates in the synthesis of several products. These compounds are essential chemicals that are widely used in food, pharmaceutical, cosmetic, detergent, plasticizer, lubricant, textile and other industrial applications. The aim of this work is the synthesis of fatty esters from mixed carboxylic fatty anhydrides using heterogeneous acid catalyst. This work describes a novel and efficient method of synthesis of fatty esters by the esterification reaction with mixed carboxylic fatty anhydrides, using heterogeneous acid catalyst. We have investigated the reactivity of some carboxylic palmitic anhydrides in the esterification reaction of primary, secondary and tertiary alcohols. We have optimized the conditions for maximum esterification yields by varying different reaction parameters. We describe a novel and efficient method for the synthesis of fatty esters by the esterification reaction of primary and secondary alcohols using resin Amberlyst-15 as heterogeneous acid catalyst. The esterification of tertiary alcohols was carried out using Lewis acid catalyst.

Synthesis and characterisation of 2,5-disubstituted 1,3,4-Oxadiazoles through Oxidative Cyclization of *N*-acylhydrazones

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The 1,3,4-oxadiazoles and related derivatives are an important group of π -conjugated heterocyclic compounds. They have attracted significant interest in many fields such as organic synthesis[1], pesticide chemistry[2] and material science [3]. Moreover, these heterocyclic scaffolds have also proven important medicinal activities as anti-inflammatory, anticonvulsant, antioxidant, and anthelmintic agents [4,5]. In this work, we describe the synthesis of a new series of asymmetrical 2,5-disubstituted 1,3,4-oxadiazole derivatives by an oxidative cyclization of β -chloro- α,β -unsaturated *N*-acylhydrazones in basic medium. The new adducts were characterized in solution using multinuclear (¹H and ¹³C) NMR and IR spectroscopies.



Keywords: β -chloro- α,β -unsaturated *N*-acylhydrazones, NMR, 2,5-disubstituted 1,3,4-oxadiazoles

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Synthesis and characterization of new tin tetrachloride complexes with β -chlorovinyl aldehydes

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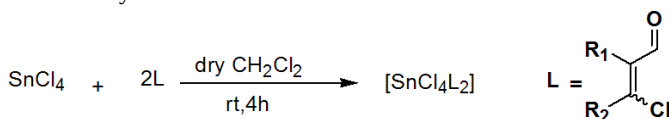
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The coordination chemistry of tin(IV) halides have attracted considerable interest due to their industrial, biological and catalytic properties¹⁻³. This has also been used in supramolecular chemistry with diverse structures and interesting properties⁴. In particular, tin(IV) complexes continue to provide fundamental information about both Lewis acid–base model and tin(IV) species reactivity^{5,6}. In this work, we report on the synthesis of a new series of octahedral complexes of tin tetrachloride with β -chlorovinyl aldehydes in anhydrous dichloromethane. The adducts have been characterized in solution using multinuclear (¹H, ¹³C and ¹¹⁹Sn) NMR and IR spectroscopy. The variable temperature NMR studies in solution showed that the magnitude and the mode of the metal–ligand interactions depend considerably on the nature of β -substituents in β -chlorovinyl aldehydes. On the basis of these results, the title aldehydes have been classified according to their Lewis basicity.



Keywords: β -Chlorovinylaldehydes, tin(IV) complex, characterization, ¹¹⁹Sn NMR.

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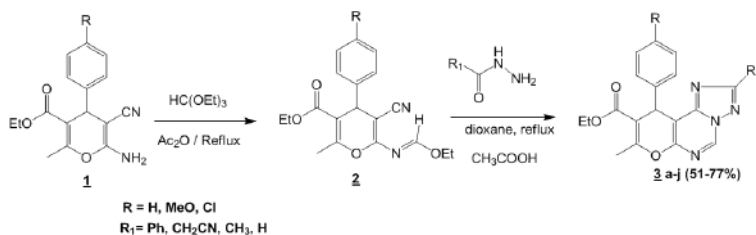
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Design and synthesis of novel pyranotriazolopyrimidine derivatives

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Heterocyclic compounds are widely prevalent in nature and important activities are associated with this class of substances. The paramount importance of these compounds has led to the search for new methods for the formation of heterocyclic systems. In particular, pyrimidines and condensed pyrimidines, which have attracted a great deal of interest owing to their broad spectrum of biological and pharmacological activities such as antidiabetic, anticancer, anti-tuberculosis and antiviral activities¹⁻³. Our work fits into this optical and consists in the synthesis of novel pyranotriazolopyrimidine **3** derivatives via the cyclocondensation reaction of α -functionalized iminoether **2**, which was obtained from 2-amino-3-cyanopyrane **1**, with a series of hydrazides (Scheme 1). Structures of all synthesized compounds were determined using spectroscopic methods including ¹H NMR and ¹³C NMR.



Scheme 1: Synthetic pathway of compounds **3**

Keywords :

2-amino-3-cyanopyrane, hydrazides, pyranotriazolopyrimidines.

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Ionic conduction of a strontium britholite doped with lanthanum and neodymium

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Britholite materials are phosphosilicate apatites obtained by a coupled substitution of the divalent cation by a trivalent lanthanide or a tetravalent actinide ion and the trivalent groupment PO_4 by a tetravalent SiO_4 groupment in the general formula $\text{Me}(\text{XO}_4)_6\text{Y}_2$ (Me: divalent cation; XO_4 : anionic groupment and Y: Monovalent anion) [1-3]. Strontium phosphosilicate apatite doped with lanthanum and neodymium and whose chemical formula $\text{Sr}_8\text{La}_{2-x}\text{Nd}_x(\text{PO}_4)_4(\text{SiO}_4)_2\text{F}_2$ with $0 \leq x \leq 2$ were physico-chemically investigated. The materials were prepared via conventional solid state reactions. The analysis and characterization of the synthesized powders were conducted by means of several techniques. The ionic conductivity σ of the samples was measured via a complex impedance spectroscopy. The results showed that the double substitution of lanthanum-neodymium in strontium phosphosilicated fluorapatite was effective and well crystallized single-phase apatites were successively obtained. The molar ratio $\frac{\text{Sr} + \text{La} + \text{Nd}}{\text{P} + \text{Si}}$ was of about 1.67 verifying the stoichiometry character of the powders. The *a* and *c* lattice parameters obtained from a structural refinement by the Rietveld method were found in decrease if the Nd content (*x*) rose. The ^{31}P NMR (MAS) exhibited a single peak and the FTIR spectroscopy revealed the characteristic bands of phosphosilicated fluorapatite. The neodymium-lanthanum substitution was total according to the small size differences of the two cations. The measured ionic conductivity σ of the samples was found to depend simultaneously on the Nd content and more intensively on the heating temperature, the maximum was $1.73 \cdot 10^{-6} \text{ S.cm}^{-1}$ obtained at 780°C for $x=2$.

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SYNTHESIS AND STRUCTURAL STUDY OF THE MONOCLINIC PHASE $\text{Na}_4\text{Co}_{7-x}\text{Al}_{0.67x}(\text{As}_{1-y}\text{P}_y\text{O}_4)_6$. ($x = 1.60$; $y = 0.116$).

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The title compound, tetrasodium hepta(cobalt/aluminium) hexa(arsenate/phosphate), $\text{Na}_4\text{Co}_{5.40}\text{Al}_{1.07}(\text{A}_{0.883}\text{P}_{0.116}\text{O}_4)_6$, was prepared by a solid-state reaction. It is a new member of isostructural compounds with the general formula $\text{A}_4\text{M}_7(\text{XO}_4)_6$ (A: Na, K; M: Ni, Co; X: P, As) and it is most similar to $\text{Na}_4\text{Co}_{5.63}\text{Al}_{0.91}(\text{AsO}_4)_6$ [1]. Its structure was determined by single-crystal X-ray diffraction: monoclinic, space group C2/m, $a=10.5797(2)$ Å, $b=14.5528(3)$ Å, $c=6.6441(3)$ Å, $\beta=105.608(9)^\circ$ and $Z=2$. The structure was solved and refined to final agreement factors $R(F^2)=3\%$, $R_w(F^2)=8.30\%$, $S(F^2)=1.07$. The obtained structural model was supported by both bond-valence-sum (BVS) and charge-distribution (CD) validation tools [2,3].

The asymmetric unit of the title compound (Fig. 1) contains seven metallic sites of which four are occupied by Na^+ cations (occupancies ranging from 0.23 to 0.50) with eight cations per unit cell, two others (noted MA and MB) are simultaneously shared by Co^{2+} and Al^{3+} ions, and one is fully occupied by Co^{2+} ions. The three-dimensional network encloses tunnels in which Na^+ cations are located (Fig. 2). The possible motion of monovalent cations in the anionic framework is simulated by means of a generalization of the BVS model.

Key words: $\text{Na}_4\text{Co}_{5.40}\text{Al}_{1.07}(\text{A}_{0.883}\text{P}_{0.116}\text{O}_4)_6$, BVS, CHARDI.

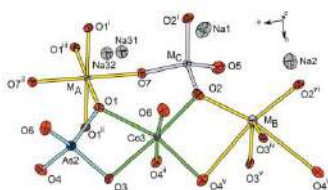


Fig. 1: The asymmetric unit of $\text{Na}_4\text{Co}_{5.40}\text{Al}_{1.07}(\text{A}_{0.883}\text{P}_{0.116}\text{O}_4)_6$

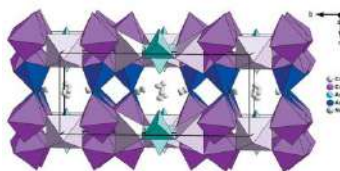


Fig. 2: Projection of structure along the [100] direction.

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C-DLTS interface defects in Al_{0.22}Ga_{0.78}N/GaN HEMTs on SiC: Spatial location of E2 traps

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In this work, we identify the spatially trapping mechanism by C-V measurements and further characterize the properties of the traps in AlGa_{0.22}N/GaN heterostructures on SiC by means of DLTS spectroscopy. The C-V analysis have been recorded in the 20–320 K temperature range and exhibit an increase in the pinch-off voltage by an amount of 300 mV once the temperature exceeds 200 K. A hysteresis phenomenon has been observed in the C-V spectra by sweeping the gate voltage V_{gs} forth and back between -5 and 0 V. This parasitic effect has identified to be related to trapping and detrapping mechanisms occurring in the GaN-HEMT device. DLTS results have proved the presence of two traps, labeled E1 and E2, with activation energies of 0.31 eV and 0.525 eV and capture cross sections of $3.86 \times 10^{-18} \text{ cm}^2$ and $2.75 \times 10^{-15} \text{ cm}^2$, respectively. The major E2 trap seems to be nitrogen anti-sites, possibly located in the buffer layer near to the interface AlGa_{0.22}N/GaN. It has been reported that there exists a good correlation betwixt the anomalies in C-V-T characteristics and DLTS measurements.

**Synthesis, structure and characterization
of a hybrid centrosymmetric material
(4-Dimethylaminopyridinium nitrate gallic acid monohydrate).**

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New hybrid material: 4-Dimethylaminopyridinium nitrate gallic acid monohydrate abbreviated DNGA monohydrate has been successfully synthesized by slow evaporation method at room temperature. X-ray diffraction (XRD) on a single crystal showed that the latter was crystallized in P-1 space group. Likewise, thermal analyses demonstrated the stability of our crystal up to 80°C. Besides, the analysis of the infrared spectrum (FTIR), allowed us to confirm the presence of the different groups present in the structure. Furthermore, by studying the UV-Visible spectrum, the transparency of our crystal was proven. The stability and cohesion of the structure is ensured via hydrogen bonds.

Synthesis, crystal structure, phonon, magnetic and electrical properties of new molybdate $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$

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The single crystals of $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$ were successfully grown using the solid-state method. This compound crystallizes in a triclinic system with $P\bar{1}$ (C_i) space group. Its structure can be described as a three-dimensional anionic framework of Mn_2O_{10} double octahedra units sharing edges with the MoO_4 tetrahedra. The Na^+ ions are disordered and located in the voids forming infinite channels running along the [100], [010] and [001] directions. The structural model was validated by the bond valence sum (BVS) and charge distribution (CHARDI) methods. Polycrystalline powder of $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$ was prepared as well using citrate process. The obtained sample was characterized by X-ray powder diffraction, infrared spectroscopy and Raman scattering at room temperature. Vibrational study confirms the existence of the MoO_4^{2-} functional group. Thermal stability of the studied material was analyzed using differential scanning calorimetry. The $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$ compound is thermally stable up to 500°C. Magnetic susceptibility measurements reveal that the title compound is antiferromagnetic with Néel temperature $T_N = 6.5(5)$ K. At higher temperatures, its susceptibility follows a Curie–Weiss law. Electrical measurements of this material were studied by means of the impedance spectroscopy technique, in 0.1 Hz–4 MHz frequency and in 443–691 K temperature ranges. The conductivity of $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$ is $2.30 \mu\text{Scm}^{-1}$ at 691 K and is thermally activated with energy of 0.47 eV. The $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$ compound can be classified as a medium ionic conductor.

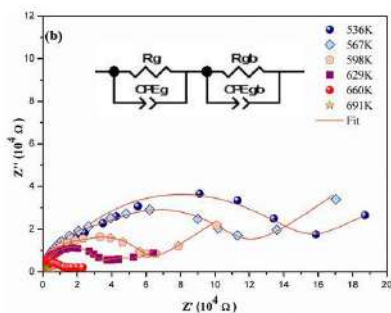


Fig. 1 Plots of the impedance data at 536–691 K for the $\text{Na}_2\text{Mn}_2(\text{MoO}_4)_3$.

Key words: Molybdate, X-ray diffraction, Rietveld, Magnetic measurements, Ionic conductivity.

Sol-gel synthesis and characterization of monolith and transparent Sr, Fe and Al doped TiO₂.

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Transparent monoliths of Al, Fe and Sr doped TiO₂ were synthesized through a modified sol-gel way from titanium isopropoxide as precursor. By controlling the hydrolysis of this precursor through the intermediate of the esterification reaction between acetic acid and solvent at room temperature. The monoliths xerogels prepared by this method were transparent in the wavelengths between 500 nm and 800 nm. The Alumina and Iron-doped TiO₂ samples have a crystalline part without calcination. Powder X-ray diffraction confirmed the amorphous-to-anatase and the anatase-rutile/brookite phases transformations. Only anatase TiO₂ could be observed in the samples annealed at T<500°C. BET analysis showed that transparent gels have an important surface area.

Key words : TiO₂, Sol-gel, Transparent, Monolith, Metal doped.

ELABORATION, STRUCTURE, SPECTROSCOPY STUDY AND THERMAL BEHAVIOR OF PIPERZINEDIIUM TRIAQUATRICHORO IRON(III) CHLORIDE

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A new organic-inorganic hybrid material $(C_4H_{12}N_2)[FeCl_3(H_2O)_3]Cl_2$, has been synthesized and crystallographically characterized by single-crystal X-ray diffraction. It crystallizes in the monoclinic system, space group $P2_1/m$, with the following unit cell parameters: $a = 6.889(16)$; $b = 16.0298(38)$; $c = 7.0524(17)$ Å; $V = 717,84(17)$ Å³ and $Z = 4$. The title compound is built of $[FeCl_3(H_2O)_3]$ neutral entities, piperazinediium cations and chloride anions. The crystal cohesion is ensured by hydrogen bonds established between the different entities. Raman and infrared spectra of the title compound were recorded in the range of 25–400 and 400–4000 cm^{-1} , respectively. The thermogravimetric study showed that the thermal decomposition of precursor occurs in several stages and leads to the formation of the iron oxide as a final product at 900 °C.

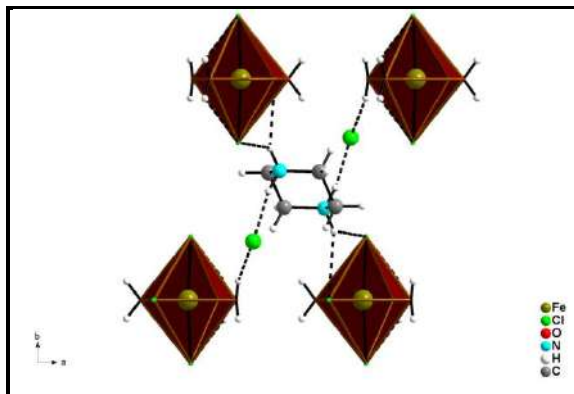


Figure. Projection of the structure of the title compound along the c-axis.

Keywords: Hybrid material, 0D structure, IR and Raman spectroscopy, Thermal behavior.

Spark plasma sintering of $\text{Ti}_{0.7}\text{W}_{0.3}\text{C}$ powders prepared by mechanical alloying

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$\text{Ti}_{0.7}\text{W}_{0.3}\text{C}$ composites have been obtained from a mixture of elemental powder of titanium, tungsten and graphite milled by high energy planetary ball mill for different durations to produce our nanosized particles.

After that, its densification were obtained by SPS at different temperatures.

Then, we have to characterize the microstructure of the prepared materials and to study the mechanical alloying temperature effects on the $\text{Ti}_{0.7}\text{W}_{0.3}\text{C}$ carbide formation by SPS.

The results shows that the relative density and the micro-hardness of the powder milled for 20h and sintered at 1170°C for 5 min under 100 MPa reach respectively 81% and 1761.5 HV.

So, the novel carbides (substitution with 0.3% W) haven't good mechanical properties compared with TiC ($\text{HVN}=27\text{GPa}$)¹ and $\text{Ti}_{0.9}\text{W}_{0.1}\text{C}$ ($\text{HV}0.3=2978$)².

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Structural characterizations and mechanical behavior of activated clay-based $\text{Si}_5(\text{PO}_4)_6\text{O}$ and SiP_2O_7 compounds

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Pure, well-crystalline and low-cost silico-phosphate materials were prepared by a simple procedure, different from that previously reported by sol-gel method. In this case, the $\text{Si}_5(\text{PO}_4)_6\text{O}$ and SiP_2O_7 compound have been synthesized from the mixtures of activated clay $-\text{H}_3\text{PO}_4$ (70 wt% H_3PO_4 and 80 wt% H_3PO_4). The structural changes induced by thermal treatment, have been studied by X-ray diffraction (XRD), Fourier transformed infrared (FTIR) spectroscopy, ^{31}P , ^{29}Si MAS-NMR techniques and by the mechanical Brazilian test. The XRD results showed that the well-crystalline $\text{Si}_5(\text{PO}_4)_6\text{O}$ material has been synthesized from a heat treatment at 800°C. When, the well-crystalline SiP_2O_7 material has been obtained after a heat treatment at 500°C. These results were confirmed by ^{31}P and ^{29}Si MAS-NMR. the mechanical Brazilian test results showed that the silicophosphates SiP_2O_7 has high mechanical properties compared to $\text{Si}_5(\text{PO}_4)_6\text{O}$. At 900°C, the mechanical strength has been increased from 6.58 for $\text{Si}_5\text{O}(\text{PO}_4)_6$ to 21.5 MPa for SiP_2O_7 .

Keywords: Activated kaolin; Phosphoric acid; silicophosphate.

Thermal Stability of AA6060 Aluminum Alloy after Equal Channel Angular Pressing

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The annealing behavior of AA 6060 aluminum alloy deformed by equal-channel angular pressing (ECAP) was studied experimentally. The material was subjected to extrusion through die with channels intersecting at an 90° angle. Samples were pressed for up to 8 passes using route B_C, then cut into slices and subsequently annealed for 1 hour at temperatures from 150°C to 450°C. Hardness measurements were performed on each slice. Microstructure of material was analyzed by means of Electron Backscatter Diffraction (EBSD). Grain size and disorientation distributions were estimated. ECAP caused significant improvement of hardness, with stabilization after 4 passes. Refinement of microstructure was obtained with the increasing amount of passes. Material properties were stable during annealing at temperatures lower than 150°C. Annealing at higher temperatures caused a decrease in hardness corresponding to an increase of the grain size.

Keywords: ECAP; Hardness; EBSD; Recrystallization

**Structural, magnetic and the thermal stability characterizations
of the nanostructured Fe₅₀Co₂₅Ni₁₅B₁₀ alloy
prepared by mechanical alloying**

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Structural, magnetic characterizations and the thermal stability of the nanostructured Fe₅₀Co₂₅Ni₁₅B₁₀ alloy were followed by X-ray diffractions (DRX), SQUID magnetometer at 300 K and differential scanning calorimetry (DSC). The final product of the mechanical alloying process was nanocrystallized solid solution. The dissolution of the non-magnetic boron atoms crystallized in the lattice of iron was effected in the magnetization of saturation. From the magnetic field, one can notice that the hysteresis loops show low coercive force, which implies the soft ferromagnetic behavior. Likewise, as increasing the milling time a slight diminution of the saturation magnetization, M_s, was also found. In addition, the squareness ratio (M_r/M_s) increases at higher milling times. The DSC differential calorimetric analysis shows the existence of more intense exothermic peaks after 100 hours of milling.

Keywords: FeCoNiB alloy; nanostructure; Magnetic properties.

Synthesis, characterization and study physical propertie of iron oxide Fe₃O₄

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To meet the increasing demand for electrochemical capacitors with higher energy density and power density, many research attempts have been made to explore new materials. Much attention has been focused on the study of nano-sized transition– metal oxides and their carbon nanocomposites as anode materials for supercapacitors including magnetite (Fe₃O₄).

The magnetite Fe₃O₄ samples have been successfully synthesized via hydrothermal method using PEG, SDS and Triton as surfactants. The morphology and structural of the obtained products were characterized by powder X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). UV-vis spectroscopic study showed a change in the energy band gap of Fe₃O₄ with the surfactant nature. The electrochemical properties of the as-prepared samples are investigated as advanced electrode materials using cyclic voltammetry. It is found that the Fe₃O₄/CTAB nanomaterials displays much higher specific capacitances and better cycle stability than those of Fe₃O₄/SDS and Fe₃O₄/Triton materials.

Preparation, crystal structure and Hirshfeld surface analysis of vanadium(V) complex, 4-isopropylpyridin-1-ium decavanadate hydrate ($\text{C}_8\text{H}_{12}\text{N}$)₆ $\text{V}_{10}\text{O}_{28}\cdot 16\text{H}_2\text{O}$

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The crystals of vanadium(V) complex, 4-isopropylpyridin-1-ium decavanadate hydrate ($\text{C}_8\text{H}_{12}\text{N}$)₆ $\text{V}_{10}\text{O}_{28}\cdot 16\text{H}_2\text{O}$ (**1**) were obtained from a mixture of vanadium(V) oxide and piperidine-2,6-diylidimethanamine in water with the respective molar proportions 1: 3. The structure of this compound was elucidated using single-crystal X-ray diffraction. It crystallizes in the triclinic system, $P\bar{1}$ space group with the cell parameters: $a=11,258(4)\text{\AA}$, $b=11,783(3)\text{\AA}$, $c=15,060(2)\text{\AA}$, $\alpha=93,43(2)^\circ$, $\beta=102,52(3)^\circ$, $\gamma=100,69(5)^\circ$, $V=1905,9(4)\text{\AA}^3$ and $Z=1$. The asymmetric unit consists of one half-decavanadate anion of C_i symmetry, three organic cations and eight water molecules (**Fig. a**). In the crystal, molecules are linked into a three-dimensional network by N-H...O, C-H...O and O-H...O hydrogen bonds and by π - π interactions. The prevalence of these interactions is illustrated by an analysis of the 3D-Hirshfeld surface and by 2D-fingerprint plots. In the shape-index map (**Fig. b**), the adjacent red and blue triangle-like patches show concave regions that indicate π - π stacking interactions.

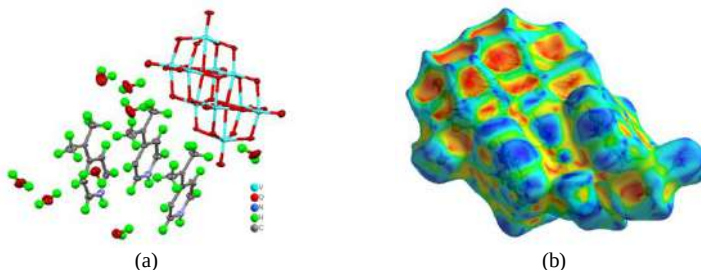


Fig. The molecular structure of (**1**) (**a**) and a view of the 3D- Hirshfeld surface mapped overshape index (**b**).

Key words: Crystal structure; Decavanadate; Hirshfeld surface; Fingerprint plots

ELECTROCHEMICAL BEHAVIOR OF A POROUS TiNiCu BIOMATERIAL

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Porous Ti-Ni alloys are promising implant materials. They have advantages over conventional implants for two main reasons. First, open porosity can improve bone growth and, therefore, improve fixation at the interface between bone and implant. On the other hand, the porosity decreases the effect of the difference in stiffness between the bone and the implant; therefore, by reducing the effects of shielding stress which decreases the life of the implant through bone resorption and loosening, the addition of third element namely copper whose objective is to improve the corrosion resistance, to avoid the release of nickel in the body fluid, to stabilize the superelastic properties and to increase the mechanical performance of the implants. Several techniques have been used for the production of porous Ti-Ni-Cu parts, such as hot isostatic pressing, the MIM (Metal Injection Molding) process, and solid phase sintering, in which we have developed our samples. To this end, this work aims to study the process of elaboration, structural and electrochemical characterization in a physiological medium of this biomaterial by varying the copper content from 0 to 8%. The results of investigation confirm at the level of the structure the formation of an alloy more less homogeneous with the presence of the majority phase TiNi. Concerning the electrochemical behavior the study allowed us to determine the passivation capacity of these alloys as well as the kinetics of formation of a protective film and the different parameters of corrosion. The addition of copper considerably improves the electrochemical parameters and the kinetics of corrosion.

**Program of
Tuesday
18 December 2018**

Crystal structure, physico-chemical studies, Hirshfeld surface analysis and theoretical calculations of a novel hybrid material, bis(2,6-diaminopyridinium) hexachloridostannate(IV)

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A novel hybrid compound, bis(2,6-diaminopyridinium) hexachloridostannate(IV) formulated as $(C_5H_8N_3)_2[SnCl_6]$ was synthesized by slow evaporation. The title compound crystallizes in the monoclinic system, $P2_1/c$ space group, with the following unit cell parameters $a = 7.148$ (4) Å, $b = 11.116$ (6) Å, $c = 12.453$ (1) Å and $\beta = 104.69$ (6)°. The atomic arrangement shows alternation of organic and inorganic entities. The cohesion between these entities is ensured by N-H...Cl and C-H...Cl hydrogen bonds that build a three-dimensional network (**Fig.1**). The 3D Hirshfeld surface and the associated 2D fingerprint plots were performed to gain insight into the behavior of the intermolecular interactions. The powder XRD data confirms the phase purity of the crystalline sample (**Fig.2**). The vibrational absorption bands were identified by IR spectroscopy and have been discussed. Optical-properties were studied by measuring the diffuse reflectance. Theoretical calculations were performed using density functional theory with the B3LYP level for studying the molecular structure and vibrational spectra of the title compound. Overall, very good agreement between theoretical and experimental frequencies was achieved.

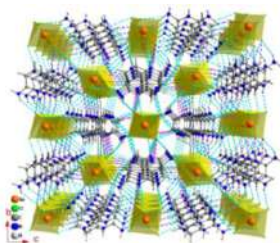


Fig.1. Three-dimensional network of $(C_5H_8N_3)_2[SnCl_6]$

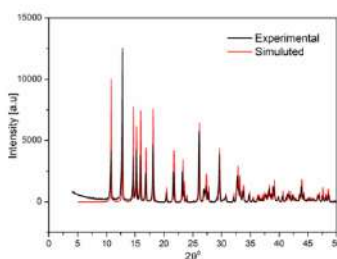


Fig.2. Simulated and experimental powder XRD patterns of $(C_5H_8N_3)_2[SnCl_6]$

Key words: crystal structure, organic hexachloridostannate(IV), Hirshfeld surface, DFT calculations

Structural properties of $\text{Ho}_{1-x}\text{Ba}_x\text{CrO}_3$ ceramics

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$\text{Ho}_{1-x}\text{Ba}_x\text{CrO}_3$ nanoparticles with different Ba concentrations ($x = 0.0, 0.1, 0.2, 0.3$) were synthesized via the sol-gel process. The Rietveld refinements of the XRD data reveal that these samples crystallise with orthorhombic distorted structure (Pnma) in single phase. The schematic representations of the perovskite structure are generated using VESTA program. The octahedral tilting observed can be explained in terms of tolerance factor and cooperative Jahn Teller effect.

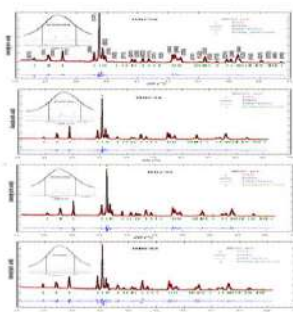


Figure 1 : Rietveld fit of XRD patterns

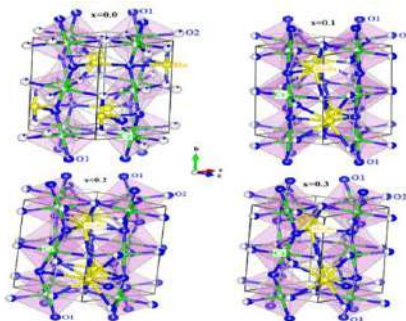


Figure 2 : The graphical representation of the samples

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A novel inorganic-organic hybrid material based on β -Anderson Polyoxomolybdate: Synthesis and physico-chemical characterization

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In the structural study of hetero polyoxometalates the isomerism attracts a considerable interest and make POMs more and more multiple and diverse.[1] Anderson as a characteristic kind of polyoxometalate have two isomers α and β [1]. The first Anderson β - isomer heteropolyanion was discovered 30 years ago by Ogawa and his co-workers [2]. Anderson framework is fundamentally planar however β -Isomer is not planar. It is a bent structure such as the heptamolybdate. [3] In order to extend the POMs family and enrich the background of hybrid materials a new organic-inorganic hybrid compound based on β -Anderson polyoxomolybdate $(C_6H_{14}N_4)_2(NH_4)_2[H \beta -SbMo_6O_{24}].6H_2O$ has been synthesized and characterized by single-crystal X-ray diffraction. This compound crystallized in the orthorhombic system, space group $Pnma$, with $a = 23.6649(6)$ Å, $b = 19.5394(5)$ Å, $c = 8.6683(2)$ Å, and $Z = 4$. The new hybrid material is characterized by infrared spectroscopy, ultraviolet spectroscopy, cyclic voltammetry.

The infrared spectrum fully confirms the X-ray crystal structure. Furthermore, the UV spectrum and the electrochemical behavior were investigated. Hirshfeld surface analyzes all the intermolecular interactions within the structure, which are important to stabilize the structure.

Key Words: Hybrid inorganic-organic material, β - Anderson Polyoxomolybdate, Crystal Structure, characterization

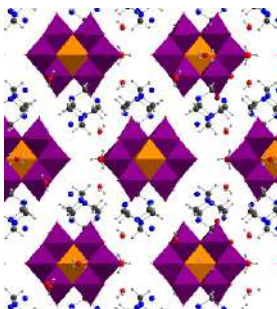


Fig. View along c axis of the new hybrid compound

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Luminescent properties of co-doped Eu³⁺/Eu²⁺ calcium aluminosilicate glass-ceramics: A potential tunable luminophore

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Eu³⁺ and Eu²⁺ doped calcium aluminosilicate glass-ceramics have been successfully prepared from the initial calcium aluminosilicate glass, containing 50 wt% of silica, under heat-treatment. Structural and optical properties of glass and obtained glass-ceramics were investigated. Control of crystallization using X-ray diffraction and Raman spectroscopy allowed to identify two main crystalline phases: anorthite [CaAl₂Si₂O₈] as the major phase and melilite [Ca₂Mg_{0.75}Al_{0.5}Si_{1.75}O₇] as the minor phase. Luminescent properties were investigated by emission spectra, lifetime measurements and color point analysis. The results showed that, Eu²⁺ is incorporated into the crystalline phases after reduction of Eu³⁺ during annealing or in the melilite phase. This incorporation, increasing with time of heat-treatment, enhanced Eu²⁺ luminescence. The color coordinates shift after annealing suggesting that crystallization process appears to be a useful technique to obtain phosphors with a tunable emission.

Integration of Natural Fluorapatite as a raw material for cement production

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One of the highest man made CO₂ emission from industry is due to Portland cement production [1]. Roughly 800 kg of CO₂ is emitted for every ton of Portland cement [2,3]. So one way to reduce the CO₂ emissions could be the use of none carbonated calcium sources as natural fluorapatite. Thus, the purpose of this study is to investigate the effect of the integration of natural fluorapatite in the raw meals with percentages ranging from 0 up to 15% on the mineralogy and the reactivity of clinkers. The samples were characterized by infrared spectrometry, X-ray diffraction and microscopy techniques. The distribution of phosphorous and fluorine into clinkers minerals was determined by MEB/EDS mapping. The mineralogical composition was determined by XRD/Rietveld and the samples reactivity followed by isothermal microcalorimetry. It has been found that fluorine stabilizes C₃S and β-C₂S which still are found with high levels of P₂O₅. Cements obtained from up to 8 % natural fluorapatite incorporation still present acceptable properties. Natural fluorapatite could have an important potential as decarbonised source of CaO contributing to decrease the CO₂ emission in cement industry.

Keywords: Natural fluorapatite, clinker mineralogy, reactivity.

References

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Synthesis and characterization of two organic-inorganic salts: Sulfates of diphenyl sulfone derivatives

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Crystal engineering of hydrogen bonded organic-inorganic hybrid materials has attracted tremendous attention emerging as a key strategy for the development of low-cost, stable and functional new materials applied in various fields.

Prompted by aryl sulfones' use as building blocks for some drugs and their ability to be good hydrogen bond acceptors, we have synthesized two new organic sulfates based on 3,3'-diaminodiphenyl sulfone and 4,4'-diaminodiphenyl sulfone.

The crystal structures, identified by means of single crystal X-ray diffraction, confirm an atomic arrangement that consists of inorganic layers built by $[\text{SO}_4]^{2-}$ isolated tetrahedron between which crystallographically independent organic cations $[\text{C}_{12}\text{H}_{14}\text{N}_2\text{O}_2\text{S}]^{2+}$ are inserted. $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds assured the formation of the resulted three-dimensional networks.

Moreover, the first compound was found to crystallize in the monoclinic system with the non-centro-symmetric space group $\text{P}2_1$. Its unit cell dimensions are: $a=10.6218$ (4) Å, $b=9.6697$ (4) Å, $c=14.1442$ (5) Å, $\beta=106.322$ (4)°, $V=1394.20$ (10) Å³ and $Z=2$. The second compound, however, crystallizes in the same system but with a centro-symmetric space group $\text{P}2_1/c$ with those unit cell dimensions: $a=30.1122$ (18) Å, $b=11.7047$ (5) Å, $c=8.0292$ (3) Å, $\beta=96.307$ (5)°, $V=2812.8$ (2) Å³ and $Z=4$.

Furthermore, ^{13}C NMR study was conducted for the grown crystals. Functional groups present in the compounds were also identified by IR spectral study. ATG coupled to DSC analysis were carried out to study the thermal behavior of the prepared materials. Finally, the optical study was investigated through UV-Vis absorption.

Keywords: Hybrid material, Dapsone, Sulfuric acid, Spectroscopic study, organic-inorganic materials, X-ray diffraction, UV-Vis.

Hydrothermal synthesis, Crystal structure, thermal behavior and vibrational studies of the novel hybrid iron fluoride (III), $\text{FeF}_6(\text{C}_2\text{N}_5\text{H}_6)_3\text{FH}$

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The new organic-inorganic iron fluoride compound, $\text{FeF}_6(\text{C}_2\text{N}_5\text{H}_6)_3\text{FH}$, was successfully prepared by hydrothermal method using EtOH as solvent at 120°C. The crystal structure was solved by single-crystal X-ray diffraction and the bulk was characterized by thermal analyses (TG- DSC) and vibrational spectroscopy (FTIR, Raman). The crystal structure of $\text{FeF}_6(\text{C}_2\text{N}_5\text{H}_6)_3\text{FH}$ crystallizes in the monoclinic system space group $\text{P}2_1/\text{c}$ with $a = 15.907(2)\text{Å}$, $b = 9.898(1)\text{Å}$, $c = 11.651(1)\text{Å}$, $\beta = 90.686(3)^\circ$, $Z = 4$ and $V = 1834.63(9)\text{Å}^3$. The structure is built up from isolated octahedral FeF_6 separated by monoprotonated $[\text{C}_2\text{N}_5\text{H}_6]^+$ cations and hydrogen fluorides groups. Thermal analysis was investigated. Infrared absorption and Raman scattering have been carried out used to confirm the presence of all the fundamental modes of organic and inorganic part of our material.

Key words: hydrothermal synthesis, Iron fluoride, thermal analysis, vibrational spectroscopy

Alkali-activated mortar based on phosphate washing waste

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During the extraction of phosphate ore, the phosphate sludge is generated as a waste with huge amount. This waste become a pollution source in many different countries. As a solid waste management, the phosphate washing waste was used as a precursor for alkali activated materials. The aim of this study was to investigate the effect of the calcination on the phosphate washing waste and its activation with alkali solution to produce geopolymeric mortars. The powder was calcined at 3 different temperatures 600 °C, 700 °C and 800 °C and then characterize with X ray powder diffraction (XRD), Fourier transform infrared (FTIR) with attenuated total reflectance (ATR), Differential Scanning Calorimetry and Thermogravimetric analysis (DSC-TG), Magic Angle Spinning Nuclear Magnetic Resonance (MAS-NMR) and Scanning Electron Microscope (SEM). Then the obtained powders were activated with a solution of sodium hydroxide and sodium silicate. The samples were cured for 7 and 28 days and studied by XRD, SEM and compressive strength. The results show that the geopolymeric mortar based on phosphate washing waste calcined at 700°C presents the best compressive strength needed for masonry application.

Synthesis of new copper(I) complexes with hydrophilic aminomethylphosphines

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Inorganic compounds have had an enormous impact on medicine [1], in particular in the treatment of cancer. In the research of novel metal based drugs useful for addressing anticancer therapy, recent findings have demonstrated that copper(I) complexes represent good alternatives to platinum drugs [2]. What is more, numerous literature reports confirming that phosphines and their metal complexes, especially copper(I), exhibit promising antimicrobial, anticancer and antiarthritic properties [3].

Lipophilic and hydrophilic aminomethylphosphines were prepared in excellent yield by the condensation of tetrakis hydroxymethyl phosphonium chloride (THPC) with a variety of secondary amines under nitrogen atmosphere such as N-methyl-piperazine (Fig.1).

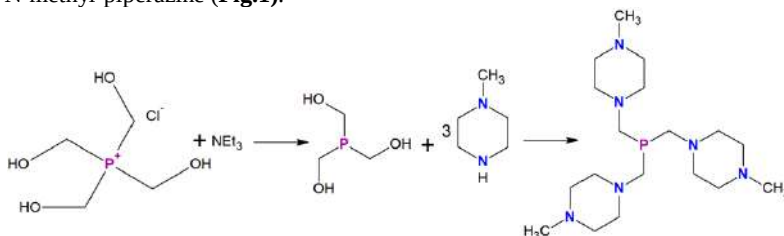


Fig.1. Formation of aminomethylphosphines.

The chemical structures of these new complexes were determined in solution by means of NMR ¹H ³¹P{¹H} and ¹³C{¹H} NMR, elemental analyses and mass spectrometry.

Keywords

Phosphines, Copper(I) complexes, THPC and N-methylpiperazine

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A study on organic templated metal halides: Structure, thermal analysis and magnetic properties.

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Two complexes with the general formula $L_2[MX_4]$ (with L is organic cation, M is metal, and X= Cl, Br) have been grown by the slow evaporation method at room temperature. These compounds were subjected to the following characterization techniques: single crystal X-ray diffraction, thermal analysis and temperature dependent magnetic susceptibility measurements. Organic cations connected to the inorganic sheets by means of hydrogen bonds. Thermal analyses were carried out to highlight the possible phase transitions and the thermal stability of the compounds. The compounds exhibit weak antiferromagnetic interactions.

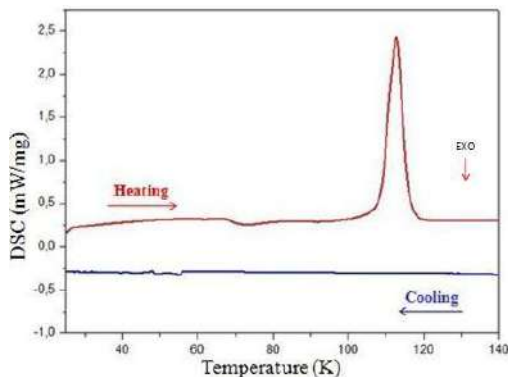


Fig: DSC curves obtained upon cooling and heating processes

Key words: Metal halides, intermolecular interactions, thermal behavior, Magnetic properties.

Electrical conductivity and dielectric behaviour of nanocrystalline $\text{La}_{0.6}\text{Gd}_{0.1}\text{Sr}_{0.3}\text{Mn}_{0.75}\text{Si}_{0.25}\text{O}_3$

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An $\text{La}_{0.6}\text{Gd}_{0.1}\text{Sr}_{0.3}\text{Mn}_{0.75}\text{Si}_{0.25}\text{O}_3$ ceramic was prepared via a solution-based chemical technique. X-ray diffraction study confirms the formation of the compound in the orthorhombic structure with the *Pnma* group space. Dielectric properties have been investigated in the temperature range of 85–290 K with the frequency range 40 Hz to 2 MHz. The conductivity spectra have been investigated by the Jonscher universal power law: $\sigma(\omega) = \sigma_{\text{dc}} + A\omega^n$, where ω is the frequency of the ac field, and n is the exponent. The deduced exponent 'n' values prove that a hopping model is the dominating mechanism in the material. Based on dc-electrical resistivity study, the conduction process is found to be dominated by a thermally activated small polaron hopping (SPH) mechanism. Complex impedance analysis (CIA) indicates the presence of a relaxation phenomenon and allows us to modelize the sample in terms of an electrical equivalent circuit. Moreover, the impedance study confirms the contribution of grain boundaries to the electrical properties.

SYNTHESIS AND CHARACTERIZATION OF ZN-DOPED MESOPOROUS TiO₂ NANOPARTICLES AS EFFICIENT MATERIAL FOR PHOTOCATALYTIC APPLICATIONS

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Mesoporous, nanocrystalline, Zinc-doped TiO₂ nanoparticles were synthesized by surfactant-assisted sol–gel method. The samples were characterized, using SEM, XRD, UV-vis, FTIR, and electrical measurements. The SEM micrographs revealed agglomerated spherical-like morphology. From the optical studies, there is a red-shift in the absorption edge that can be attributed to the presence of Zn in the TiO₂. For Zn doped TiO₂ nanoparticles the optical band gap varies between 3.3 and 3.1 eV with the increase of doping concentration. XRD pattern confirmed the tetragonal structure of synthesized samples. Average grain size was determined from X-ray line broadening using the Debye–Scherrer relation. The crystallite size was found to vary from 25 to 20 nm. The TiO₂ conductivity determined from impedance measurements showed characteristic behavior which is compatible with disordered materials where conductivity is ensured by hopping processes and characterized by a power law behavior at high frequencies. Photocatalytic activity of the synthesized nanomaterials was successfully tested for photodegradation of rhodamine B as model pollutant under UV light. The obtained results show an enhancement of photocatalytic activity of TiO₂ nanopowder with Zn-doping.

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Hydrothermal synthesis, characterization and crystal structure of new inorganic-organic hybrid materials based on metatungstate type units

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A new organic–inorganic hybrid compound $(C_7H_{11}N_2)_6 [H_2W_{12}O_{40}].2H_2O$, have been isolated under autogenous pressure method and characterized by Fourier-transform infrared spectra (FTIR) UV-visible spectroscopy, single-crystal X-ray diffraction analysis, cyclic voltammetry and Thermogravimetric analysis (TGA). The single-crystal X-ray diffraction study shows that the compound crystallizes in monoclinic crystal system with space group $P 2_1/c$ and cell constants of $a = 13.898 \text{ \AA}$, $b = 20.844 \text{ \AA}$, $c = 27.014 \text{ \AA}$, $\beta = 97.8354^\circ$, $Z = 2$, $V = 7752.95$. Crystal structure of the title hybrid material is constituted of $[H_2W_{12}O_{40}]^{6-}$ clusters linked to each other's by organic cations $(C_7H_{11}N_2)^+$ by hydrogen bond interactions between N atoms of the organic molecules and the O atoms of the polyanions as well as between the O atoms of the water molecules and N atoms of organic cations.

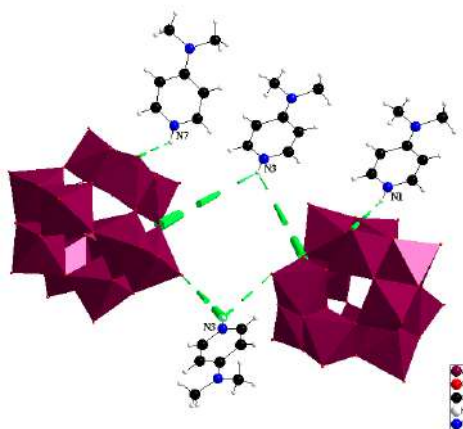


Figure: A-View showing the strong hydrogen-bonding interactions between organic cation, terminal oxygen atoms of polyoxoanions

Keywords: Polyoxometalate; Hybrid materials; Crystal structure; Infrared spectroscopy; Thermogravimetric Analysis

Electrical and vibrational properties studies of $\text{Na}_{0.45}\text{K}_{1.55}\text{Cu}_3(\text{MoO}_4)_4$

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Single crystals of a new triple molybdate, sodium potassium copper(II) tetra-[molybdate(VI)], $\text{Na}_{0.45}\text{K}_{1.55}\text{Cu}_3(\text{MoO}_4)_4$ have been synthesized by a solid-state reaction and its crystal structure has been determined by X-ray diffraction. This compound crystallizes in the monoclinic space group P21/c with $a = 5.097$ (2) Å, $b = 14.594$ (3) Å, $c = 19.905$ (3) Å, $\beta = 94.00$ (2)°, $V = 1476.9$ (7) (Å³), $Z = 4$, $R(\text{F}_2) = 0.025$ and $wR(\text{F}_2) = 0.063$. K2 and Na1 cations are located at the same general site with occupancies of 0.55 and 0.45 respectively. The structural model is supported by bond-valence-sum (BVS). The electrical properties of the title compound are investigated using complex impedance spectroscopy taking into account the contributions of grains, grain boundaries and electrode. A factor group analysis of $\text{Na}_{0.45}\text{K}_{1.55}\text{Cu}_3(\text{MoO}_4)_4$ leads to the determination of internal and external modes. The infrared and Raman vibrational spectra have been investigated. The three crystallographically independent Cu^{2+} cations adopt the $[4 + 2]$ CuO_6 Jahn-Teller distortion giving rise to an intense d-d transition in UV-vis absorption spectra. The nature and value of the band gap have been determined.

Key words: X-ray diffraction; Bond valence analysis; Structure; Charge Distribution

Electrical properties, phase transitions and conduction mechanisms of $\text{Tl}_{1.90}\text{Rb}_{0.10}(\text{SO}_4)_{0.92}(\text{SeO}_4)_{0.08}\cdot\text{Te}(\text{OH})_6$

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The new mixed compound $\text{Tl}_{1.90}\text{Rb}_{0.10}(\text{SO}_4)_{0.92}(\text{SeO}_4)_{0.08}\cdot\text{Te}(\text{OH})_6$ (TlRbSSeTe) has been synthesized in order to determine the temperature transitions and to study the electrical properties as well as the conduction mechanism. It is obtained by slow evaporation at room temperature and found to crystallize in the monoclinic system with $\text{P2}_1/\text{c}$ space group using X-ray diffractometer data. The main feature of these atomic arrangements is the coexistence of three different anions (SO_4^{2-} , SeO_4^{2-} and TeO_6^{6-} groups) in the unit cell, connected by

O–H...O hydrogen bonds building up the crystal.

Thermal analysis (DSC, DTA and TG) of the title compound confirms the presence of the phase transitions and the temperature of the decomposition of the studied salt. In order to characterize the phase transitions, Raman spectra have been recorded at various temperatures in the wave number range from 50–1200 cm^{-1} . Detailed dielectric and electrical properties of the material have been analyzed as a function of frequency (100 Hz–10 MHz) and temperature (383–518 K). Besides, the analysis of Nyquist plots were well fitted to an equivalent circuit consisting of a series of combination of grains and grain boundary elements.

The variation of the DC and AC conductivity confirms all the transitions of our sample. Furthermore, the frequency dependence of alternative current (AC) conductivity is interpreted in terms of Jonscher's law (developed). The alternative current (AC) electrical conduction in TlRbSSeTe material is accounted for in terms of two processes that can be attributed to a hopping transport mechanism. These processes are the correlated barrier hopping (CBH) model in some regions, as well as the non-overlapping small polaron tunneling (NSPT) model in the other regions. The conduction mechanism for each phase is determined with the help of Elliot's theory.

**Anticorrosive Effects of Curcuma extract
Against the Corrosion of Iron:
An electrochemical and Computational Study**

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The inhibition effects of Curcuma Rhizomes extract on iron in 0.5 M NaCl was investigated using gravimetric technique, the electrochemical impedance spectroscopy as well as the quantum chemical calculations.

The experimental result allowed concluding that the Curcuma Rhizomes extract acted as an inhibitor for chloride-induced corrosion of iron. The inhibition efficiency increased when the electrolyte extract content increased. However, it decreased when temperature increased.

Inhibitor adsorption characteristics were predicted following Langmuir adsorption isotherm at the concentrations and temperatures studied.

Quantum chemical calculations were performed using the density functional theory at B3LYP/6-311G (d,p) level of theory to find out whether a clear link exists between the inhibitive effect of the extract and the electronic properties of its main constituents.

Keywords: Iron, EIS, Green inhibitor, DFT calculations.

Removal of nickel (II) using a novel synthetic bis(2-pyridylmethyl)amino-chloroacetyl chloride-ethylenediamine-grafted GO sheets.

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The functionalization of graphene oxide sheets by ethylenediamine (EDA) was accomplished followed by the grafting of bis(2-pyridylmethyl)amino group (BPEN) onto the activated graphene oxide sheets in the presence of chloroacetyl chloride (CAC) produced a magnetic graphene-based composite [(Go-EDA-CAC)-BPEN]. The physic-chemical properties of [(Go-EDA-CAC)-BPEN] composites were investigated by Fourier transform infrared (FT-IR) Vibrating sample magnetometer (VSM), Scanning electron microscopy (SEM), Thermogravimetric analysis (TGA). Moreover, [(Go-EDA-CAC)-BPEN] was used for removing Ni(II) ions from aqueous solutions using a batch process. The effect of pH, contact time and temperature were investigated, however weakly dependent on ionic strength. The chemical adsorption involving the strong surface complexation of metal ions with the nitrogen and oxygen containing groups on the surface of graphene oxide. The maximum adsorption capacity values of Ni(II) on the [(Go-EDA-CAC)-BPEN] at the pH of 6 is 3.05 mmol.g⁻¹. To examine the underlying mechanism of the adsorption process, pseudo-first, pseudo-second-order and intraparticle diffusion models were fitted to experimental kinetic data. Results showed that the pseudo-second-order equation was appropriate to describe the Ni(II) adsorption by [(Go-EDA-CAC)-BPEN]. Adsorption data were further analyzed by the Langmuir and Freundlich adsorption approaches. Additionally, the adsorption properties of the [(Go-EDA-CAC)-BPEN], their reusability (more than 10 cycles) and durability in the aqueous solutions open the path to removal of Ni(II) from water solution. Based on the results obtained, we conclude that [(Go-EDA-CAC)-BPEN] can be an effective and potential adsorbent for removing Ni(II) ions from an aqueous solution.

Keywords: Graphene oxide, bis(2-pyridylmethyl)amino, adsorption kinetics, isotherms.

Mineralization of Nanofiltration Concentrate of Landfill Leachate by Electrochemical Advanced Oxidation Processes

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In order to mineralize nanofiltration (NF) concentrate from landfill leachate, a heterogeneous electro-Fenton (HEF) process was implemented. An undivided electrocatalytic cell using a $\text{Fe}^{\text{II}}\text{Fe}^{\text{III}}$ layered double hydroxide (LDH)/ carbon felt (CF) cathode and a sub-stoichiometric titanium oxide (Ti_4O_7) anode was employed to carry out the HEF of NF concentrate. Excellent mineralization of NF concentrate was achieved by HEF with Pt anode after 8h of electrolysis, while homogenous EF with the addition of catalyst (Fe^{2+}) and adjustment of pH at 3 showed lower mineralization. Comparative studies at low current density using Ti_4O_7 anode led to higher mineralization rate compared to Pt anode. The toxicity of NF concentrate was evaluated along the mineralization process using Microtox method to show the detoxification capacity of the process. The identification and quantification of carboxylic acids and released inorganic ions, as a consequence of mineralization process, were achieved using gas chromatography–mass spectrometry (GC/MS) and ionic chromatography (IC).

DEGRADATION OF METHYLENE BLUE USING ZnO PHOTOCATALYST IN WATER PURIFICATION

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Current environmental protection concerns the quality of water and air. This strong tendency to control the purity of the water leads to the design of sensors. In this work, we study the degradation of methylene blue in the presence of the ZnO photocatalyst. The photochemical behavior of this molecule depends a lot on the conditions and the nature of the reaction medium; especially the pH of the solution to be degraded and the concentration of the pollutant. We apply the photocatalysis of the dye (at room temperature) under visible light and using a UV lamp. The photocatalytic efficiency was calculated from absorption spectra using UV-visible spectroscopy.

Keywords: ZnO, Photocatalysis, Methylene Blue, Water UV-Visible Spectroscopy

Application of Polyaniline Nanoparticles Modified Screen Printed Carbon Electrode as a Sensor for Determination of Hg(II) in Ground Water Samples

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We have described the development of electrochemical nano sensor for the detection of mercury ions from aqueous solutions based on the formation of polyaniline nanoparticle films. Screen printed carbon electrodes were modified with polyaniline nanoparticles. Electropolymerization of polyaniline nanoparticles was performed by the pulsed potentiostatic method. The sample of polyaniline nanoparticles was prepared by repeating the potential step process three times. Structural and morphological characterization of polyaniline nanoparticles modified screen printed carbon electrode was performed using Fourier Transmission infrared (FTIR), X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). PANI nanoparticles were spherical shaped having an apparent diameter varying from 20 to 45 nm.

Square wave anodic stripping voltammetry was used for the detection of Hg(II) on PANI NPs modified screen printed carbon electrode under optimized conditions. Hg(II) was deposited for 60 seconds by the reduction of Hg(II) in buffer solution: (citric acid and sodium chloride pH 2.30), followed by Hg stripping between 0.3 and 0.8 V at the following parameters: scan rate: 100 mV s⁻¹, frequency: 60 Hz, amplitude: 0.025 V and increment: 4.0 mV. it was found that the PANI NPs modified screen printed carbon electrode had a highest anodic stripping peak current in solution of pH 2.30. The limit of detection value for Hg(II) was found to be 2.50 ±0.03 ppb. The limits of detections determined are below the corresponding guideline value from the World Health Organization (WHO). In addition, the modified nano electrode exhibited excellent reproducibility and high stability. The developed method was successfully applied to determine Hg(II) in real water samples with satisfactory results.

Key words : electrochemical nanosensor, polyaniline nanoparticles, mercury sensor, modified electrode, voltammetry.

Casting of PLA mixed with natural dye

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PLA is a biodegradable and compostable thermoplastic obtained from renewable resources such as starch and sugar, generally used in the medical field and has mechanical performances compared to traditional polymers used for the manufacture of rigid packaging (Carlotta et al.). He is known for his ease of implementation. Like other petrochemicals, PLA can be processed by various methods such as injection molding, sheet extrusion, blow molding and thermoforming. PLA films can be made by various methods such as extrusion, thermocompression and casting method. This method has been widely used for the preparation of biopolymer films because PLA is known by its solubilisation in different solvents (Carlotta et al). The goal of this work is to prepare PLA films mixed with natural dye in order to produce products that respect the environment.

Key words: Natural dye, casting, poly acid lactic.

Physical properties, electrochemical stabilities and molecular dynamics study of novel ionic liquids based on N-allyl-N, N-dimethylethylammonium cation.

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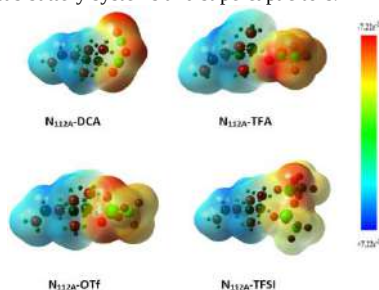
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A series of novel ionic liquids (ILs) based on N-allyl-N,N-dimethylethylammonium (N_{112A}^+) are synthesized and characterized. Their physical properties and electrochemical stabilities were investigated and discussed toward the anion constituents. Herein, four anions were studied including one non-fluorinated and planar structured anion (DCA⁻) and three fluorinated anions (TFSI⁻, OTf⁻, TFA⁻). The experimental properties were compared to those predicted by molecular DFT dynamics simulations. All salts were found to be low melting compounds, while being all-liquid at room temperature. N_{112A} -TFSI is found to be the most thermally stable ($T_d = 329^\circ\text{C}$) while N_{112A} -TFA is the least stable ($T_d = 158^\circ\text{C}$). The ILs transport properties have been determined versus temperature and discussed using the ionicity and Angell's fragility, concepts. Among the good and fragile prepared ILs, N_{112A} -DCA exhibits outstanding transport properties in terms of low dynamic viscosity (19.97 mPa.s) and high ionic conductivity (19.20 mS.cm^{-1}) at 298 K. These suitable properties are explained, from DFT computational calculations, by the lower intermolecular interactions of ion-pairs in N_{112A} -DCA, and quantified by the decreased value of dispersion ion-pairs interaction energy (-6 kJ.mol^{-1}) compared to the others ones. The ILs electrochemical stability window (ESW) seems strongly affected by the cation structure, while their values are found to decrease in the following order N_{112A} -TFSI (4.40 V) > N_{112A} -OTf (3.80 V) > N_{112A} -DCA (3.00 V) > N_{112A} -TFA (2.18 V). Taking into account of the most likely oxidation and reduction reactions, these trends were discussed and validated by the SMD calculation model. The experimental values of ESWs are also very close to the predicted ones. Overall, the results show that, these ILs are suitable as electrolytes for electrochemical devices as battery systems and supercapacitors.



Optimized structures of selected ILs with the electrostatic potential map (isovalue 0.0004, scale -0.0722 ; $+0.0722$).

DEGRADATION EFFICIENCY AND TOXICITY EVOLUTION OF EMERGING CONTAMINANTS IN WATER SOLUTIONS

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Applying gamma irradiation is an effective advanced oxidation process for removing pharmaceutical contaminants from wastewater as an alternative to conventional water treatment technologies. In this purpose, the degradation efficiency of several detected contaminants under gamma irradiation was evaluated. In fact, radiolysis of organic pollutants in aqueous solutions produces powerful reactive species, essentially hydroxyl radical ($\cdot\text{OH}$), able to destroy recalcitrant pollutants in water. In this study the basic principles of radiolytic treatment of organic pollutants in water specifically electron beam and Cobalt-60 processing will be illustrated. Many applications, highlighting the technology's strong points and operational conditions are described, with a presentation of the main advantages of this technology. Pharmaceuticals considered in this study are aqueous solutions of paracetamol, diclofenac and fumaric acid, which were treated with different doses. Moreover, the catalytic oxidation of these compounds by gamma irradiation was investigated using hydrogen peroxide (H_2O_2) as a convenient oxidant. In the aim to release high degradation efficiency of considered pharmaceuticals, an optimization of the main parameters influencing this process, namely irradiation doses, initial concentration and oxidant volume were investigated. Significant modifications attributed to these parameters appeared in the variation of degradation efficiency, chemical oxygen demand removal and concentration of radio-induced radicals, confirming them synergistic effect to attempt total mineralization. Pseudo first order reaction kinetics could be used to depict the degradation process of these compounds. A sophisticated analytical study was released to quantify the detected radio-induced radicals (EPR). All results showed that this process is effective for the degradation of pharmaceutical products in aqueous solutions due to strong oxidative properties of generated radicals. Furthermore, the addition of optimal amount of H_2O_2 was efficient to improve the oxidative degradation and contribute to high performance of this process at very low doses.

Keywords: wastewater, pharmaceuticals, radiolysis, HPLC, EPR.

Biocidal effect of *Melia azedarach* seed oil encapsulated on devastating insect species and environmental protection

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Synthetic chemical pesticides are often found as residues in food and pose risks to human health and the environment. In order to reduce the harmful effects of synthetic products. It is interesting to move towards control by the use of active substances and non-polluting. *Melia azedarach* seed oil can act as an effective and natural pesticide that has strong anti-insect pest and regulate the growth substance. The aim of this study is to validate the use of *Melia azedarach* seed oil of Algerian origin extracted by soxhlet and encapsulated by lyophilization's method "freeze-drying". The manufacture of the capsules is obtained in two stages (emulsification and lyophilization) in order to characterize their physicochemical properties. In vitro controlled release of encapsulated *Melia azedarach* seed oil was achieved for the first time. We also evaluated the insecticidal potential of encapsulated *Melia azedarach* seed oil on two devastating insect species: Rice weevil (*Sitophilus oryzae*) and Grain capuchin (*Rhyzopertha dominica*). The results of the insecticidal activity of the encapsulated *Melia azedarach* oil indicate that this oil exhibits an effective toxicity against *Rhyzopertha dominica* (F.) and *Sitophilus Oryzae* which reach 100 % for the following doses 0.05, 0.1, 0.3 and 1g of capsule. The result of this study shows that *Melia azedarach* seed oil has very interesting insecticidal properties against pests and could be used as an alternative to synthetic chemical pesticides.

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2. Bagle, A. V.; Jadhav, R. S.; Gite, V. V.; Hundiware, D. G.; Mahulikar, P. P. Controlled Release Study of Phenol Formaldehyde Microcapsules Containing Neem Oil as an Insecticide. International Journal of Polymeric Materials and Polymeric Biomaterials 62 (2013) 421–425.

Keywords: encapsulated *Melia azedarach* seed oil, in vitro release, insecticide, *Rhyzopertha dominica* (F), *Sitophilus Oryzae*.

**Tunisian Palm (*Phoenix dactylifera* L.) leaves:
Anti-corrosive activity against the corrosion of steel in acidic media**

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This work is devoted to examine the corrosion inhibition ability of solvent extract of *Phoenix dactylifera* L. leaves for the corrosion of steel in industrial corrosive media (H₂SO₄ 1M) by electrochemical techniques. Results show that the extract is a good inhibitor and acts as mixed type inhibitor. Indeed, the inhibition efficiency calculated from polarisation curves and electrochemical impedance spectroscopy reached 96%. Also, we have tested the effect of temperature in aim to determine the adsorption model. Results show that the Adsorption of *Phoenix dactylifera* leaves aqueous extract on the steel surface follows the Langmuir isotherm.

Keywords:

Anti-corrosive; solvent extract; *Phoenix dactylifera* L.; electrochemical techniques.

Chemometric optimization and validation of a novel method for the simultaneous separation of five antihistaminic in pharmaceutical formulations by UPLC-UV.

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The antihistamine drugs, such as of Dexchlorpheniramine, Promethazine, Cyproheptadine, Cetirizine and Desloratadine have been widely prescribed to alleviate symptoms associated with allergic.

A new method for the simultaneous separation and determination of five antihistaminic by ultra performance liquid chromatography (UPLC-UV) was developed and optimized with the use of experimental design. The analyzed factors were pH of mobile phase, percentage of trifluoroacetic acid (TFA) and the flow rate. These significant variables were optimized using Box Behnken matrix. The influence of these independent variables on resolutions of Cyproheptadine - Cetirizine peaks and time of analysis were evaluated.

The best resolution was achieved by means of a Waters Acuity UPLC C18 (2.1 x 150 mm, 1.7 μ m) analytical column under isocratic conditions using a mobile phase consisting of TFA (pH 2.5)-acetonitrile (60:40, v/v) at a flow rate of 0.3 mL min⁻¹, column temperature of 30 °C and UV detection at 235 nm.

The separation method was validated using accuracy profile to confirm specificity, precision, accuracy, detection and quantification limits. The potential of method for the routine analysis of antihistaminic in pharmaceuticals formulations has been demonstrated.

Keywords: Chemometric, Validation, Accuracy profile, UPLC, Antihistaminic

Electrostatic complexation of polyelectrolytes in aqueous solution

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Polyelectrolytes (PEs) have remained one of the most attractive subjects of scientific research in recent decades owing to their great importance in advanced technologies and molecular biology. A PE is defined as a macromolecular material that has repeating units and dissociates into a highly charged polymeric molecule after its solubilisation in a polar solvent such as water, to form either a positively or negatively charged polymeric chain and counter ions of opposite charge.

The electrostatic attraction between cationic and anionic macromolecules leads in general to the formation of macroscopic precipitates, or more rarely to stable colloidal complexes (PECs). The structure of PECs mainly depends on the degree of ionization of the PEs, their concentrations, mixing ratio [+/-], molecular weight, hydrophobicity,... Two structural models of PECs are proposed : nonstoichiometric watersoluble and stoichiometric insoluble PECs. Although these systems have been studied for a long time, only few structural studies have been carried out on these complexes in aqueous solution. Therefore, the goal of this work is to determine structural properties of polyelectrolyte complexes formed by strong polyelectrolytes such as poly(diallyldimethylammonium chloride), 'PDADMAC' : polycation and poly(styrene sulfonate), 'PSSNa', and evaluate the effect of some parameters like **hydrophobicity**, polymerization degree and charge density on these complexes.

We are concerned in this study with different degrees of polymerization either for the cationic PE 'PDADMAC': 2174, 1242, 621; or for the anionic PE, 'PSSNa': 2692, 1846 and 337. Thereafter, we varied the charge density of PSSNa between 35% and 100%, while we used $f=100\%$ for PDADMAC. Hydrophobicity of PSSNa depends on its charge density (when f increases, hydrophobicity decreases). On the other hand, we modified the hydrophobicity of PDADMAC by substituting a methyl group by an alkyl C5 or C12 chain. Polyelectrolytes were chemically characterized by RMN ¹H and ¹³C, elemental microanalysis of carbon, sulfur and nitrogen, and atomic emission spectroscopy for sodium. The second step of our study consists in plotting state diagrams for each pair of PE in order to delimit the zones of solubility and insolubility. We have explored the state diagrams of the complexes PSSNa 100% (N=337)/PDADMAC 100% (N=621) and PSSNa 35% (N=337)/PDADMAC 100% (N=621). The results show that the solubility zone widens as f decreases, i.e hydrophobicity increases.

Keywords: polyelectrolytes complexes, aqueous solution, hydrophobicity, structure, stability.

Removal of amoxicillin in fixed-bed column packed with activated carbon derived from date palm

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Activated carbon obtained from date palm by chemical activation was used as adsorbent for the removal of amoxicillin from aqueous solutions. Activated carbon was characterized using Scanning Electron Microscopy, thermo gravimetric analysis, FTIR Spectroscopy, surface area measurement (BET), zero point charge measurement (pH_{PZC}). For column study, the four breakthrough models, namely, Adams–Bohart, Thomas, Yoon–Nelson and Yan were used for the correlation of breakthrough curve data along with the evaluation of model parameters. The experimental breakthrough data, including the saturation adsorption capacities, breakthrough times were determined.

Keywords: activated carbon, adsorption, fixed-bed column, amoxicillin.

REMOVAL OF ARSENIC (III) FROM AN AQUEOUS SOLUTION BY ADSORPTION ON COAL RAW AND TREATED RESULTING FROM DATE PITS

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The objective of this study is the valorization of a lignocellulosic natural residue «the date pits» and its application in elimination by adsorption and electrosorption of the arsenic (III) contained in water. The chronological stages of obtaining coal were: cleaning, drying, crushing and finally two types of treatments: a thermal treatment by pyrolysis at 900°C (CAP1), and a chemical pretreatment with iron oxide of the natural residue followed by a carbonization at 600°C (CAP2). The characterization of the carbonaceous and activated matter showed properties comparable with those of many industrially produced coals. The retention tests optimized in static mode of arsenic (III) on the two obtained materials, gave a maximum capacity of adsorption, about 25 mg/g for the chemically activated carbon and 21 mg/g for that thermally activated. The adsorption capacity of pyrolyzed material at 600°C without preliminary pretreatment is approximately 2 mg/g. The study of the influence of the pH and temperature of the medium showed that with a neutral pH and at ambient temperature (T=20°C), the optimal adsorption of arsenic (III) suitably follows the Langmuir and Freundlich models. The kinetics of adsorption is slow, and it is of type pseudo-second order. The dynamic study in adsorption and electrosorption of arsenic (III) on prepared coals, showed a clear improvement of adsorption in absence of applied potential; it is that ~ 86 mg/g for the activated grain carbon chemically treated and ~ 76 mg/g for the activated grain carbon thermally treated. The application of negative potential (-2V) at saturation, increases the adsorption of the CAG2 at 111 mg/g and 97 mg/g for CAG1, initial concentration of arsenic (III) being of 50 mg/l.



Figure 1 : Raw date pits

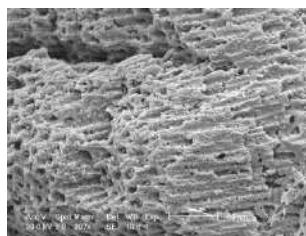


Figure 2 : Scanning electron microscope image of the prepared coal

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Iron-Catalyzed the solventless etherification under green conditions

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Chemists are very passionate about the area of green chemistry and are increasingly to design a careful planning of chemical synthesis and molecular design to reduce adverse consequences [1]. In this context, we present the solventless etherification in environmentally conditions in the presence of $\text{Fe}(\text{SO}_4)_3 \cdot 5\text{H}_2\text{O}$ as a catalyst. The use of simple, cheap, and readily available iron (III) sulfate makes this protocol highly attractive and environmentally benign that meet the principles of green chemistry [2]. Thus, all the structures were confirmed by spectroscopic studies.

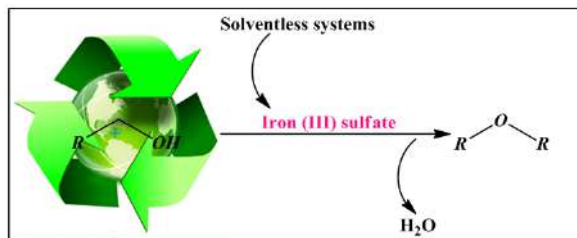


Fig. 1

Key words: green chemistry, etherification, environmentally, catalyst, cheap, iron (III) sulfate.

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Synthesis of some novel Pyrazolines derivatives through 1,3-Dipolar cycloaddition between Dialkyl (allyloxymethyl)phosphonate and nitrile imines

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Jacques LEBRETON^b, Hedi M'RABET^a.

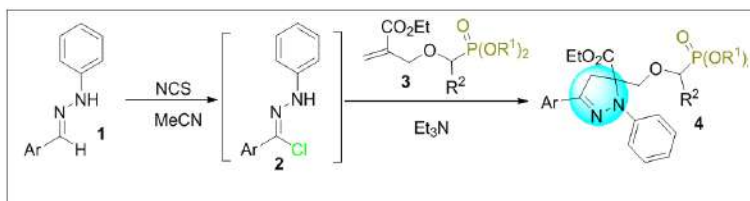
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Pyrazolines are a major class of five-membered nitrogen heterocycles and are important core components in natural products and valuable molecules in the pharmaceutical industry.¹ Several protocols have been reported in the literature for the synthesis of these compounds and the presence of this core in any molecule plays a key role in enhancing the activity.² Among the methods employed in the synthesis of pyrazolines, there is an efficient procedure based on the 1,3-Dipolar Cycloaddition of nitrile imines and dipolarophiles. As a part of our ongoing studies, a new pyrazolines derivatives **4** were synthesized with good yields by the 1,3-Dipolar cycloaddition between Dialkyl (allyloxymethyl)-phosphonates **3** and nitrile imines generated *in situ* from the corresponding hydrazoneyl chloride **2**.



Scheme: 1,3-Dipolar cycloaddition between nitrile imine and dialkyl (allyloxymethyl)phosphonates.

Key words: 1,3-Dipolar cycloaddition, Pyrazolines, Nitrile imines, Hydrazoneyl chlorides.

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Molecular weight degradation, rheological properties and antioxidants activities of polysaccharides from *Zizyphus lotus* fruit under ultrasonic treatment

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This study investigates the effect of ultrasonic treatment of polysaccharides isolated from *Zizyphus lotus* fruits (ZLP) with high molecular weight on the chemical composition, rheological behavior and antioxidant activities of polysaccharides. Results showed that molecular weight (Mw) was decreased from 2.72×10^6 to 1.69×10^6 g/mol for 120 minutes without modification in the primary structure as revealed by chemical analysis and FTIR spectrum. Rheological analysis showed that ZLPs solutions (2.5mg/mL) exhibited a pseudoplastic flow behavior. Besides, during the ultrasonic depolymerization time, a decrease in the apparent viscosities for each shear rate value was observed for ZLPs solutions which attributed to the reducing in the molecular mass. In addition, the apparent viscosities of ZLPs solutions decreased with the acidic pH (2.0) or alkaline pH (8.0) which was further raised with the temperature increment. The addition of monovalent and divalent salts modified significantly the apparent viscosities of ZLPs. Furthermore, our results exhibited that ZLPs could be valorized as gelling agent and stabilizer in the food industry. Antioxidant activity assays *in vitro* indicated that the degraded fraction with low molecular weight had a stronger 2,2-diphenyl-1-picrylhydrazyl scavenging ability, reducing power and anti-lipid peroxidation activities.

Keywords: *Zizyphus lotus* fruits, polysaccharides, depolymerization, rheological properties, antioxidant activities.

3-acetyl-coumarin *N*-benzoylhydrazone: Synthesis and biological activity

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In the present work, we are particularly interested in the synthesis of 3-acetyl-coumarin *N*-benzoylhydrazone and their biological activity. **Two-step synthesis** method has been used: (i) the Knoevenagel condensation between salicylaldehyde and methylacetoacetate. (ii) The resulting 3-acetyl coumarin was then reacted with benzohydrazide in ethanol in the presence of acetic acid as a catalyst. The structure of the new compound was confirmed by IR and NMR (¹H, ¹³C, HMBC) spectroscopy. On the other hand, we are interested in the pharmaceutical effect of this compound in Wistar rats with acute coronary syndrome following the injection of isoproterenol [1]. The results obtained revealed that the administration of our compound induces a net improvement in heart injury, significantly reduces total cholesterol and triglyceride levels. In addition, a decrease in fibrinogen level. Therefore, the use of this synthesized molecule enhances the ventricular remodeling process.

Key words: 3-acetyl-coumarin *N*-benzoylhydrazone, isoproterenol, total cholesterol, triglyceride levels, fibrinogen level

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Synthesis, conformational analysis of new diastereomeric cyclophosphamides

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Cyclophosphamides are an important class of organic compounds that exhibit various medicinal properties^[1,2].

Thioxo, Oxo, Seleno, diastereomeric cyclophosphamides containing 1,3,2-dioxaphosphorinanes are prepared by a one step chemical reaction. Their structural determination is carried out by means of NMR (³¹P, ¹H, ¹³C), MR-SM. The conformational study of diastereomeric products is described. DFT calculations allowed the identification of preferred conformations.

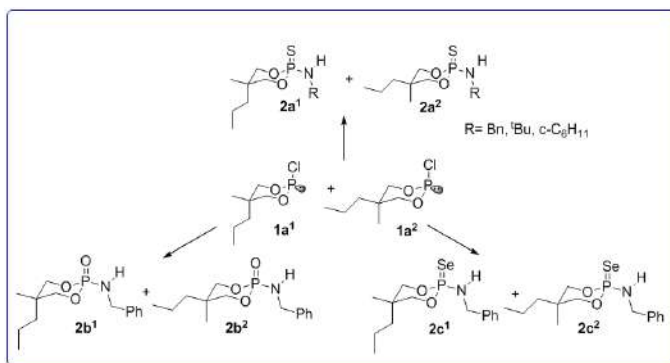


Fig 1. Synthesis of diastereomeric thioxo, Oxo, Seleno, diastereomeric Cyclophosphamides

Key words: Cyclophosphamide, dioxaphosphorinane, diastereomeric products, heterocyclic synthesis.

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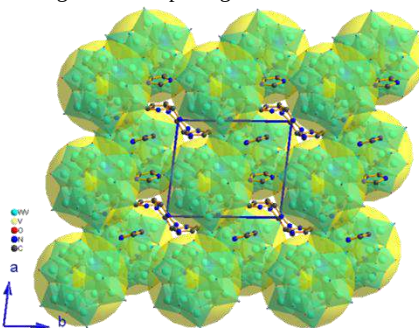
Synthesis, characterization and antimicrobiol activity of a novel fluorescent tetra-V- substituted kegggin heteropolyoxotungstate decorated with imidazolium cations

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Heteropolyoxometalates (HPOMs), which are inorganic mixed-metal oxide cluster anions are considered as a great class of polyoxometalates. Their intriguing topological structures have been extensively studied in recent years due to their large variety of applications in many fields such as medicine, biology, catalysis, material sciences and chemical analysis specially those displaying the Keggin structure. Recently, Salts of mixed-metal anions $[V_nW_{12-n}O_{40}]^{(2+n)-}$, in which one or more tungsten (VI) atoms are substituted by vanadium (V), are distinguished by their electronic properties and their excellent chemical reactivity as well as their antibacterial activity. The synergy of those inorganic species and organic cations is beneficial for synthesizing functional materials.

In light of this reason, we explore a new-fangled tetra-V-substituted Keggin-type polyoxotungstate associated to a pentacyclic aromatic compound with tow potential N-donor sites, the imidazolium cations. The synthesized compound has been characterized by powder and single-crystal XRD methods, ICP-AES, IR, UV-Vis and photoluminescence spectroscopy measurements. X-ray diffraction analysis show that $(ImH)_6[V_4W_9O_{40}]$ with $ImH = C_3N_2H_5$; crystallizes in the triclinic system with space group $P\bar{1}$ with $a = 10.297$ (5) Å, $b = 12.015$ (5) Å, $c = 21.231$ (5) Å, $\alpha = 83.205$ (5)°, $\beta = 83.788$ (5)° and $\gamma = 82.980$ (5)° and its crystal packing shows that kegggin anions and ImH^+ cations assemble into a porous 3-D hydrogen-bonded host framework in which the independent cations reside in the channel voids balancing charge and participating in the extensive hydrogen-bonding 3D-supramolecular network. Furthermore, the electronic properties and the optical band gaps have also been investigated well confirming the semiconductor behavior and photoluminescent property of reported material. In addition, the complex shows promising antimicrobial and antifungal activities against some pathogenic microbes.



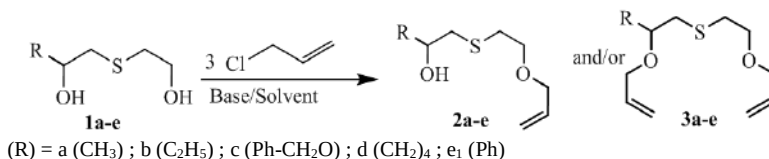
A porous 3-D supramolecular network of ImV4W9 viewed along c-axis

An efficient synthesis of new allyloxy- β -hydroxy and bis(allyloxy)sulfides

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Allyloxy- β -hydroxy sulfides constitute an important class of organic compounds¹. Owing to their stability in both acid and basic media, they are frequently used as protective groups for amines and alcohols. They are also used as intermediates in the synthesis of several compounds having interesting biological properties², such as antitumor, antiviral and antifungal agents. These compounds also constitute the starting material for the synthesis of pharmaceutical products, dendrimers, biodegradable polymers and a large variety of biomedical molecules³. In a previous work, we have described the synthesis of a series of thioetherdiols⁴. Herein, we report on their reactivity *via* the condensation reaction with allyl chloride in basic medium for the preparation of new allyloxy- β -hydroxy sulfides through a regioselective reaction.



Key words: Allylic substitution, Dihydroxy sulfides, Allyloxy- β -hydroxy sulfide, bis-(Allyloxy)sulfides, regioselectivity.

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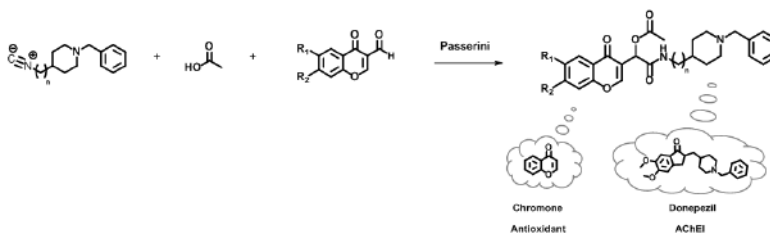
Synthesis of donepezil-chromone hybrids via the Passerini reaction

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New α -acyloxycarboxamides were easily obtained in a one step by the Passerini multicomponent reaction of carboxylic acid, aldehyde and isocyanide. They were designed based on the Multi-Target-Directed Ligand (MTDL) approach, by combining the N-benzylpiperidine pharmacophore present in the acetylcholinesterase inhibitor (AChEI) donepezil currently used for Alzheimer's disease treatment, with a chromone which is a well-known antioxidant. These hybrids proved to be potent cholinesterase inhibitors showing moderate antioxidant properties.



Key words: Donepezil, Chromone, Passerini reaction, Cholinesterase inhibitor, Antioxidant.

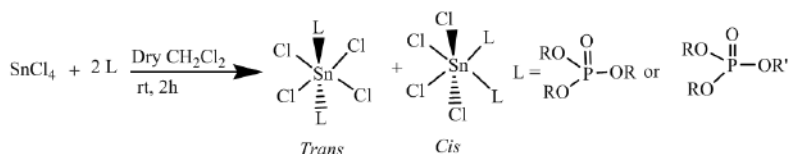
PREPARATION AND CHARACTERISATION OF TIN(IV) COMPLEXES WITH BIOLOGICALLY RELEVANT ORGANOPHOSPHATES

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Organophosphates have found a variety of applications in the areas of industrial, agricultural and medicinal chemistry due to their biological and physical properties as well as their utility as synthetic intermediates [1-3]. In particular, dialkyl aryl phosphates were shown to be excellent inhibitors of both acetylcholinesterase (AChE) and butyrylcholinesterase (BChE), with a preference for the latter enzyme, surpassing in some cases the inhibitory activity of the currently approved Alzheimer's disease medications, rivastigmine and galantamine [4]. In a previous work, we have shown that tin coordination of phosphoramidates bearing aryl groups could be used to evaluate their possible biological activity [5, 6]. In this work, we show that trialkyl phosphates and dialkyl aryl phosphates (L) bearing long chain alkyl groups readily form stable octahedral complexes with tin (IV) chloride to yield new tin complexes. These adducts have been characterized by multinuclear (¹H, ³¹P and ¹¹³C) NMR and IR spectroscopy. The solution NMR data of these complexes showed the presence of a mixture of *cis* and *trans* isomers with the proportion of the former isomer being more pronounced for dialkyl aryl phosphates. The difference between the two types of phosphoryl ligands could be interpreted in terms of the electronic effects of the substituents on the phosphorus atom of the ligand.



Keywords: Organophosphates, dialkyl aryl phosphates, tin(IV) complex, ³¹P NMR.

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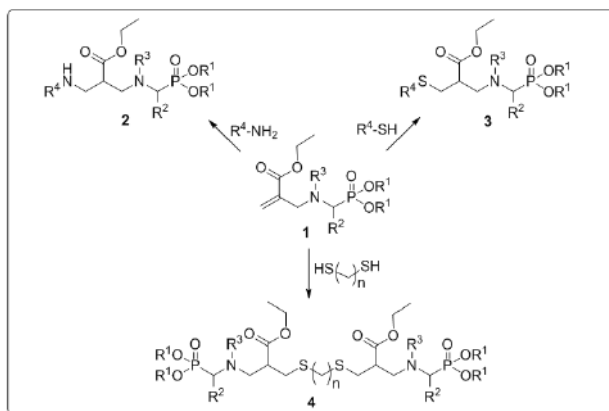
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Reactivity of β -ethoxycarbonylated *N*-methylphosphonate allylamines with amines, thiols and dithiols.

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The Michael addition is one of the most exploited reactions in synthetic organic chemistry.¹ This reaction is widely reported as an essential step for the preparation of several natural products and compounds that exhibit biological and pharmaceutical interests.^{2,3} In this context, we describe an efficient conjugate addition of amines, thiols and dithiols to β -ethoxycarbonylated *N*-methylphosphonate allylamines **1** using triethylamine as catalyst. Michael adducts **2-4** were obtained in good yields and were characterized by (¹H, ¹³C and ³¹P) NMR spectroscopy.



Scheme 1. Conjugate addition of amines, thiols and dithiols to β -ethoxycarbonylated *N*-methylphosphonate allylamines **1**.

Keywords: β -ethoxycarbonylated *N*-methylphosphonate allylamines, conjugate addition, amines, thiols, dithiols.

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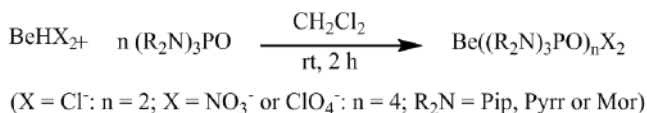
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SYNTHESIS AND CHARACTERISATION OF BERYLLIUM (II) COMPLEXES WITH PHOSPHORAMIDES BEARING DIFFERENT CYCLIC AMINO GROUPS

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Beryllium chemistry is still comparatively underdeveloped due to its extreme toxicity [1]. However, it is a vital component in a variety of technological and consumer industries and its usage continues unabated despite its toxicity [2]. Therefore, it is imperative that there are chemical agents for remediation and as therapies for individuals exposed to beryllium poisoning [3]. On the other hand, phosphoramides are increasingly attracting considerable attention due their potential applications in coordination chemistry as versatile ligands, in industry as flame retardants, in medicine as prodrugs, in catalysis and synthesis as chiral ligands [4, 5]. In this work, we report on the synthesis of beryllium (II) complexes with phosphoramides containing different cyclic amino groups of the type $(R_2N)_3P(O)$. These complexes were fully characterized by multinuclear (^1H , ^{13}C and ^{31}P) NMR, IR spectroscopy and conductivity. The effect of the substituents of the phosphorus atom on the stability of the complex formed will be also presented.



Keywords: Phosphoramides, cyclic amine, beryllium complex, ^{31}P NMR.

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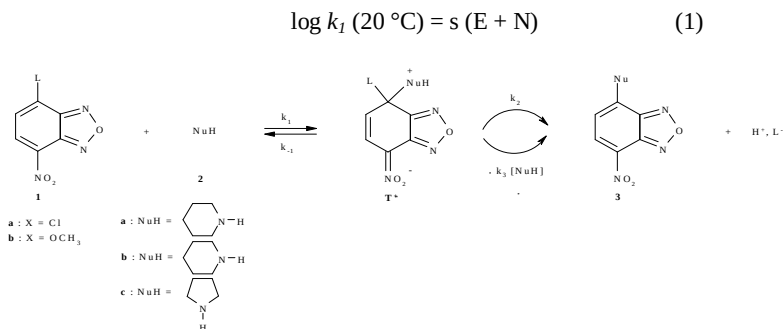
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Electrophilicities of benzofurazans and correlations structure-reactivity

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The kinetics of the nucleophilic aromatic substitution reactions S_NAr of 7-L-4-nitrobenzofurazans **1** (L = Cl, and OCH₃) and secondary cyclic amines (morpholine, piperidine, and pyrrolidine) **2a-c** have been measured in acetonitrile solution at 20 °C and monitored by UV-visible spectroscopy (Scheme 1). The derived values of second-order rate constants (k_I) have been employed to determine the electrophilicity parameters E for both benzofurazans **1a** and **1b** according to the linear free enthalpy relationship (equ.1) and to include them into the comprehensive electrophilicity scale of Mayr.



Scheme 1

As will be seen, the effect of amine basicity on the reaction rate has been examined quantitatively and discussed. On the other hand, the high values of β_{nuc} have been interpreted in terms of a single electron transfer mechanism.

Keywords: S_NAr Mechanism, Electrophilicity, Brønsted's equation, Benzofurazans, Kinetic, Mayr's approach.

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Efficient N-Heterocyclic Carbene Palladium (II) Catalysts Formed In Situ For Carbonylative Suzuki Coupling Reaction Of Arylboronic Acids With 2-Bromopyridine Under Co Pressure Leading To Unsymmetrical Arylpyridine Ketones: Synthesis, Characterization And Cytotoxic Activities

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The palladium NHC complexes are one of the most interesting and widely investigated complexes in different catalytic transformations, especially C–C bond formation reactions such as Suzuki¹, Heck², and Sonogashira³ reactions. Thus, the use of N-heterocyclic carbenes associated to palladium has been reported as efficient catalysts for the carbonyl coupling under mild and varied conditions⁴. Herein, we report the synthesis, characterization and cytotoxic activities of two new families of benzimidazolium salts. Then we studied the use of this class of benzimidazolium salts as a ligand in the carbonylative cross coupling of 2-bromopyridine with different boronic acids under CO atmosphere to form unsymmetrical arylpyridine ketones. **Figure 1**

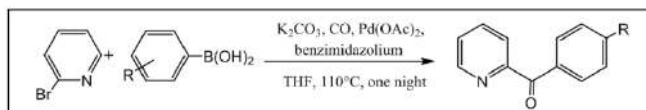


Figure 1: Pd-NHC complexes catalyzed carbonylative Suzuki cross-coupling reaction of arylboronic acids with 2-bromopyridine

Key words: NHC-Pd(II) catalysts, carbonylative suzuki cross-coupling reaction, arylboronic acids, 2-bromopyridine, unsymmetrical arylpyridine ketones.

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Synthesis and reactivity of 3-amino-propiolate derivatives

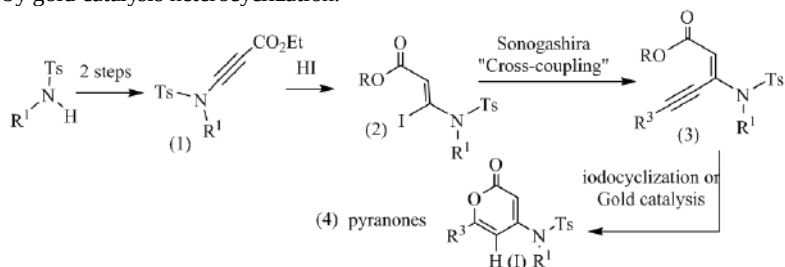
Dhouha Sghairi^{a,b}, Moufida Romdhani-Younes^a, Jérôme Thibonnet^b

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Ynamines are versatile functionalities that are found to be useful in an increasing array of transformations, indeed, many methods of preparation are described in the literature [1,2]. Their popularity can be attributed to the advent of several methods for their synthesis over the last decade [3].

In the present work, we have been able to isolate compounds resulting from the addition of HI on 3-amino-propiolate derivatives **1**, this addition reaction was found to be regio- and stereoselective. The vinyl iodide **2** was then engaged in Cross-coupling reactions, in particular by a Sonogashira reaction. The obtained enynes **3** were used to access new pyranones **4** by iodolactonization reactions or by gold catalysis heterocyclization.



Keywords: ynamines, pyranones, vinylic iodide, Sonogashira Cross-coupling reaction

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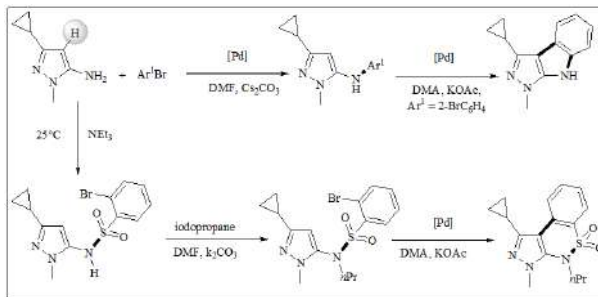
The formation of 5- and 6-membered rings through Pd-catalyzed intramolecular direct arylations of 5-aminopyrazoles bearing 2-bromoaryl substituents on the amino group

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The synthesis of polycyclic aromatics *via* sequential palladium-catalysed amination followed by intramolecular direct arylation of 3-cyclopropyl-1-methylpyrazol-5-amine has been developed. Moreover, from 1,2-dibromobenzene and 2-bromobenzenesulfonyl chloride, the 5-aminopyrazoles bearing N-2'-bromoaryl or 2'-bromobenzenesulfonamide substituent on the amino group were obtained in good yields, without cleavage of the second C-Br bond of the aryl on the pyrazolyl derivatives. Then, an intramolecular Pd-catalyzed direct arylation of bromo-substituted *N*-arylpyrazoles allowed the formation of tricyclic compounds by formation of 5- or 6-membered rings in very high yields.



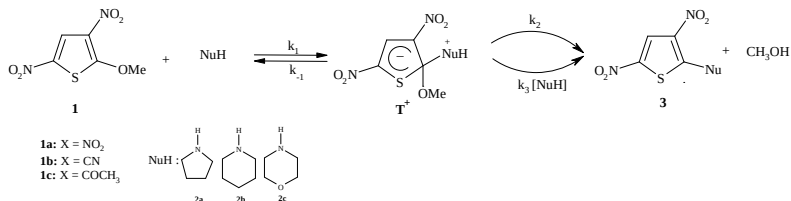
Keywords: intramolecular arylation, amination, pyrazole, tricyclic compounds.

QUANTIFICATION OF THE ELECTROPHILIC REACTIVITIES OF SUBSTITUTED THIOPHENES AND CORRELATIONS STRUCTURE-REACTIVITY

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The kinetics of S_NAr reactions of thiophenes **1a-c** with references secondary cyclic amines have been investigated in acetonitrile and methanol containing 9 vol % acetonitrile as a cosolvent at 20 °C (Scheme 1).



Scheme 1

The derived rate constants have been used to evaluate the electrophilicities parameters E for these series of thiophenes **1a-c** by the linear free energy relationship $\log k_1$ (20 °C) = s_N ($E + N$).

As can be seen, correlation of E values determined in this work and some thiophenes reported recently by Echaieb and co-workers with the corresponding $pK_a^{H_2O}$ values for water addition to these neutral thiophenes in aqueous solution has been constructed and discussed.

Key words: Kinetics, S_NAr Mechanism, Mary's Equation, Electrophilicity, Thiophenes, σ -complexation.

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DOES THE LIMESTONE (CaCO_3) ADDITION AFFECT THE HYDRATION KINETICS OF RESISTING SULFATE (RS) PORTLAND CEMENT?

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The effect of limestone additive on resisting sulfate (RS) Portland cement hydration has been often studied, but there is no general agreement on the relative effects of different amounts of calcium carbonate on the cement paste hydration kinetics [1,2]. The objective of the present work is to assess the effect of various amounts of calcium carbonate on the hydration of RS cement in order to explain the physico-chemical changes occurring during hydration. This study is assured by using a number of commercial RS Portland cements. The hydration kinetics was followed after 1, 2, 7 and 14 days by using by X-ray diffraction technique (XRD), Fourier Transformed Infra-Red spectroscopy (FTIR), Thermogravimetric analysis (TGA), Scanning electron microscopy (SEM) and isothermal calorimetry. We determined the degree of hydration by using two different methods: calculation the ultimate chemically bound water (Non-evaporate water= W_i) and the measurement of the cumulative heat released during hydration after a time t . The results show on the one hand, that the hydration kinetics of the samples containing high calcite contents was delayed and the formation of monocarboaluminate calcium takes place after 7 days of hydration in the cement pastes containing more 5 % of CaCO_3 , on the other hand.

Key words: RS Portland cement, limestone addition, Calcite, hydration kinetics, degree of hydration.

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Structural, elastic, vibrational and thermodynamic properties of Cerium oxide CeO₂. A combined experimental and ab initio investigation

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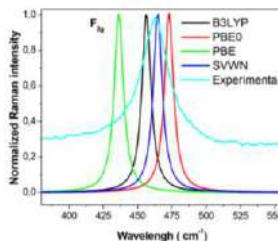
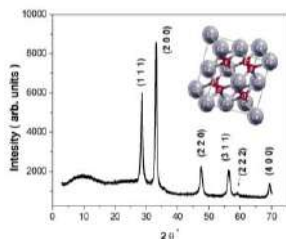
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This work outlines the structural, the vibrational dynamics, the elastic and the thermodynamic properties of Cerium oxide CeO₂ studied by both experimental and ab initio quantum mechanical simulations with various one-electron Hamiltonian by employing different density functionals (B3LYP, PBE0, PBE and SWVN). The structure of the as prepared CeO₂ thin films synthesized by means of the chemical spray pyrolysis route is investigated by X-ray diffraction and compared with the optimized DFT structure. X-ray diffraction (XRD) measurements and the scanning electron microscopy (SEM) analyses revealed the polycrystalline nature of all samples. DFT Electronic properties indicated that B3LYP hybrid functional band gap is closer to the experimental results obtained by UV-Vis NIR spectrophotometry measurements. Except for the PBE prediction, the simulated IR and Raman frequencies and intensities of cubic CeO₂ are consistent with our experimental spectra. The effect of pressure on the elastic constants and related properties (Young's modulus E, bulk modulus K, Poisson ratios ν , and shear modulus G) have been investigated for all mentioned functionals. The lattices parameters, thermal expansion and isothermal bulk modulus of Cerium oxide are carried out in the quasi-harmonic lattice dynamical computation implemented in the CRYSTAL17 code at simultaneous pressure up to 8 GPa and temperatures up to 2000 K.

The effect on the above simulated properties of four density functionals is also explicitly examined. Taken together, the results in this investigation show that cerium oxide is an interesting material for novel electronic devices used at extreme conditions.



Keywords: DFT theory; vibrational modes; Elastic properties; quasi-harmonic approximation.

SYNTHESIS, STRUCTURAL DETERMINATION AND PHYSICO-CHEMICAL PROPERTIES OF $C_{24}H_{36}Cl_6CuN_4O_8S_2$

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Crystals of the new hybrid compound, $C_{24}H_{36}Cl_6CuN_4O_8S_2$, have been synthesized by the slow evaporation method at room temperature. The structure is analyzed by various techniques: single crystal X-ray diffraction, spectroscopy and thermal analyses. This compound crystallizes in the triclinic system with P-1 space group. Its cell dimensions are: $a=6.9530 \text{ \AA}$, $b=11.6200 \text{ \AA}$, $c=12.7000 \text{ \AA}$, $\alpha=111.906^\circ$, $\beta=96.918^\circ$, $\gamma=106.413^\circ$ and $Z=1$. The Cu atom adopts a distorted octahedral geometry. The structural arrangement characterized by an alternation between the organic and the inorganic layers. The IR, Raman and UV-visible spectroscopies were also used to characterize the title compound. Indeed, the thermal stability of the grown crystal was evaluated using thermogravimetric and differential thermal analysis.



The asymmetric unit of $C_{24}H_{36}Cl_6CuN_4O_8S_2$

Keywords: Copper, Hybrid material, thermal analysis, X-ray diffraction.

+Electrical conductivity and dielectric properties of Ln_{1.8} Sr_{0.2} CuO₄ (Ln=La, Pr and Nd)

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In this work we are interested in the study of electric conduction and dielectric properties of Ln_{2-x}Sr_xCuO_{4-δ} (Ln=La,Nd,Pr) family's which are synthesized by the conventional technique of solid state chemistry at 1100°C. The comparison between these oxides was investigated. In fact, X-ray diffraction (XRD) was used to determine the structures and the group spaces. It shows that La_{1.8} Sr_{0.2} CuO₄ and Pr_{1.8} Sr_{0.2} CuO₄ belong to tetragonal structure while Nd_{1.8} Sr_{0.2} CuO₄ is crystallized in orthorhombic structure. The transition phase in the temperature range from 50°C to 600°C was verified by the differential scanning calorimetric (DSC). It shows a significant endothermic anomaly in La_{1.8} Sr_{0.2} CuO₄ and Pr_{1.8} Sr_{0.2} CuO₄ at about 370°C and 250°C respectively, however, Nd_{1.8} Sr_{0.2} CuO₄ does not have any anomaly. The activation energy of the oxide La_{1.8} Sr_{0.2} Cu O₄ (Ea= 0.366 eV) is low compared to the two others oxides Pr_{1.8} Sr_{0.2} Cu O₄ (Ea= 0.503 eV) and Nd_{1.8} Sr_{0.2} Cu O₄ (Ea= 1.47eV). Detailed studies of dielectric properties of the compounds as a function of frequencies at different temperatures (270°C-500°C) show that La_{1.8} Sr_{0.2} CuO₄ and Pr_{1.8} Sr_{0.2} CuO₄ have a very high dielectric constant $\epsilon' > 10^5$ compared to Nd_{1.8} Sr_{0.2} CuO₄ ($\epsilon' \approx 5$). While La_{1.8} Sr_{0.2} CuO₄ and Pr_{1.8} Sr_{0.2} CuO₄ own an important dielectric loss (≈ 65 -70) compared to Nd_{1.8} Sr_{0.2} CuO₄ which has a very low value (≈ 0.65).

Keywords: Cuprates, Structural Analysis, Dielectric Studies, dielectric constant, dielectric loss and modulus studies.

Synthesis, characterization and optical properties of core/shell AgInS₂/ZnS quantum dots

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Ternary I-III-VI₂ quantum dots (QDs) have gained high attention not only for fundamental studies but also their for potential applications in light-emitting diodes, biomedical labeling, solar cells and photocatalysis [1-3]. These QDs exhibit long photo-luminescence (PL) lifetimes and low toxicity compared to Cd-containing QDs.

In this study, the aqueous synthesis, the characterization and the optical properties of ternary AgInS₂ (AIS) and quaternary core-shell AgInS₂/ZnS (ZAIS) QDs are presented. Various synthetic parameters such as the Ag/In molar ratio, the capping ligand and the pH of the reaction medium were varied. The X-ray diffraction (XRD) patterns of AIS QDs show that the nanocrystals exhibit the tetragonal chalcopyrite structure. After the growth of the ZnS shell at the periphery of the AIS core, the diffraction peaks move towards the standard position of the ZnS blende structure. This result proves the formation of the core/shell structure and indicates the diffusion of Zn²⁺ ions into the AIS core, which results in a change in the crystalline network parameters of the AIS nanocrystals. Transmission electronic microscopy (TEM) analyses show spherical ZAIS QDs with an average diameter of about 4 nm. The photoluminescence (PL) spectra of the samples (AIS and ZAIS) were recorded at different stages of the nanoparticles growth in order to optimize their optical properties by adjusting the synthetic parameters. For the Ag/In = 1/5 ratio, the PL spectrum of the AIS QDs shows an emission band centered at 601 nm. After the ZnS shell introduction, a blue shift of the PL peak is observed and the PL emission is located around 563 nm, which further confirms the formation of quaternary alloyed nanocrystals (Figure 1). By in-creasing the Ag/In molar ratio, the emission band of QDs ZAIS shifts gradually from 560 nm to 530 nm. The PL quantum yield for AIS QDs varies between 10% and 40% and increases to 50-70% for ZAIS QDs. These PL quantum yields are the highest reported to date for ZAIS QDs

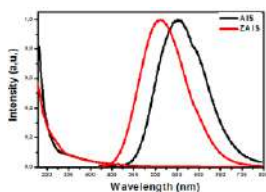


Figure 1: UV-visible absorption and PL emission spectra of AIS and ZAIS QDs prepared in aqueous solution (pH=8.5) with 3-MPA as capping ligand.

Keywords: Quantum Dots, Core/shell, aqueous syntheses, AgInS₂/ZnS, photoluminescence.

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Structural and microstructural studies of Cobalt-based compounds and iron obtained by mechanical alloying

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In this research work, $\text{Co}_{31}\text{Fe}_{31}\text{B}_{30}\text{Ta}_8$ alloy was prepared by mechanical alloying (MA) under argon gas atmosphere. This obtained alloy have been investigated by using X-ray diffraction (XRD) in reflection mode using Cu K- α the morphological study was also studied by scanning electron microscopy (SEM). The MAUD refinement program is used to carry out the structural study. The evolution of the phase transformation during milling time is reported. The results showed that it is possible to produce a solid solution Fe (B) and Co (B) after 5h of milling time. Up to 15h of milling, microstructure consisted of nanocrystalline bcc-(Fe, Co) phases and Ta. After 45h milling time the Co_2Ta phase was formed and it was disappear after 135h milling time. However, the main peak of the bcc-(Fe, Co) phase still persists to 200 hours. The evolution of the lattice parameter and the size of the phase crystals that appear during the mechanical alloying process were studied.

Structural, Spectroscopic Analysis and Photocatalytic Activity of $\text{K}_2\text{Co}_2(\text{MoO}_4)_3$

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In this contribution, potassium cobalt (II) molybdate $\text{K}_2\text{Co}_2(\text{MoO}_4)_3$ was synthesized by a solid-state reaction process. The morphology, the microstructure and the optical properties of prepared compound have been studied by means of scanning probe microscopy, X-ray diffraction (XRD), FTIR and Raman spectroscopy respectively. Also, this material was studied by photoluminescence (PL) and UV-vis spectroscopy. X-ray diffraction analysis reveal that $\text{K}_2\text{Co}_2(\text{MoO}_4)_3$ crystallizes in the monoclinic system with $P2_1/c$ space group and lattice parameters: $a=7.038(8)$ Å, $b=8.987(9)$ Å, $c=20.573(3)$ Å, $\beta=112.19(3)^\circ$, $V=1204.9(7)$ Å³ and $Z=4$. This structure can be described by the presence of tetramers linked with each other by MoO_4 tetrahedra giving a three-dimensional crystal structure containing channels in which K^+ ions reside (Fig. 1). Obtained Raman and IR lines were assigned to different normal vibration modes. This work suggests a good photocatalytic activity of $\text{K}_2\text{Co}_2(\text{MoO}_4)_3$, which may be of interest to develop a safe, cost-effective solar water treatment process.

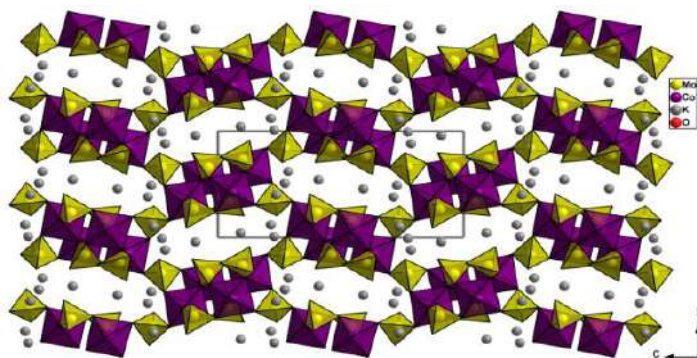


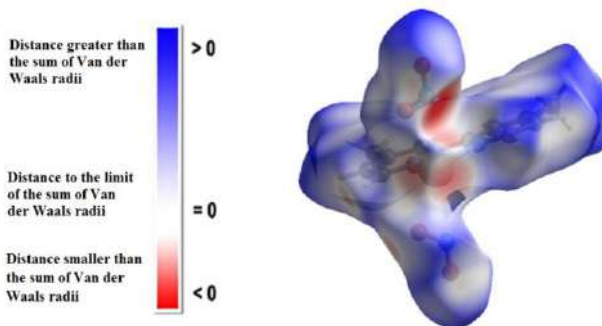
Fig. 1: Projection of the structure along the direction $[100]$.

A HIRSHFELD SURFACE ANALYSIS, CRYSTAL STRUCTURE AND PHYSICOCHEMICAL STUDIES OF A Cd (II) COMPLEX WITH THE 4,4'-DIMETHYL-2,2'-DIPYRIDYL LIGAND

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The Cd(II) complex $[\text{Cd}(\text{NO}_3)_2(\text{C}_{12}\text{H}_{12}\text{N}_2)_2]$ with the bidentate ligand 4,4'-dimethyl-2,2'-dipyridyl has been synthesized in ethanol solution and its structure has been determined by single crystal X-ray diffraction, elemental analysis, CP-MAS NMR and IR spectroscopy. The Cd(II) atom is eight-coordinated by four nitrogen atoms from two bidentate 4,4'-dimethyl-2,2'-dipyridyl ligands and by four oxygen atoms from two nitrate groups leading to a distorted CdO_4N_4 polyhedron. The CdO_4N_4 polyhedra and the nitrate anions are located parallel to the (a, b) plane at $x = n/2$ and the organic residues are located between them. The crystal packing is stabilized by intermolecular O-H...O, N-H...O and C-H...O hydrogen bonds which link the molecules into a three-dimensional network. Intermolecular interactions were investigated by Hirshfeld surfaces. The ^{13}C CP-MAS NMR spectrum was reported and the vibrational absorption bands were identified by infrared spectroscopy. Electronic properties such as HOMO and LUMO energies were derived from theoretical calculations.



Hirshfeld surface around the asymmetrical unit colored according to d_{norm} and color gradient used to cover these surfaces

Keywords: Cd(II) complex; X-ray diffraction; Coordination compound, Hirshfeld surface, contact enrichment ratio; DFT calculations.

Synthesis, electrical and dielectrical properties of phosphate-sulfate fluorapatites $\text{Ca}_{10-x}\text{Na}_x(\text{PO}_4)_{6-x}(\text{SO}_4)_x\text{F}_2$

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In recent years, apatites with different compositions have been attracting a considerable interest as the solid electrolytes for solid oxide fuel cellsSOFCs [1-3]. A series of new phosphate-sulfate fluorapatites $\text{Ca}_{10-x}\text{Na}_x(\text{SO}_4)_x(\text{PO}_4)_{6-x}\text{F}_2$ ($0 \leq x \leq 6$) has been synthesized by the solid-state reaction at high temperature. The samples were characterized using X-ray diffraction, Infrared spectroscopy and Raman scattering spectroscopy. X-ray diffraction study shows that these materials crystallize in the hexagonal system with $\text{P6}_3/\text{m}$ as space group. Infrared and Raman spectra are reported and band assignments are made [4].

An impedance analysis has been used to analyze the electrical behavior of samples as a function of frequency at different temperatures. Evidences of temperature-dependent electrical relaxation phenomena have been observed. The bulk resistance decreases with increasing temperature, showing a typical negative temperature coefficient of resistance (NTCR). Ac-Conductivity measurements have been performed on a wide range of frequencies and temperatures. The complex impedance analysis suggests the presence of non-Debye relaxations that would be associated with correlation on ions motion. The ionic conductivity obeys the Arrhenius and the Jonscher laws.

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Physico-chemical characterization, Hirshfeld surface analysis and opto-electric properties of a new hybrid material: Tris (2-amino-5-chloropyridinium) hexachlorobismuthate(III)

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One novel bismuth (III) hybrid compound with 2-amino-5-chloropyridine was prepared. The crystal was grown by slow evaporation method at room temperature. The structure was determined by single-crystal X-ray diffraction. It crystallizes in the triclinic space group *P*-1, with the following parameters: $a = 7.5076(4)$ Å, $b = 12.3682(6)$ Å, $c = 15.1265(6)$ Å and $\alpha = 98.893(2)^\circ$, $\beta = 95.779(2)^\circ$, $\gamma = 106.459(2)^\circ$ with $Z = 2$ and $V = 1315.26(11)$ Å³. The structure was solved with a final $R = 0.03$ for 5983 independent reflections. The crystal arrangement consists of $[\text{BiCl}_6]^{3-}$ anions surrounded by $[\text{C}_5\text{H}_6\text{ClN}_2]^+$ cations. Complex hydrogen bonding interactions between $[\text{BiCl}_6]^{3-}$ and organic cations through $\text{N}(\text{C})-\text{H}\cdots\text{Cl}$ hydrogen bonds form a three-dimensional network. The crystal packing is stabilized by $\text{Cl}\cdots\text{Cl}$ interactions. Hirshfeld surface calculations were conducted to investigate intermolecular interactions, associated 2D fingerprint plots and enrichment ratio, revealing the quantitatively relative contribution of these interactions in the crystal packing. Thermal behavior was characterized by TG-DSC showing the decomposition of the compound at 180°C. Furthermore, Impedance spectroscopy study in the temperature range from 298 K to 443 K and in the frequency range between 5 and 13 MHz revealed that the temperature dependence of DC conductivity follows the Arrhenius law. Moreover, the frequency dependence of conductivity follows Jonscher's dynamical law. Nyquist plots (Z'' versus Z') are well fitted to an equivalent circuit model which consists of a parallel combination of a bulk resistance R_b and constant phase elements CPE.

Relationship between crystal structure and electric properties of LiFePO_4 , and cations conduction pathways simulation is approved by the bond valence sum.

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LiFePO_4 crystallizes in orthorhombic space group $Pnma$ with lattice parameters of $a=10.3290(2)\text{\AA}$, $b=6.0065(2)\text{\AA}$, and $c=4.6908(1)\text{\AA}$. The structure consists of FeO_6 octahedra and PO_4 tetrahedra sharing corners and edges to form a three-dimensional framework. This arrangement leads to intercrossed tunnels along b and c directions where Li^+ cations reside [1]. This compound seems to be a good candidate for applications as positive electrode in lithium batteries [2]. The BVS model (Bond Valence Sum) and the BVSM (Bond Valence Sum Map) [3] are extended to simulate the ionic migration pathways of lithium cations in the crystal bulk (Fig. 1). The result thus obtained will be discussed and compared with experimental measurements.

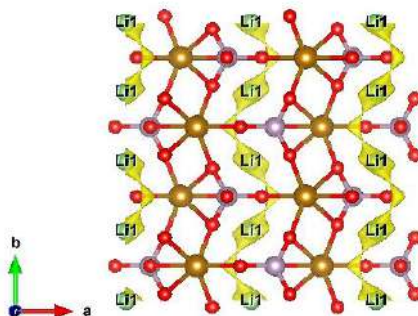


Fig. 1: 1D pathways link Li^+ along b -axis

Keywords: Bond valence sum; Crystal structure; Conduction pathways; Bond valence sum map; Simulation.

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Dielectric Properties of $\text{Ca}_{0.9}\text{Sr}_{0.1}\text{Cu}_{2.9}\text{Mg}_{0.1}\text{Ti}_4\text{O}_{12}$ (CSCMTO) – x SrTiO_3 (STO) Composites prepared by solid-state reaction

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Recently, a new material has been discovered by Subramanian et al named $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ (CCTO) [1]. This material presented a giant permittivity (10^4 - 10^5) and show nearly temperature independent behaviour in the temperature and frequency range 100–400K and 100–100 Hz respectively [2, 3].

A novel strategy was proposed by combining two oxide phases to create a new system: (1-x) $\text{Ca}_{0.9}\text{Sr}_{0.1}\text{Cu}_{2.9}\text{Mg}_{0.1}\text{Ti}_4\text{O}_{12}$ (CSCMTO) – x SrTiO_3 (STO) composite ceramics (with x= 1, 2 and 3 weight %) in order to enhance the dielectric and electrical properties of CCTO. All the composite ceramics were prepared by a conventional mixed oxide method and sintered at 1100°C for 6h only. Raman measurements revealed the formation of CCTO phase at grains. These results are consistent with that observed by XRD analysis. Moreover, adding of 1% weight.% STO can promote the grain growth size, but further addition of STO lead to decrease the grain size. The control of grain growth can be explained by the ratio of Sr^{2+} occupation in the lattice. A clear improvement of dielectric constant accompanied by a great decrease of dielectric loss. According to nonlinear properties, it can be seen that E_b and α enhanced considerably with addition of STO ratio by comparing to CCTO and CSCMTO. This enhancement is correlated to the microstructure as well as the resistance of grain boundaries.

Key words: CCTO ceramics, composites, SEM, resistance of grain and grain boundaries.

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Microstructural characterization and thermistor behavior of lead-free $x \text{ NaNbO}_3 - (1-x) \text{ BiFeO}_3$ electroceramics

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Electroceramics are advanced ceramic materials, displaying a wide variety of electric, optical and magnetic properties which find attractive applications as capacitors, sensors, dielectrics, thermistors, electronics, multiferroics, etc. In particular, the most known electroceramics bismuth ferrite (BiFeO_3 , BFO) and sodium niobate (NaNbO_3 , NNO), of perovskite type structure, have attracted enormous research works in the past decades and the study of the corresponding solid solution has attracted great interest [1-3]. Having in mind these precedent works, up to our knowledge, an electrical study of the NNO-BFO system in a wide enough composition range focusing on both dielectric and thermistor response has not been previously approached. Therefore, we have been interested in synthesizing nanoparticulated NNO-BFO ceramics by a facile route and in reinvesting these materials aiming to study the structural, compositional and microstructural features in relation to their electrical properties [4]. The electroceramics of the $x \text{ NaNbO}_3 - (1-x) \text{ BiFeO}_3$ ($x=0.25, 0.50, 0.75, 1$) system (NBNFO) have been prepared by the ceramic method at moderate temperatures (600 °C). Microstructural analysis from high resolution electron microscopy reveals the existence of small crystals (10–150 nm), which agglomerate leading to micro-sized crystals. All the NBNFO compounds show perovskite-type structure and a transition from rhombohedral (S.G. $R3c$) to orthorhombic (S. G. $P2_1ma$) mean macroscopic symmetry takes place for $x=0.50$, as analyzed by refinement of XRD data. Nevertheless, at the microstructural scale, the system can be described by a compositional-segregation picture in which structural heterogeneity is present. The materials show a positive temperature coefficient of resistivity (PTCR)-thermistor behavior above room temperature for $x \geq 0.50$, up to maxima temperature values of 410, 393 and 463 K for x values of 0.50, 0.75 and 1, respectively. Above these temperatures, in the NTCR temperatures-region, conduction and polarization phenomena are analyzed from impedance and modulus formalisms in terms of two mechanisms implying different charge carriers: polaron hopping and/or diffusion of cation and oxygen vacancies. The activation energy values, E_a , corresponding to these processes are of about 0.50 and 1 eV, respectively. Finally, in the dielectric response displayed by the NBNFO ceramics, the development of a FE contribution as x increases is detected, which can be interpreted considering microstructural features.

Keywords: Perovskites, Microstructure, Electrical properties, Impedance, Thermistors.

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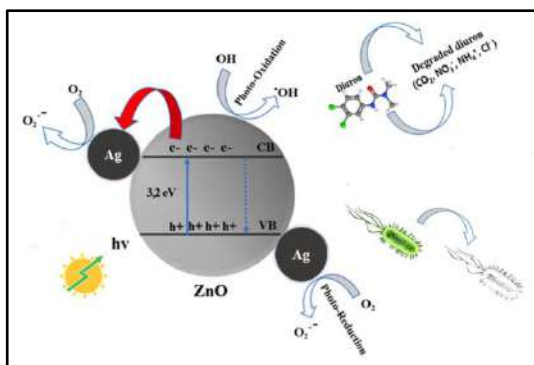
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Facile Synthesis of Ag/ZnO photocatalysts on the degradation of diuron herbicide under solar light and the investigation of its antibacterial activity for waste-water treatment

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Nanocrystalline Ag/ZnO powders have been successfully prepared by a modified polyol process using triethylene-glycol (TEG) as solvent, reducing and stabilizing agent. The synthesis procedure has been conducted without any post-synthesis thermal treatment. The structural and optical properties have been characterized by X-ray diffraction, transmission electron microscopy, N₂ adsorption study, inductively coupled plasma optical emission spectroscopy and UV-Vis diffuse reflectance spectroscopy. The photocatalytic activity of Ag/ZnO materials have been studied by analyzing the degradation of an herbicide, diuron, under solar light. Ag/ZnO photocatalysts with optimized $x = 0.7$ % Ag content showed 14 times higher rate of degradation than that of unmodified ZnO. We attribute these observations to the addition of silver nanoparticles allowing interfacial oxide-to-metal electron transfer within the hybrid Ag/ZnO photocatalyst. The inhibitory and bactericidal activities of samples have been tested against Gram-negative bacteria; *Escherichia coli*, *Salmonella typhimurium* and gram-positive bacteria; *Staphylococcus aureus*, *Enterococcus faecium* and *Candida albicans*. The results showed that the Ag/ZnO can be used as photocatalysts and antibacterial agents for potential practical applications in the wastewater treatment.



SHEMA 1. Schematic of the proposed photocatalytic and bactericidal mechanism of Ag/ZnO nanostructure.

Key words: ZnO; Ag; Nanoparticles; Photocatalysis; Antibacterial; wastewater treatment

Structural, thermal and dielectric properties of phosphoric acid-based geopolymer with Metakaolin

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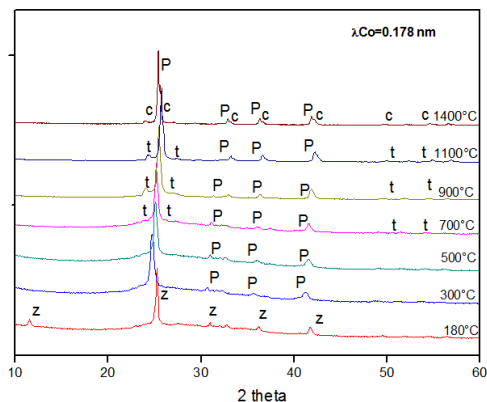
In this work, a new geopolymer was prepared by using metakaolin and phosphoric acid solution. Microstructural properties were investigated by X-ray powder diffraction, while thermal properties were evaluated by differential thermal analysis and thermogravimetry. Finally, the conductivity of geopolymer and dielectric properties were investigated.

The results showed that the onset temperature of crystallization of the Zeolite phase occurs at 180°C. This phase is converted into phosphocrystalite phase at 300°C and persists until 1400°C. From the temperature of 700°C, a new crystalline phase was observed: tridymite SiO₂.

The amount of phosphocrystalite and tridymite crystals reaches a maximum at approximately 1100 °C, then, further exposure to 1400 °C showed that tridymite phase is converted to cristobalite.

The conduction properties of geopolymer indicates first very low solid-state conductivity ($\sigma \approx 10^{-10}$ S/cm), and then above 625°C, the conductivity begins to rise rapidly, reaching 10^{-7} S.cm⁻¹.

Keywords: Geopolymer, Rietveld refinement, Thermal analysis, Electrical Conductivity



z: zeolite (AlPO₄.(H₂O)_{2.53}); c: cristobalite SiO₂; P: phosphocrystalite AlPO₄; t: tridymite SiO₂.

Figure. Phase evolution of geopolymer at elevated temperature

**Program of
Wednesday
19 December 2018**

π -Chem & Go! π -Stack on DNA and go to the best place

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The interaction of the $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ metal complex synthesized in our group [1] with DNA has been studied at computational level by docking, semi empirical methods including dispersion, QM/MM and DFT. The $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ metal complex exists as two main isomers in solution. Indeed, in one isomer phenanthroline (phen) is coordinated in the equatorial plane (EqEq), whereas in the other one N of phen is coordinated in an equatorial position and the other N in an axial one (EqAx). Although the EqEq structure is more stable, there is not a great difference between the energy of the isomers and we studied both systems, EqEq and EqAx, interacting with DNA to explain the experimentally found cytotoxicity.[1] We also took into account two different modes of interaction with DNA, that is, groove binding and intercalation, since such competition has been recently described in the bibliography for metal complexes with flat ligands interacting with DNA.[2-4] PM6-DH2 hamiltonian and QM/MM methods by using M11L/6-31+G(d,p): AMBER were calibrated with the intercalated 1n37 structure of PDB and were observed to perform excellently. On the other hand, for the $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ metal complex, it is observed that the system prefers the intercalation via minor groove than through the major groove. Moreover, once the bases experimented the rise movement to allocate the metal complex, the groove binding mode became unstable and the intercalation more likely.

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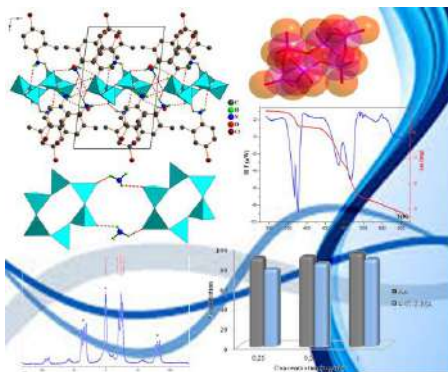
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Biophysicochemical Study Of A Hybrid Cyclohexaphosphate

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The new hybrid $[4\text{-Cl-2-(CH}_3\text{)}_6\text{H}_3\text{NH}_3]_6\text{P}_6\text{O}_{18}\cdot 2\text{H}_2\text{O}$ was synthesized under normal conditions of temperature and pressure. Single crystal X-ray diffraction study was used to identify its structure. It revealed that this organic cyclohexaphosphate crystallized in the $P\bar{1}$ triclinic space group. In the crystal framework, the assembling of the three dimensional (3D) structure is formed by intermolecular hydrogen bonds and Van Der Waals interactions. A spectroscopic characterization was carried out to elucidate the structure (UV-Vis, FTIR, ^{31}P MAS-NMR and fluorescent properties). The thermal stability was studied by TG-DTA diagrams under argon atmosphere. This compound was also evaluated for its antioxidant activity; four tests were done, in vitro, 1,1-diphenyl-2-picrylhydrazyl (DPPH•), hydroxyl scavenging ability ($\text{OH}^\bullet$), ferric reducing power (FRP) and ferrous ion chelating (FIC) ability, using ascorbic acid as a control.



Keywords: Crystal structure; X-ray diffraction; Spectroscopic study; Thermal properties; Antioxidant activity.

Bias dependent dielectric properties study of $\text{La}_{0.8}\text{Ba}_{0.1}\text{Ca}_{0.1}\text{Mn}_{0.85}\text{Co}_{0.15}\text{O}_3$ at room temperature

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The $\text{La}_{0.8}\text{Ba}_{0.1}\text{Ca}_{0.1}\text{Mn}_{0.85}\text{Co}_{0.15}\text{O}_3$ sample was prepared by polymerization complex sol-gel method. The crystallographic study indicates that our sample crystallizes in the rhombohedral structure with the R-3c space group, at room temperature. The dielectric properties of this material were studied, in the frequency range of 500-10⁶ Hz and a bias voltage range of 0- 2 V, using the impedance spectroscopy analyzer, at room temperature. The imaginary part of the complex impedance frequency dependence revealed one relaxation peak. The Nyquist plots were modelled with grain and grain boundary resistance by introducing proper ac equivalent circuit. The impedance loss plot showed that the relaxation peak shifts towards the higher frequency, with increasing bias voltages. This implies the possibility of a charge hopping between the localized charge states. High frequency dielectric constant of our sample are found to be in the order of 10⁵. The dielectric loss at different bias voltages shows the possibility of hopping mechanism for electrical transport processes in the system. Our results are interesting and indicate that this material can be a potential candidate in some applications.

Synthesis and characterization of composite material based on magnesium phosphate cement for cesium retention.

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The pollution sources are numerous and varied, reflecting the diversity of activities, materials used and manufacturing processes. Industrial pollution in all its forms is a direct threat to the environment and the quality of life. In particular, water pollution is an alteration that renders its use dangerous and disrupts the aquatic ecosystem. This is done when its equilibrium is modified by too large a supply of more or less toxic substances, of natural origin or resulting from human activities. Especially radioactive pollution with Cs, which is the major radioactive waste contaminants, and is radiotoxic because of their 30 year period which is considered too long for the decay to occur naturally. One of the most adopted techniques for this treatment is the adsorption and as adsorbent we chose the zeolite chabazite for the treatment of Cs. But the disadvantage of the adsorbent mentioned above, they are not recoverable after adsorption. With this in mind, we have thought of a material that can be alloyed with these compound while keeping their performance and will also be used for the recovery of zeolites after the adsorption of pollutants, this material is the phosphate magnesium cement (MPC) which was prepared with magnesia oxide (MgO), potassium dihydrogen phosphate (KH₂PO₄) and some retarders. This type of cement has taken great care for its advantages: fast setting, low permeability, accelerated resistance development, excellent bonding with almost any clean and dry surface. The obtained optimal conditions were examined and analysed by X-ray diffraction (XRD) and scanning Electronic Microscopic (SEM), BET and atomic adsorption.

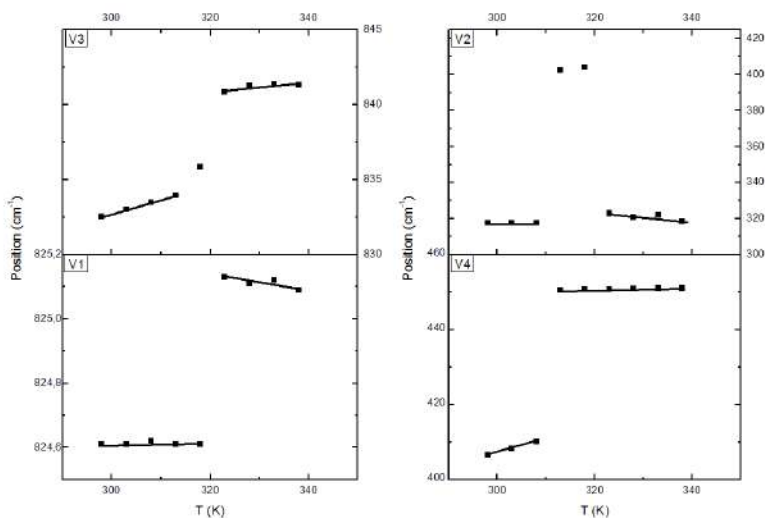
Key words: Magnesium phosphate cements (MPC), zeolite, adsorption, and cesium.

Order-disorder phase transition in the Cesium SelenateTellurate material at high temperature.

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The $\text{Cs}_2\text{SeO}_4\cdot\text{H}_6\text{TeO}_6$ material presents an order-disorder phase transition at $T = 320$ K confirmed by thermal analyses, crystal structure and vibrational spectroscopy studies. Indeed, at room temperature it crystallizes in the monoclinic system, space group $P2_1/c$, with the following parameters: $a = 12.817(6)$ Å, $b = 7.519(3)$ Å, $c = 12.432(5)$ Å, $\beta = 111.16(2)^\circ$ and $V = 1117.3(8)$ Å³. While at $T = 360$ K it crystallizes with the **trigonal** system, space group $R\bar{3}m$, with $a = b = 7.535(8)$ Å, $c = 8.554(8)$ Å, $\gamma = 120(2)^\circ$ and $V = 450.55(10)$ Å³. The crystal structure is built from isolated (SeO_4^{2-}) tetrahedra and (TeO_6^{6-}) octahedra, they form tunnels where Cs^+ cations and some hydrogen atoms are placed. The high temperature vibrational studies, carried out in the temperature range of 289 to 353 K, confirm the presence and the nature of the transition detected by DSC at 320K.



The temperature dependence of the position vibration modes related to tetrahedron group in the $\text{Cs}_2\text{SeO}_4\cdot\text{H}_6\text{TeO}_6$ material.

Synthesis, structure and physico-chemical studies of a novel oxalate material $C_8H_{14}N_2(C_2O_4)$

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A new oxalate material with the general formula: $C_8H_{14}N_2(C_2O_4)$, has been synthesized by slow evaporation at room temperature and the structure was determined by single crystal X-ray diffraction analysis, Hirshfeld surface analysis, IR, UV visible and Thermal analysis. This sample has been crystallized in the monoclinic system, space group $C2/c$, with $a = 13.3936(6)$, $b = 7.0339(3)$, $c = 12.1983(5)$ Å, $\beta = 112.446(2)^\circ$, $V = 1062.13(8)$ Å³ and $Z = 4$.

The asymmetric unit of the title compound contains a half of the m-xylylenediaminium cation, and half oxalate anion. The structure is built up from anionic chains parallel to the b-axis and interconnected by the organic cations via N–H...O and C–H...O hydrogen bonds so as to build a three dimensional arrangement. The intermolecular interactions of this salt were also evaluated by using the three-dimensional Hirshfeld surfaces and two-dimensional fingerprint plots. The hydrogen bonding interactions associated to N–H...O and C–H...O represent the top fraction of 51.6 % followed by those of the H...H type contributing 39.2 %.

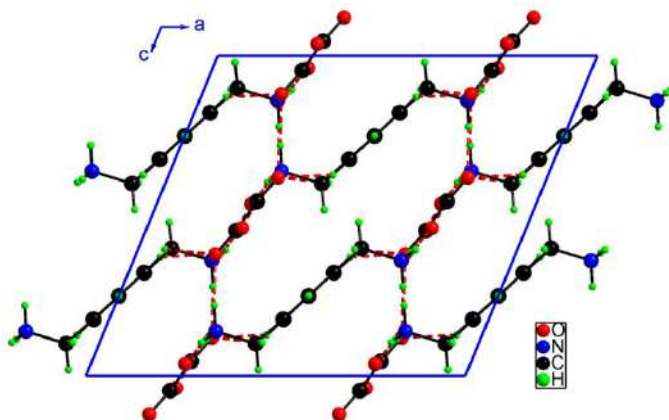


Fig. Projection of $C_8H_{14}N_2(C_2O_4)$ along the b-axis.

Keywords: crystal structure, m-xylylenediaminium, oxalate, Hirshfeld surface analysis, fingerprint maps.

Structure, thermal decomposition and spectroscopic characterization of a new hybrid iron fluoride $\text{Fe}_4\text{F}_{18} \cdot (8\text{-Hydroxyquinoline})_6$

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The hydrothermal synthesis of a new hybrid compound base on iron, fluoride and 8-Hydroxyquinoline molecule has been described. This new material was characterized by single crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), Hirschfeld surface, spectroscopy measurement, thermal study and photoluminescence properties.

$[\text{8Hqn}]_6 \cdot (\text{F}_4\text{F}_{18})$ crystalized in trigonal space group R3c with cell parameters $a=17.9239(5)\text{\AA}$, $b=17.9239(5)\text{\AA}$, $c=30.6196(11)\text{\AA}$, $V=8519.1(5)\text{\AA}^3$ and $Z=6$. The structure of $\text{F}_{18}\text{Fe}_4(\text{HQN})_6$ is built up from $[\text{Fe}_4\text{F}_{18}]^{6-}$ isolated tetramers surrounded by six cations HQN^+ . The cohesion between these entities is performed via N-H... F and O-H...F hydrogen bonds to form a three-dimensional network. Hirshfeld surface analysis was used to investigate intermolecular interactions, as well 2D finger plots were conducted to reveal the contribution of these interactions in the crystal structure quantitatively.

Thermal analysis of the title compound showed that the decomposition introduced three steps. IR spectra confirmed the presence of 8-hydroxyquinoleine molecules. The photoluminescence properties of the compound investigated in the solid state, at room temperature, exhibited one band at 364 nm and a strong fluorescence at 552 nm.

Keywords: structure, hybrid, fluoride, thermal, spectroscopic

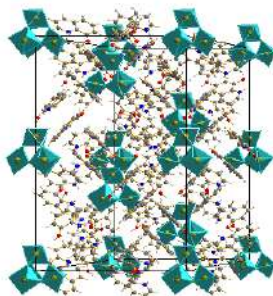


Figure 1: Crystal structure representation of the $\text{Fe}_4\text{F}_{18} \cdot 6(\text{C}_9\text{H}_8\text{NO})$ compound

Crystal structure, Vibrational spectroscopy, Optical properties and Hirshfeld surface analysis of adeninium dichromate and trichromate

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The structures of adeninium dichromate ($\text{C}_5\text{H}_6\text{N}_5$)₂ [Cr_2O_7] and trichromate ($\text{C}_5\text{H}_7\text{N}_5$)[Cr_3O_{10}] were grown by the slow evaporation technique and characterized by X-ray diffraction data. These compounds crystallize in the triclinic system, space group P-1 with $Z=2$ and $a=11.685(1)\text{\AA}$, $b=11.753\text{\AA}$, $c=14.560(1)\text{\AA}$, $\alpha=83.96(1)^\circ$, $\beta=70.48(1)^\circ$, $\gamma=61.86(1)^\circ$ for the dichromate and in the triclinic system also for the trichromate with space group P-1, $Z=2$ and $a=8.15(2)\text{\AA}$, $b=9.842(3)\text{\AA}$, $c=10.474(4)\text{\AA}$, $\alpha=75.93(1)^\circ$, $\beta=72.35(1)^\circ$, $\gamma=72.27(1)^\circ$. These two compounds were characterized by IR spectroscopy, RAMAN, UV spectroscopy and Hirshfeld surface.

The X-ray analysis shows that dichromate and trichromate compound possess a 3D framework, which is built up by isolated $\text{Cr}_2\text{O}_7^{2-}$ anions and $\text{C}_5\text{H}_6\text{N}_5^+$ cations for the dichromate and $\text{Cr}_3\text{O}_{10}^{2-}$ anions and $\text{C}_5\text{H}_7\text{N}_5^{2+}$ cations for the trichromate, the extensive net hydrogen bonds between cations and anions contribute to the crystal packing.

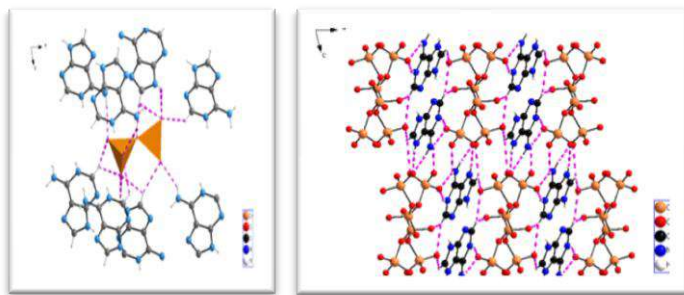


Fig. Projection of the two structures of ($\text{C}_5\text{H}_6\text{N}_5$)₂[Cr_2O_7] and ($\text{C}_5\text{H}_7\text{N}_5)[Cr_3O_{10}] along b axis$

Keywords : X-ray diffraction, IR spectroscopy, RAMAN, UV spectroscopy, Hirshfeld surface.

Study of the influence of synthesis parameters on the physico-chemical properties of hydroxyfluoroapatite via the Taguchi method

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The hydroxyfluoroapatite nanoparticles ($\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})\text{F}$) were synthesized by means of the mechano-synthesis method using planetary ball milling. In order to develop mathematical models describing the physicochemical properties of the hydroxyfluoroapatite, the Taguchi method was applied. X-ray Diffraction (XRD), Infrared Spectroscopy (IR), Energy Dispersive X-ray spectroscopy (EDX), Scanning Electron Microscopy (SEM) and Brunauer-Emmett-Teller (BET) method were employed to characterise the synthesis products. Four factors were studied: disc velocity, number of balls, final mass of powder and milling time. The Signal-to-Noise ratio (SN) was used to determine the most influent factors. The physicochemical properties of the hydroxyfluoroapatite: crystallite size, specific surface area, Ca/P atomic ratio and percentages of apatite and calcite were evaluated.

Keywords: Mecanosynthesis, Taguchi method, apatite, nanocrystallites.

Synthesis by the Sol-Gel Autocombustion Method and Physicochemical Characterizations of Ferrimagnetic Nanoferrites of $\text{Ni}_{0.2}\text{Cu}_{0.4}\text{Co}_{0.4}\text{Fe}_2\text{O}_4$

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The nanomaterial $\text{Ni}_{0.2}\text{Cu}_{0.4}\text{Co}_{0.4}\text{Fe}_2\text{O}_4$ was synthesized via simple, economic and environmentally friend sol-gel auto-combustion method. The obtained black powder has been characterized by different physicochemical techniques. The X-Ray Powder Diffractogram (**Figure 1**) has been indexed in the spinel cubic system which is in good agreement with TEM study (**Figure 3**), whereas the magnetic measurement results (**Figure 4**) have highlighted the ferrimagnetic and superparamagnetic behavior at and below the room temperature of the studied material. Furthermore, the spinel structure has been also confirmed by FT-IR study results which indicate the presence of two characteristic peaks, at 407.212 cm^{-1} and 569.634 cm^{-1} , in the corresponding spectrum (**Figure 2**).

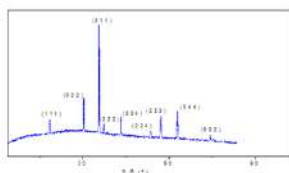


Figure 1: The X-Ray Powder Diffractogram of the Nanomaterial $\text{Ni}_{0.2}\text{Cu}_{0.4}\text{Co}_{0.4}\text{Fe}_2\text{O}_4$

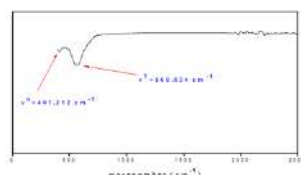


Figure 2: The Infrared Absorption Spectrum of the Nanomaterial $\text{Ni}_{0.2}\text{Cu}_{0.4}\text{Co}_{0.4}\text{Fe}_2\text{O}_4$



Figure 3: TEM Image of the Nanomaterial $\text{Ni}_{0.2}\text{Cu}_{0.4}\text{Co}_{0.4}\text{Fe}_2\text{O}_4$ annealed at 900°C

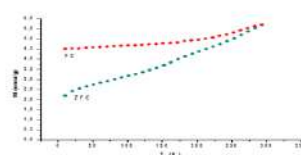


Figure 4: The ZFC-FC Magnetization curves of the Nanomaterial $\text{Ni}_{0.2}\text{Cu}_{0.4}\text{Co}_{0.4}\text{Fe}_2\text{O}_4$

Electrochemical oxidation of crystal violet using a BDD anode with a solid polymer electrolyte

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This paper explores the applicability of an innovative electrochemical cell with a solid polymer electrolyte (SPE) with mesh electrodes for the electrochemical oxidation of a low conductivity solution (0.022 mS/cm) containing crystal violet (CV) dye compound as model pollutant in a range concentration of 25–100 mg/L. The system anode/membrane/cathode is formed by Nafion membrane sandwiched between a Ti/RuO₂ cathode and a BDD anode. The dependence of applied current, stirring rate, supporting electrolyte and temperature has been investigated. The experimental results showed that the electrochemical cell with SPE is suitable for the treatment of solution with a very low conductivity since the CV solution was completely mineralized with an energy consumption of about 60 kWhm⁻³. Furthermore, the process was under charge transfer control for low applied current, becoming mass transfer control around 1 A. The addition of supporting electrolyte as Na₂SO₄ (0.6 and 1 g/L) and NaHCO₃ (1 g/L) to the solution decreased the removal rate due to the presence of competitive reaction and scavengers media. The evolution of nitrogen compounds during the electrolysis shows that at the end of the process the 80% of initial N has been converted in nitrate and ammonium, indicating the formation of volatile compound.

Toxicity assessment of Pesticide use in Tomato production : Case study of a Tunisian-Dutch soilless greenhouse

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Pesticides are applied to agricultural fields to optimise crop yield and quality. On the other hand, pesticides have numerous negative impacts on ecosystems and human health as a result of fractions not reaching the intended target. In current Life cycle assessment (LCA) practices, quantifying pesticide emissions from agricultural fields is not aligned with characterizing related potential toxicological impacts on humans and the environment. This leads to incomplete and often misleading and hardly interpretable LCA results in the agri-food sector and moreover makes it impossible to assess and compare the environmental performance profiles of different pest management systems and practices. To address this challenge, this study takes advantage of the latest recommendations for pesticide emission inventory and impact assessment. Here, freshwater ecotoxicity and human toxicity impacts of tomato production in the south of Tunisia are evaluated during a 2-year period. The assessment is mainly based on the consensus model Usetox. Results showed that the main aspects influencing the impacts are the interface between inventory estimates and impact assessment, and the consideration of intermediate processes, such as crop growth development and pesticide application method.

Keywords: Pesticides, Freshwater ecotoxicity, Human toxicity, Characterization factor, Tomato production

The optimization of wastewater treatment using ultrafiltration process

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Tunisia is characterized, in most regions, by a semi-arid to arid climate. The country suffers as much from inadequate rainfall as their uneven distribution in time and space. The global demand for quality water, whether for purposes of drinking, sanitation, irrigation, and industrial use, has been on a continuous rise. Thus, to satisfy all the needs of the country in order to preserve water and water quality in drinking water to ensure better public health and protect the environment, the need to promote domestic and industrial wastewater treatment is important. In this context, the use of treated wastewater has become a necessity and an integral part of the current strategy to mobilize all available resources.

Conventional wastewater treatment processes, physicochemical (chemical consumers) and biological processes remain ineffective and limited by the emergence of micropollutants and / or biologically recalcitrant. Hence the need to develop other methods to offer interesting alternatives such as membrane separation processes (Microfiltration (MF), Ultrafiltration (UF), Nanofiltration (NF), Reverse Osmosis (RO), Electrodialysis (ED) Cross-Ionic Dialysis (IIC) and advanced oxidation processes (POA)).

In this work, the adaptation of membrane separation techniques to the treatment plant of a pharmaceutical industry is the main objective. The second objective is to improve the performance of the membranes in terms of limiting the clogging phenomenon and improving the quality of treated water through steps of modification of their active surfaces.

The first experimental part consists in characterizing, the supplied pharmaceutical effluent and the used (unmodified) membranes with several analytical techniques such as : X-ray diffraction, atomic force microscopy (AFM), scanning electron microscopy (SEM), etc. The table 1 describes the results of the physicochemical analysis of the pharmaceutical wastewater.

Table 1. Industrial wastewater characteristics

Parameter	Value
pH	7.95
Turbidity	60.5 NTU
Salinity	2.25 g/L
Conductivity	4.07 mS/cm
TDS	2.05 g/L
DCO	143 mg O ₂ /L
Cl ⁻	550 mg/L
NO ₂ ⁻	0.18 mg/L
NO ₃ ⁻	0.5 mg/L
PO ₄ ³⁻	16.94 mg/L
Na ⁺	626.1 mg/L
K ⁺	327.0 mg/L
NH ₄ ⁺	53.1 mg/L

The membranes used in this work are polyamide-polysulphone ultrafiltration membranes SEPA-GH and SEPA-GK with molecular weight cut-off (MWCO) 1 KDa and 2 KDa respectively. The evaluation of membrane efficiency by adjusting the parameter of transmembrane pressure was reported. After a series of membrane filtration experiments, the results showed that for GH membrane the maximum rejection rates were obtained at $\Delta P = 5$ bar. In fact, the increase in transmembrane pressure from 2 to 6 bars has a significant effect on the rejection rates and a slight decrease was observed after 5 bars.

Elimination of phenolic compounds from waste air by absorption and enzymatic biodegradation

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Phenolic compounds have become a frequent source of air pollution due to their large use in different industries. This study reports a new technique of remediation of waste-air containing a model molecule of volatile phenolic compounds, 2-chlorophenol (2-CP). The process is based on absorption of the compound in silicone oil (PDMS 47V20) then its enzymatic degradation with cross-linked enzyme aggregate (CLEA).

The process started by evaluating the absorption capacity of PDMS throw measuring the partition coefficient air /PDMS of 2-CP. Results show that in PDMS, 2-CP is characterised by a partition coefficient five times lower than its value in water. On the other hand, it was found that inside a pure organic medium, BRP-CLEAs kinetics follow Andrews's model with K_m and V_{max} equal to 23.71 mg.L⁻¹ and 0.115 mg.L⁻¹. min⁻¹ respectively.

The biodegradation essays of 2-CP revealed an optimal contact time of 100 min and optimal concentration of 2-CP and H₂O₂ of 80 mg.L⁻¹ and 6mM respectively leading to a maximum removal yield of 69%.

ELECTROCHEMICAL OXIDATION OF CHLORTETRACYCLINE ANTIBIOTIC ON A NICKEL FOAM ELECTRODE: BIODEGRADABILITY IMPROVEMENT

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This project deals with the electrochemical oxidation coupled with biological treatment of biorecalcitrant antibiotic: chlortetracycline (CTC). This organochlorine compound releases from pharmaceutical industrial waste into the environmental water and usually causes suspected undesirable effects in aquatic organisms. The pre-treatment was performed in a home-made flow cell involving nickel foam as a working electrode at potential of 0.5 V/saturated calomel electrode (SCE). The electrolysis through the percolation cell led to a more than 99% conversion yield of chlortetracycline in oxidation in alkaline conditions. The evolution of the concentration during treatment was followed up by Ultra Performance Liquid Chromatography (UPLC). Cyclic voltammetry with a nickel electrode revealed a significant electrochemical activity of chlortetracycline. Total Organic Carbon (TOC) analyses of the electrolyzed solution revealed that the level of mineralization remained low, underlying the interest of a combined electrochemical and biological treatment. The biodegradability, based on the biological oxygen demand over 5 days (BOD₅)/ the chemical oxygen demand (COD) ratio, was studied at the oxidation potential of 0.5 V/ SCE. The electrolyzed solutions were biodegradable. Moreover, a simultaneous generation of chlorides was observed and intermediates were identified and monitored during 4h of electrolysis.

Keywords: Chlortetracycline, biodegradability, electro-oxidation pretreatment, percolation cell.

Substitution of chemical coagulants by biopolymers for the treatment of tannery wastewater

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As part of water resources management, the Tunisian state has imposed in the last decade a rigorous and tight legislation to industries in order to apply a good governance of the water and reduce pollution caused by sewage and effluents discharged. Our work falls in this context, the leather industry is a major producer of wastewater and solid waste containing potential water and soil contaminants.

In this context, the conventional biological treatment does not always achieve satisfactory performance due to the toxicity of the tannery effluents that affects the development of the bacteria. In addition, conventional physical chemical processes are comparatively expensive, and may lead to secondary pollution because it needs additional chemicals.

Our study was conducted to treat the tannery wastewater through coagulation-flocculation. It was based on the investigation of the performance of biopolymers such as chitosan, Alginate, Cactus Opuntia Ficus Indica, olive tree leaf. The optimization of the coagulation/flocculation process was conducted by design experiments. Several operating parameters such as the duration and the stirring speed, the type and dosage of coagulant and flocculant, and other parameters were investigated. The first stage of our study is a screening to identify the significant parameters. the Plackett-Burman plan (1st order) was adopted. In the second step, attention is paid to the determination of the optimum conditions for coagulation/flocculation in order to guarantee a quality of pretreated water respecting the favorable conditions for the biological treatment operation. A Box Behnken experimental design (2nd order) was used.

The construction of the matrix of experimental design was established using Statistica 8.0 software. The matrix consists of 16 tests. For each response we obtained significant factors, which have an influence on the response, and non-significant factors which haven't a significant effect on response variation and are eliminated in the next order plan.

The optimum conditions were subsequently determined using the response surface plots and contour plots for all significant parameters.

The optimal conditions results are as follow:

- X1: Coagulant dosage: 123.5 mg/L	- X4: Flocculant dosage: 2mg/L
- X2: Mixing rate of coagulant: 216 rpm	- X7: Settling: 40.1 min

Olive tree leaf have shown there efficacy as biopolymer for the treatment of the tannery effluents.

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Spectroscopic and thermal studies, theoretical investigation and photocatalysis application of 2-aminobenzimidazolium tetrachlorocobaltate(II)

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In this study we present the crystal structure, spectroscopic and thermal behavior, Hirshfeld surface analysis, DFT calculations and photocatalytic activity of new organic-inorganic hybrid compound $(C_7H_8N_3)_2[CoCl_4]$ (**1**) (**Fig.**). The X-ray diffraction structure determination prove that this compound crystallize in the centrosymmetric space group *P*-1 of triclinic system. The structure can be described by the alternation of two different, cationic-anionic layers parallel to (110) plane. This complex is assembled into 3D supramolecular architecture through N-H...Cl hydrogen bonds and $\pi\cdots\pi$ interactions. Hirshfeld surface analysis and their relative fingerprint plots are used for decoding intermolecular interactions in the crystal network and contribution of component units for the construction of the 3D architecture. The optimized structure and calculated frequencies of the title compound were obtained by density functional theory (DFT) using B3LYP functional and 6-311+G(2d,2p) basis set for H, C, N, Cl atoms and LANL2DZ for Co. The experimental and theoretical results confirmed the proposed molecular structure for the new synthesized compound.

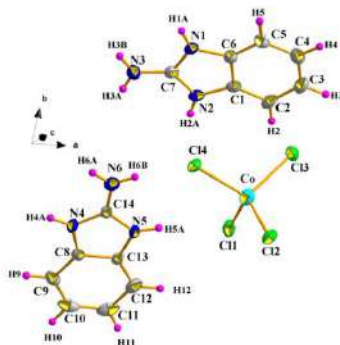


Fig. The asymmetric unit of the crystal structure of (**1**)

Keywords: Crystal structure, Hirshfeld surface, spectroscopy, thermal analysis, DFT study, photocatalytic activity

Elaboration and Characterization of a Poly (HEMA) Network and an Interpenetrated Polymer Network Based on Cellulose and HEMA Application to Wastewater Remediation by Colorant Retention

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In this work, we are interested in the development of a crosslinked polymer network based on Hexyl Ethyl Methyl Acrylate (HEMA) and Interpenetrated Polymer Network based on Cellulose and Hexyl Ethyl Methyl Acrylate (HEMA) by the technique of photo-polymerization with UV, in the presence of a crosslinking agent 1,6-hexane-diol-di-acrylate (HDDA), an initiator photo 2-hydroxy-2-methyl-propiophenone (Darocur1173) and epichlorohydrin. Characterization by the TF IR spectroscopy method. The swelling study in an aqueous medium in which the type and the dye content are varied makes it possible to demonstrate the dye retention capacity of these polymeric materials. The initial composition of the products and the conditions of preparation have a great influence on obtaining the final compound.

Key words: UV photo-polymerization, Cross-linked network, Interpenetrated Polymer network, Cellulose

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Influence of potassium permanganate treatment on the mechanical properties and thermal behavior of palm fibers reinforced polyvinyl chloride composites

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Natural fibers arouse great interest because of their particular properties and numerous advantages. Indeed, these species are renewable, respectful to the environment and have a low cost; they are widely used in the reinforcement of polymeric composites. The low density and high strength of natural fibers are attractive factors for the manufacture of lightweight and resistant materials.

This study devoted to the valuation of lignocellulosic waste, a particular interest was brought to date palm fibers, as a load in the manufacture of polyvinyl chloride (PVC) matrix composite materials with a load ratio of 0, 5 and 25 wt%. We were particularly interested in the problem of adhesion to the fiber / matrix interface. In addition, a method of treatment has been chosen. This is the modification with potassium permanganate (KMnO₄). The highlighting of the modification was examined by the FTIR analysis, and the impact of the treatments on the physico-mechanical and thermal properties of the composites was likewise studied.

Key words: polyvinyl chloride, palm fibers, mechanical properties, thermal properties.

UV accelerated aging of biobased/kenaf fibres composite: Viscoelastic behaviour in molten state & thermal properties.

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This part of work is based on the study of the effect of UVA and UVB radiations, on the rheological and thermal behaviour of starch-grafted-polypropylene matrix and composite reinforced with kenaf fibres.

Evaluation of the viscoelastic behaviour in the molten state has shown a reduction of the complex viscosity for UVB irradiated samples, however, slight change was observed for UVA irradiated ones. The Cole-Cole diagrams of UV irradiated matrix sample, illustrated an increase in curve slop with reformation of arc cycle giving lower limit viscosity with irradiation times. This suggests an occurrence of chain scission reactions in matrix samples after UVA and UVB irradiation. In contrast, composite irradiated samples have shown an increase in the line slop for UVA irradiated composite due to formation of crosslinking network. On the other hand, reduction in molecular weight was observed for UVB exposed composite.

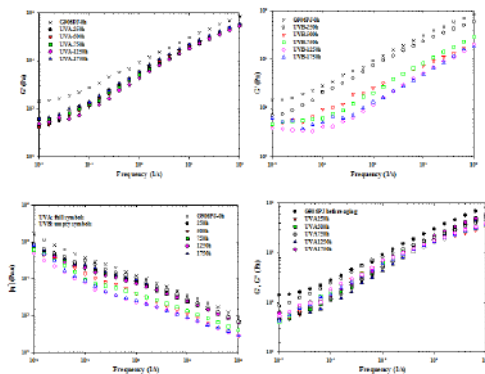


Fig.1: Complex viscosity of UV irradiated matrix and composite.

A shift to lower values of loss and storage modulus was observed for irradiated samples. The shift was more accentuated for UVB exposed matrix with formation of plateau at lower frequency, and UVA exposed composite. Evaluation of MFI confirmed the undergoing of chain scission reactions for UVB exposed matrix and eventual co-existence of crosslinking and scission chains for UV exposed composite samples. The stability of the matrix was more affected than composite especially after UVA exposition.

A simple and green synthesis of thiazolines and oxazolines

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Far from the use of toxic solvents, expensive catalyst, hard conditions, here we describe a new and soft method to access to thiazolines and oxazolines that are important scaffolds present in a great number of natural products^{1,2}. This straightforward approach allows high conversion for a broad range of nitriles and an easy isolation of the desired products.

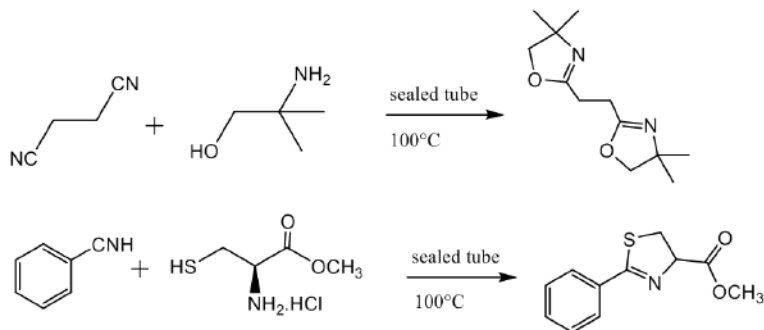


Fig. synthesis of oxazolines and thiazolines

Key words: Green synthesis, thiazolines, oxazolines, sealed tube

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Synthesis and optical properties of new pentacyclic helicenes

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Helicenes constitute a fascinating class of ortho-annulated polycyclic aromatic or heteroaromatic compounds endowed with inherent chirality due to the helical shape of their π -conjugated system¹, they have nowadays reached a high degree of appeal within the scientific challenges to manifold applications in different areas of science². These non-planar helical molecules exhibit unique electronic³, and chiro-optical properties⁴. They are potential candidates for chiral catalysts⁵, helical ligands⁶, and have been used as building blocks for helical conjugated polymers⁷. We report here the preparation of novel chiral thiahelicene bearing a cyano group at selected position (Fig.1) *via* a four-step sequence. The optical properties of the pentacyclic helicene have been investigated and show interesting behavior.

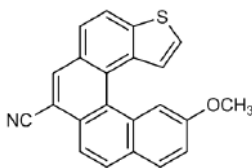


Fig 1. Synthesis of new [5]thiahelicene

Key words: Helicenes, couplings, Photocyclization.

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SOLUBILITY ENHANCEMENT OF POORLY SOLUBLE DRUGS BY SOLID DISPERSION TECHNIQUE

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The improvement of solubility and oral bioavailability of poorly water-soluble drugs by formation of amorphous solid dispersion strategy represents one of the actual alternatives to a drug development scientist. The aim of this work is to highlight the possibility of formation of thermodynamically stable amorphous solid dispersions of drug molecules (ibuprofen) in presence of polymer (PVP) by comilling at room temperature. The milled mixtures characterization was carried out using powder X-ray diffraction (PXRD), Fourier transform infrared spectroscopy (FTIR), scanning electronic microscope (SEM) and differential scanning calorimetry (DSC). Thus, the obtained results revealed the existence of intermolecular H-bonds between drug molecules and polymer which has an anti-plasticizing effect on the milled blend. Therefore, it was shown that physical stability and solubility amelioration of milled mixtures (drug/polymer) are achievable at room temperature by comilling technique.

Keywords: bioavailability, ibuprofen, celecoxib, thermodynamically stable amorphous solid dispersions, poorly water-soluble drugs, comilling, PVP.

Extensive study of Tunisian *Lycium arabicum* Boiss. by UHPLC/HR-ESI-MS/MS and evaluation of its antioxidant and anti-lipase activities.

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Nine different extracts from Tunisian *Lycium arabicum* [1] investigated in terms of their total phenolic and total flavonoid contents, phytochemical composition as well as their antioxidant [2] and anti-lipase activities. The in vitro antioxidant property investigated using three complementary methods such as DPPH, ferric reducing antioxidant power (FRAP), and β -carotene-linoleic acid bleaching assays, while anti-lipase activity was evaluated using 4-methylumbelliferyl oleate method. Methanolic extracts, especially those of stems and leaves, presented the most potent activities from all of the tested extracts. In order to investigate their chemical composition and to highlight the possible correlation of their constituents with the observed activities, an UHPLC/HR-ESI-MS/MS analysis [3] performed (Fig.1). Several compounds belonging to different chemical classes were tentatively identified such as rutin and kampherol rutinoides, the major constituents of the leaves, and N-caffeoyltyramine, lyciumide A, N-dihydrocaffeoyltyramine as well as fatty acids: trihydroxyoctadecadienoic acid and hydroxyoctadecadienoic acid isomers detected abundantly in the stems. These results showed that the MeOH extracts of stems and leaves of *L. arabicum* can be considered as a potential source of biological active compounds.

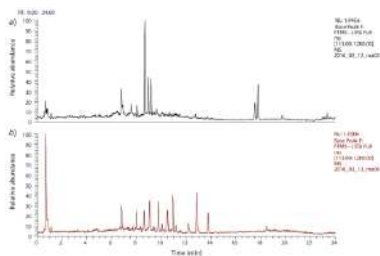


Figure 1. UHPLC/HR-ESI(–)-MS/MS based peak chromatogram
of components from *Lycium arabicum* leaves
a) and stems b) MeOH extracts.

Key words: *Lycium arabicum*, UHPLC/HR-ESI-MS/MS, Antioxidant activity, Anti-lipase activity, Polyphenols.

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Optimization of polysaccharides extraction from Quince peels: Partial characterization, antioxydant and antiproliferative properties

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In this study, Box-Behnken Design used to optimize the ultrasonic extraction of polysaccharides from quince peels (QPPs) by ascorbic acid and the effect of extraction temperature, extraction time and pH evaluated. Under optimized conditions of temperature 90 °C, 60 min sonication time and pH = 3.26, the extraction yield, the galacturonic acid yield and the concentration of sample required to scavenge 50 % of 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic) acid (ABTS) values of QPPs were respectively 10.25 %, 3.86 % and 1.35 mg/mL. The QPPs extracted under optimum conditions characterized by FTIR, ¹H NMR and SEC/MALS/VD/DRI. The monosaccharide analysis revealed that arabinose was the most abundant, followed by galactose, glucose, mannose and xylose. Moreover, QPPs showed significant antioxidant activities (DPPH and FRAP) and reduced viability of human Caco-2 and murine B-16 cell lines in a dose-dependent manner. Hence QPPs could be used as antitumor agent in functional foods and pharmaceutical industries.

Effect of grinding on the thermal stability of a trihydrate atorvastatin: a CRTA study

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Atorvastatin also named 3-hydroxy- 3-methyl-glutaryl-coenzyme A ($C_{33}H_{35}CaFN_2O_5$) is a synthetic statin used as a cholesterol-lowering agent for the treatment of hypercholesterolemia [1-2].

During manufacturing the active pharmaceutical ingredients (API) are exposed to variable environmental conditions and encounter multiple stresses throughout the production cycle. Therefore, there is a significant possibility that phase transformations may occur. Similarly, solid-state changes may occur during storage. Solid-state conversions may involve a polymorphic transition from one polymorph to another, solvate formation or desolvation of a solvate, or interconversion to an amorphous form [3]. The consequences of these solid-state changes may affect the final performance of the API. As a result, the product quality, stability and also its therapeutic effects may be different to what was expected [3,4]. It is essential to follow possible phase changes during pharmaceutical development processes, and if possible, take precautions to control them, in part due to legal and commercial implications [5,6].

The present work highlights the importance of studying the thermal stability of Atorvastatin which was made using constant rate thermal analysis technique (CRTA). This technique allows to separate successive reactions, to obtain solid and accurate decompositions and specially to avoid the problems of heat transfer, mass and gas in the reactor of study provided that the rate of reaction is sufficiently slow. For the atorvastatin which is not obtained on a single crystal, the controlling of the rate of thermal decomposition during dehydration provides more reliable crystallographic data. Unlike DSC and TG curve, showing only one step dehydration [7], CRTA at constant rate and controlled water vapor pressure $P_{H_2O} = 5$ hPa accurately isolated the multiple steps of the crystal water dehydration of atorvastatin at the closes temperature (fig1). Powder XRD study revealed that the crystal lattice of atorvastatine was retained during dehydration up to 86°C.

The effect of grinding on the dehydration of crystal water of atorvastatine has been studied. The grinding reduces notably the cristallinity of atorvastatin, as supported by DSC and XRD data. CRTA, revealed the conversion of milled atorvastatin to non-stoichiometric hydrate (fig2)

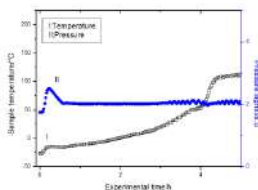


Fig.1: CRTA curves of atorvastatin

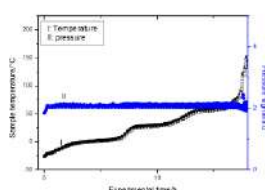


Fig.2: CRTA curves of grinded atorvastatin

Keywords: Pharmaceutical Hydrate, Atorvastatine, Dehydration, CRTA.

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Study and valorization of the active principles of some plants of southern Tunisia

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The therapeutic use of plants for the treatment of all diseases is very old and evolves with time and recently the return to "nature" is growing. In Tunisia, plants, mainly known for their richness in natural antioxidants, play a very important role in traditional medicine, they are the main sources of active ingredients used in the pharmaceutical field for the production of drugs. Indeed, there is a diversity of species with therapeutic interests, but many of them are not studied. This study is part of the valorization of Tunisian medicinal plants. Thus, six plants were selected on the basis of a study and according to their uses in traditional medicine: *Ratema raetem*, *Artemisia*, *Agropyron repens*, *Diploaxis harra*, *Lawsonia inermis* and *Kochia*. These plants, which are traditionally known for their therapeutic virtues, are extracted through a maceration with two types of solvent of different polarity and then evaluated for their extraction yield and their polyphenol content.

Key words: medicinal plants, polyphenol content, maceration.

Chemical composition, antibacterial and antioxydant activity of essential oils of *Pinus halepensis* Mill. and *Tetraclinis articulata* (Vahl) Masters.

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Through the centuries, human traditions developed the knowledge and use of medicinal plants in order to overcome suffering and improve the health of men. Indeed, the development of microbial resistance to antibiotics, also the toxicity of synthetic antioxidants used as additives in the food industry, are the source of interest generated for plants characterized by their biological properties. Different plant species have long been known for their therapeutic effects. Aromatic and medicinal plants constitute a very important natural wealth whose valorization requires a perfect knowledge of the properties to be highlighted. The medical properties of medicinal plants depend on the presence of various bioactive agents belonging to different chemical classes. These properties often due to the essential oil fraction. The use of essential oils in medicine never abandoned despite the discovery of organic synthesis processes and the birth of the pharmaceutical industry. They considered a real reservoir of basic molecules that are irreplaceable. These oils widely used in traditional therapies in Morocco and in many parts of the world. In this context we studied the chemical composition as well as the antibacterial and antioxidant properties of the essential oils of two conifers of Moroccan flora: *Pinus halepensis* Mill. and *Tetraclinis articulata* (Vahl) Masters.

Extraction of the essential oils carried out by hydrodistillation. The chemical composition analyzed by GC/MS. We used to evaluate the antioxidant activity the radical ABTS and the radical DPPH. While antibacterial activity determined by solid diffusion method and broth dilution method. The results of the biological tests show that the essential oils of *Tetraclinis articulata* (Vahl) Masters and *Pinus halepensis* Mill. have interesting antibacterial and antioxidant properties. This study scientifically validates the traditional use of these plants and reveals their interests as part of biotechnology exploitation.

Keywords: *Pinus halepensis* Mill., *Tetraclinis articulata* (Vahl) Masters, GC/MS, Antioxidant, antibacterial, DPPH, ABTS.

Magnetic properties, martensitic and magneto-structural transformations of ferromagnetic Ni-Mn-Sn-Cu shape memory alloys

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In recent years, a new type of ferromagnetic shape memory alloys (FSMA) have been becoming an important element of sensor and actuator materials due to their large magnetic-field-induced strain and shape memory effects. The Ni_{50-x} Mn₃₆ Sn₁₄ Cu_x (x=0, 1, 2) and Ni₅₀ Mn₃₆ Sn_{14-y} Cu_y (y=1) alloys were prepared by arc melting and then produced in a ribbon shape by rapid solidification using melt spinning technique.

The present study reports on the influence of the Cu doping on martensitic transition as well as magnetic properties. The crystal structures of the fabricated alloys were determined by X-ray diffraction technique (XRD). It was found that the substitution of Cu for Sn stabilized the martensite modulated structure. In addition, the characteristic transformation temperatures and the thermodynamic parameters of the samples were determined by differential scanning calorimetry measurements (DSC). The magnetic measurements were performed by a vibrating-sample magnetometer (VSM) in the temperature range 10–400 K. Experimental results indicate that the martensitic transformation (MT) temperature and Curie temperature (T_c) undergoes a slight shift towards high temperature with substituting Cu for Ni whereas, they disclose an important shift to high temperature through the substitution of Cu for Sn.

Keywords: Martensitic transformation, magnetic properties, phase transitions, Cu additions, Heusler alloys.

Optimization of composite synthesis by sintering process

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Keywords: biomedical; osteoporosis; apatite; bioactive glass; composite.

Bioactive ceramics, such as bioactive glass and dense hydroxyapatite, have been widely studied and have been developed over the last decades. Their excellent properties for the field of biomedical applications, especially in orthopaedic applications, have attracted wide attention. Calcium phosphate ceramics are currently used as biomaterials for many applications in both dentistry and orthopaedics, because they form an integrated bond with the surrounding bone tissue when implanted.

In recent years, there is a great interest in developing bioglass that contain fluoride to enhance biomaterials properties because as it is known, fluoride prevent dental decay and treats osteoporosis [1].

For this reason, we took the chose to incorporate apatites into different types of glass network that they were reported by Döhler and al [2], and are based on the composition of Bioglass®45S5.

For the preparation of these composites, different types of apatite were incorporated, hydroxyapatite ($\text{Ca}_{10}(\text{PO}_4)_6\text{OH}_2$) or magnesium fluorapatite ($\text{Ca}_{10-x}\text{Mg}_x(\text{PO}_4)_6\text{F}_2$) into different types of bioactive glass FO ($46.1\text{SiO}_2\text{-}2.6\text{P}_2\text{O}_5\text{-}37.6\text{CaO}\text{-}6.8\text{Na}_2\text{O}\text{-}6.8\text{K}_2\text{O}$ mole %) or F3 ($44.8\text{SiO}_2\text{-}2.5\text{P}_2\text{O}_5\text{-}36.5\text{CaO}\text{-}6.6\text{Na}_2\text{O}\text{-}6.6\text{K}_2\text{O}\text{-}3.0\text{CaF}_2$ mole %), the chosen sintering temperature for composites sintering is the end shrinkage temperature of each glass.

The microstructures of the sintered composites were studied using X-ray diffractometer and Fourier transform infrared spectroscopy. These results show the incorporation of apatite in the bioactive glass.

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Elaboration and characterization of Metal–Organic Frameworks thin film obtained through layer by layer deposition

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Metal-organic frameworks (MOFs) are crystalline polymeric microporous inorganic-organic hybrid materials composed of metal ions bridged by organic ligands [1]. These materials have received considerable attention in recent years because of their varied physical properties based on their uniform microporosity and their structural diversity and designability [2]. Therefore, the use of porous MOFs as thin films for the development of important future nanomaterials such as electronic, catalytic, and sensing devices is one of the challenging tasks in this research area [3]. In these circumstances, many innovative synthetic strategies for MOF thin film have been recently reported including layer-by-layer deposition on solid substrates [4]. The basis of this technique is that the reaction components are combined in a sequential manner. A distinct advantage of this growth mode is that it provides homogeneous, highly crystalline MOF films.

In this work, we describe a simple and straightforward methodology based on the in-situ conversion of metal hydroxides to MOFs thin film on glass supports using the layer by layer growth method. The obtained material was characterized by ATR-FTIR, X-ray diffraction (XRD) and optical microscopy.

Key words: metal hydroxides, MOFs, layer-by-layer deposition

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Green synthesis of copper oxide nanoparticles using biological *Cynomorium Coccineum* L. and *Nerium Oleander* extracts and study of their interaction with organic pollutants

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The synthesis of nanoparticles gained more attention due to the important characteristics that they provide including a large surface area, small size, and interesting physicochemical properties distinct from the corresponding bulk materials. These features endow nanoparticles with multiple applications in various fields. Herein, the current investigation highlights the use of an ecological synthetic procedure to reduce copper sulfate into copper oxide nanoparticles using biological molecules of either *Cynomorium Coccineum* L. or *Nerium Oleander* extracts. FTIR spectra reveal that these natural extracts were rich of carbonyl groups, phenolics, and other reducing agents which are responsible for the green synthesis of copper oxide nanoparticles. SEM analysis showed that the nanoparticles vary in size and shape distribution due to the chemical composition of the studied extracts. The purity of the metal particles was assessed by EDX analysis showing the presence of elemental copper oxide. The crystalline nature of the prepared nanoparticles has been confirmed using the XRD analyses. The as-prepared nanoparticles were further studied to interact with organic pollutants such as textile dyes. Methylene blue dye was chosen as a model molecule. Experiments were performed under the change in initial dye concentration, adsorption dose, contact time and pH value. The equilibrium adsorption capacities were 81.2 mg/g and 64 mg/g using nanoparticles synthesized from *Nerium Oleander* and *Cynomorium Coccineum* L., respectively. These levels are close to other common sorbents. In summary, biosorption effectiveness and environmental aspects of the prepared biological nanoparticles make them an ideal alternative to other expensive treatment methods.

Keywords: Nanoparticles; *Cynomorium Coccineum*; *Nerium Oleander*; Adsorption

Elaboration and characterization of germanium nanocrystals for next generation of nonvolatile memory and GeMn nanocrystals for spintronics

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In this work, we were interested to study the storage phenomenon of metal oxide semiconductor (MOS) containing germanium nanocrystals (NCs) inside SiO₂ thin layer for next-generation nonvolatile memories. The GeNCs were grown via dewetting at solid state by ultra-high vacuum (UHV) annealing at high temperature of an amorphous Ge layer. This latter was deposited by high-precision Solid Source Molecular Beam Epitaxy (SSMBE) on thermal SiO₂ and passivated with amorphous silicon before capping. By means of the C-V characterization, we noted a negative flat band voltage shift, which confirms a high degree of hole charging. We investigated also our sample using the DLTS in order to distinguish the different trap centres in the structures: indeed two traps were detected the first one (at 255 K) attributed to the dangling band and the second one (at high temperature) which is originated from minority carrier generation. No traps related to the interfaces states were detected so we have successfully fabricated MOS structures with good performance for microelectronic applications. In a second step, we were also interested in introducing manganese (Mn) in germanium nanocrystals elaborated via dewetting to improve the magnetic properties for spintronic applications. The obtained GeMn nanocrystals had a good ferromagnetic behaviour with a Curie temperature above the room temperature.

Sub-nanomolar Detection of Dopamine in Human Fluids by N-Doped Carbon dots

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Nitrogen doped carbon dots (N-CDs) were synthesized with simple and easy synthetic processes and environmentally friendly compound. In addition, a simple, rapid and highly sensitive fluorometric method for the determination of dopamine (DA) in human fluids is developed. The as-synthesized N-CDs were further characterized by TEM, HR-TEM, XRD and XPS. The maximum of the emission was centered at 350 nm. This work confirms that DA could result in an effective fluorescence quenching of N-CDs. We have also shown that the assay method adopted is linear for DA concentrations ≤ 100 ppb with a correlation coefficient of 0.9924. Finally, the developed sensing method was successfully applied to the determination of DA in human urine and serum samples.

Keywords: N-doped carbon dots, dopamine, fluorometric method, fluorescence quenching, human fluids.

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Effect of synthesis parameters on particle size of Nanocrystalline NiAl intermetallic compound

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The aim of this work is to optimize the parameters of the mechanically activated self-propagating high-temperature synthesis (MASHS) technique and the mechanically activated annealing-process (M2AP) used to produce the nanocrystalline NiAl intermetallic compound.

The as-obtained material was characterized using scanning electron microscopy (SEM) and X-ray diffraction (XRD). The morphological evolution of the mixture samples Ni50Al50, performed by SHS method as a function of milling time, shows the existence of two phases with different sizes. The milled sample 10 hrs has a very fine structure caused by the combination of mechanical activation to the rate of cooling which induced significant low section of the sample. The Rietveld refinement of the X-ray diffraction patterns, reveals the formation of two-phase β -NiAl and γ -Ni3Al intermetallic compounds that were synthesized by the mechanically activated volume combustion synthesis (MASHS). A single phase β -NiAl was formed when mechanically-activated annealing process (M2AP) was performed. The analysis has revealed the absence of any reaction between the milled elemental powders Ni and Al. It was, also, observed that there is a decrease of the crystallite size which reached a value of about 43 nm, performed by SHS method after 10 hrs of milling, as well as an increase of the atomic level strain.

Key-words : High energy ball milling, MASHS, M2AP, Ni50Al50 alloys, X-ray diffraction, Rietveld method.

APPLICATION OF HYBRIDS MAGNETIC NANOPARTICLES FOR EXTRACTION OF AROMATIC AMINES FROM ENVIRONMENTAL SAMPLES

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Since Aromatics amines (AA) [1] represent an emerging class of pollutants, it become necessary to develop a simple preparation technique to detect the residual trace in environmental matrices. There are numerous techniques for sample preparation that have been reported to isolate aromatics amines from complex matrices prior to instrumental analysis.

Magnetic solid-phase extraction (MSPE) based on magnetic nanoparticles has received increasing attention over the past few years [2,3] because of its simplicity and its easy and rapid isolation of analytes using a magnetic field. Hybrid nanoparticles (MNP-oSUD) have been previously obtained using chemisorption of sodium undecylenate oligomeric micelles (oSUD) to magnetic iron oxide nanoparticles through a single-step route in an aqueous medium. The most advantages of these oligomeric micelles adsorbed on magnetite nanoparticles (MNPs) are the excellent stability of coatings based on chemisorption [4], the high density of micelles and variety of interactions provided by this sorbent, which makes it highly efficient for the extraction of aromatic amines in a wide polarity range.

In this work, MNPs-oSUD were applied as a sorbent in MSPE to the extraction of 19 legislated carcinogenic aromatic amines [5] from urine, textile, and wastewater, prior to their quantification by LC-MS/MS [6]. The high density of micelles and variety of interactions provided by this sorbent rendered it highly efficient for the extraction of 19 aromatic amines in a wide polarity range (log K_{ow} values from -0.80 to 4.05) from textiles, human urine, and wastewater. The efficiency of these sorbents to expand the usually restricted range of extractable polarity from log K_{ow} values above 4 up to highly hydrophilic negative values has been proved by the extraction of in textiles, prior to their determination by LC-MS/MS. Recoveries in the range of 93%–123% (log K_{ow} = 1.34 to 4.05) were found for 17 out of 19 aromatic amines, independently of the type of sample and spiked concentration. These results show the high capability of MNPs-oSUD to extract compounds within a wide polarity range.

Keywords: Hybrid magnetic nanoparticles, Oligomeric micelles, Extraction, Aromatic Amines, Liquid Chromatography.

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**Program of
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20 December 2018**

The influence of water vapor in magnesium oxide carbonation

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The emission of carbon dioxide particularly anthropogenic CO₂ which comes principally from combustion of fossil fuel, has produced an increase in the atmospheric concentration of carbon dioxide from 280 ppm in 1750 to 406 ppm in 2017[1]. This increase is considered as the main cause of global warming. To avoid this threat, scientists have focused on this purpose and tried to develop solutions, the most attractive solution is the capture and storage of CO₂ coming from industrial installation. One way of CO₂ capture is the carbonation/decarbonation cycles process. Among numerous candidates (CaO, BaSiO₃, CaZrO₃...) magnesium oxide presents the advantage to be regenerable by simple heating at lowest temperature, to form a thermodynamically stable carbonate, and to be available in large quantities[2].

In this work, we are interested in synthesize mesoporous MgO via thermal decomposition method from hydromagnesite in order to use it for carbon dioxide capture at atmospheric pressure and ambient temperature.

To accelerate the reaction water vapor was added. In contrast to previous works studying this reaction at high temperatures and high pressures [3-4], our results indicate that at low temperatures (T<50°C) and atmospheric pressure, steam is no more a catalyst but it participates to the reaction giving with CO₂ an hydrated carbonated product. For the characterization of the new formed phase, ATR-FTIR and Raman spectroscopy were used as well as phase diagrams in the system MgO-H₂O-CO₂ confirming that 54% of MgO was converted to MgCO₃.3H₂O.

This reaction led to a noticeable change in the textural and morphological properties of the powder such as the decrease of specific surface, the decrease of pore volume and the shape of powder crystals; this change was investigated using MEB, BET and BJH.

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**Spectroscopic Studies, Optical Properties
and structural characterization by Rietveld
Refinements of Nano Crystal Lithium Rare Earth Polyphosphates
[LiGd_(1-x)Eu_x(PO₃)₄]**

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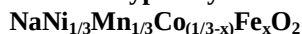
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The polycrystalline powder of the LiGd_(1-x)Eu_x(PO₃)₄ (with x= 0, 0.05 and 0.15) was synthesized by solid state reaction and was identified by X-Ray powder diffraction. The Rietveld refinement of X-ray diffraction patterns, of all compounds shows that these phases crystallized in the monoclinic system with space group I 2/a and cell parameters a= 9.635(3) Å, b= 7.035(3) Å, c= 13.191(3) Å, β= 90.082°, V= 894.214 Å³ and Z= 4. Moreover, Infrared and Raman spectra were recorded at room temperature. The observed vibrational results show the presence of the P-O-P bridges and the O-P-O groups, confirming that the structure is an infinite chain of tetrahedral (PO₃)_n. The magnetic susceptibilities of polyphosphate as a function of temperature are also reported along with corresponding magnetization measurements. All compounds exhibit a paramagnetic response. In addition, the LiGd(PO₃)₄:Eu³⁺ exhibits a higher thermal stability under 1000°C. Interestingly, Eu³⁺ doped polyphosphate can emit intense reddish orange light under the excitation of NUV light from 370 to 410 nm. This is very important for its applications in white light-emitting diodes LEDs.

Structural, Magnetic, Electrical and Electrochemical Properties of O3-Type Layered Materials:



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Herein we report the studies of different physical properties (structural, magnetic, morphologic, electrical and electrochemical) of $\text{NaNi}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3-x}\text{Fe}_x\text{O}_2$ compounds with $x = 0; 0.111; 0.222; 0.333$. Pure single-phase powders were prepared under air, using solid state synthesis method. Unit cell parameters of various compounds were refined using X-ray powder diffraction data in O3-type crystal structure and $R\bar{3}m$ space group. For all the compounds, magnetic, electrical and electrochemical properties have been also investigated. Temperature dependence of magnetic susceptibilities showed the Curie-Weiss behaviors for all compounds, and a significant change of magnetic property from antiferro- to ferromagnetic comportment with iron substitution. The magnetic hysteresis $M(H)$ loops indicated an increasing saturation magnetization from $x = 0$ to 0.333 . The electrical and electrochemical studies of the four samples also revealed enhanced polarization behavior with the substitution rate of iron.

Preparation and characterisation of tungsten oxide WO₃ thin films

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Tungsten trioxide (WO₃) thin films of 280 nm thickness have been prepared on glass substrates by spray pyrolysis technique, using a solution of aqueous ammonium tungstate with a concentration of 0.01 M. The obtained films were annealed in a programmable oven for 2 hours at temperatures 400°C, 450°C and 500°C. The thickness and the roughness parameters were checked by a profilometer. The X rays diffraction diffractogramms of the different samples showed that the films obtained are polycrystalline and crystalized in the monoclinic structure, with lattice parameters $a=8.3303\text{\AA}$, $b=8.4019\text{\AA}$, $c=3.8237\text{\AA}$ and $\beta=94^\circ$. Grains had two preferred orientations along the directions (201) and (002). It was noted that the mean grain size was about 20 nm. Optical measurements carried out in the wavelength range [190-1100 nm], revealed that the optical transmittance of the films in the visible spectrum was in the range 85-95%, and the optical band gap value was about 2.75 eV.

Keywords: Thin films; WO₃; Spray pyrolysis; XRD; Optical properties

Large magnetocaloric entropy change at room temperature in soft ferromagnetic manganite $\text{La}_{0.75}\text{Ca}_{0.05}\text{Na}_{0.20}\text{MnO}_3$

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In this paper, $\text{La}_{0.75}\text{Ca}_{0.05}\text{Na}_{0.20}\text{MnO}_3$ sample was prepared by the flux method. The crystallographic study revealed that $x=0.20$ sample crystallized in the rhombohedral structure with a $R\bar{3}c$ space group. Magnetic data, under a magnetic field of 0.05 T, indicated that our sample undergo a ferromagnetic (FM) - paramagnetic (PM) phase transition, when increasing temperature. The magnetic field dependence of the magnetocaloric properties of $\text{La}_{0.75}\text{Ca}_{0.05}\text{Na}_{0.20}\text{MnO}_3$ sample, with second phase transition, was investigated. Near room temperature, the $x=0.20$ sample exhibited a large magnetic entropy change with maxima of 6.01 and 3.12 J kg⁻¹. K⁻¹, respectively, under applied magnetic fields of 5 and 2T. Also, the relative cooling power (RCP) was calculated. According to hysteresis cycles, for our studied sample, at 10 K a typical soft FM behavior with a low coercive field was observed. These results make our sample promising candidate for magnetic refrigerators, magnetic recording, and memory devices

SYNTHESIS AND ANTIMICROBIAL EVALUATION OF NOVEL 1,3,4-OXADIAZOLE DERIVATIVES

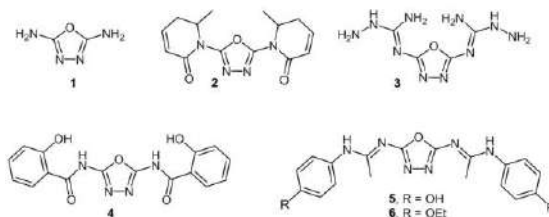
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For many years, five-membered heterocyclic compounds have attracted organic chemists due to their wide range of biological activities¹. As one of the basic five-membered aromatic heterocycles, 1,3,4-oxadiazole derivatives have been extensively studied because of their broad pharmaceutical², biological and optical activities³. We report herein, a new and efficient synthetic method for producing the 1,3,4-oxadiazole-2,5-diamine **1**, which has been used as starting materials for the synthesis of the novel symmetrical 2,5-difunctionalized 1,3,4-oxadiazole derivatives **2-6** (Scheme 1). All target compounds were screened for their in vitro antibacterial and antifungal activities using the microdilution method^{4,5}. The newly synthesized compounds **1-6** exhibit significant antimicrobial activities with different degrees and have shown moderate to high antibacterial and antifungal efficacy against several bacterial strains tested in comparison with standard drugs (Ampicillin and Nystatin). Our results suggest that the novel symmetrical functionalized 1,3,4-oxadiazole derivatives could be effective antimicrobial agents and warrant further investigation.



Scheme 1. Symmetrical 2,5-difunctionalized 1,3,4-oxadiazoles.

Key words:

Antimicrobial activities; 1,3,4-Oxadiazole-2,5-diamine; Paracetamol; Phenacetine; Salicylic acid; Thiosemicarbazide.

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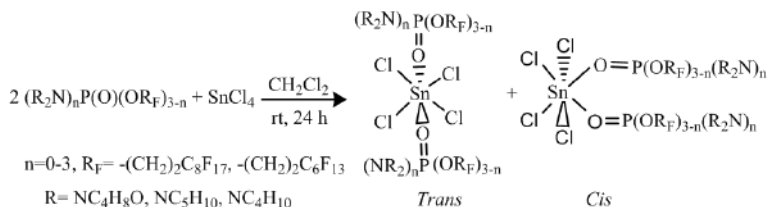
Tin(IV) chloride complexes with highly fluorinated phosphoramidates and phosphates. Synthesis and multinuclear (¹H, ¹⁹F, ³¹P and ¹¹⁹Sn) NMR characterization

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Tin compounds play an important role in inorganic and organometallic chemistry [1-3]. Studies of these compounds continue to provide fundamental information about the Lewis acid-base model, the reactivity and the Lewis acid catalytic properties of tin (IV) species [4-6]. In the present work, we report on the synthesis of new octahedral tin tetrachloride complexes with a novel series of highly fluorinated phosphordiamidates, phosphoramidates and triorganophosphates with the general formula [SnCl₄L₂] (L= (R₂N)_nP(O)(OR_F)_{3-n}). These adducts were characterized with multinuclear (¹H, ¹⁹F, ³¹P and ¹¹⁹Sn) NMR and IR spectroscopy. The NMR data show that these complexes exist in solution as a mixture of *cis* and *trans* isomers with the latter isomer being the predominant form. Moreover, 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.



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

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Thermal and viscoelastic behavior of green composite reinforced with fibrous networks obtained from *Opuntia* (Cactaceae)

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In this study, green composites were elaborated using a thermoplastic material as matrix and natural fibrous network with intricate structure obtained from *Opuntia* (Cactaceae) as filler. A new "ecofriendly" process was used to isolate cellulosic fabric with good mechanical and thermal properties. Composites with different levels of fibrous networks were produced and characterized by thermogravimetric analysis (TGA), differential scanning calorimetry (DSC) and dynamic mechanical analysis (DMA). The DMA was performed to determine the viscoelastic behavior. The obtained composites exhibit high thermal stability and good mechanical properties.

Keywords: *Opuntia* (Cactaceae), fibrous networks, green composites, thermal stability, viscoelastic behavior.

Thermotropic Liquid Crystalline Poly(azomethine-ether)s Based on 1-Phenethyl-4-piperidone

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A new thermotropic liquid crystalline poly (azomethine-ether)s containing 1-phenethyl-4-piperidone moiety in the main chain was prepared by solution polycondensation technique of various diformyl- α,ω -diphenoxyalkanes, I-IV with 3,5-bis(m-aminobenzylidene)-1-Phenethyl-4-piperidone VI, and characterized by elemental and spectral analyses. The inherent viscosities of the new poly(azomethine-ether)s are in the range of 0.40-0.90 dL/g. All the polymers were soluble in common organic and aprotic solvents. All polymers have very good thermal stability. The transition temperatures of all polymers are confirmed by DSC technique and optical texture of the poly (azomethine-ether)s in liquid crystalline state were observed on polarizing microscope. Most of the polymers exhibit a typical nematic mesophase.

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Posters Communications' Abstracts



Microrheology of an autoassociative transitional network

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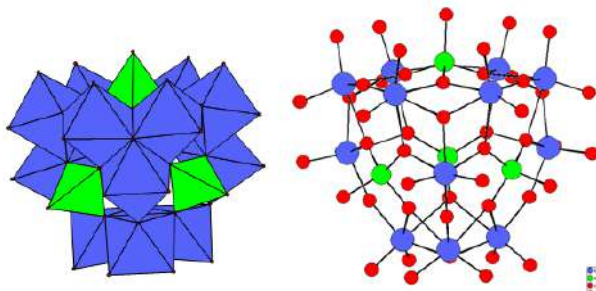
To study the viscoelastic behavior of a material, several works in the literature have used the technique of classical rheology. However, this method has several disadvantages such as the destruction of hydrophobic bonds which are fragile and the insufficiency of low frequency study. Therefore, we have proposed to use a new technique: passive light scattering microrheology (DWS) which does not have these disadvantages. The use of this method has made it possible, thanks to its cumulative effect and its resolving power, to access a dynamic whose frequency can go up to 10^5 rad / s and to use probe particles to study the internal dynamics of the system to study. The work presented is oriented particularly towards a hydrophobically modified poly (acrylic acid) polymer (HMPAA) which belongs to the family of water-soluble autoassociative polymers which are amphiphilic systems composed of a main hydrophilic (polar) chain and grafts hydrophobic (apolar). These polymers have, in an aqueous medium, particular rheological properties which are at the origin of the numerous industrial applications.

SYNTHESIS, STRUCTURE AND CHEMICAL PHYSICAL CHARACTERIZATION OF AN ARSENOMOLYBDATE CHAPED CAGE POM

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A new arsenomolybdate compound $\text{Na}_8[\text{As}_4\text{Mo}_{12}\text{O}_{50}]$ has been prepared by hydrothermal method and structurally characterized by elemental analysis, IR, UV-visible and single crystal X-ray diffraction analysis. Crystallographic data for the compound, Orthorhombic, space group $Pn\bar{m}n$: $a = 15.021$ (2) Å ; $b = 15.027$ (2) Å ; $c = 12.164$ (1) Å ; $Z = 2$. The compound consist of Na^+ ions and $[\text{As}_4\text{Mo}_{12}\text{O}_{50}]^{8-}$ shaped cage POM, which is made up by four Mo_3O_{13} groups sharing summits. The AsO_4 tetrahedra were located in the outside of the POM at the triangular windows. Whereas in other structures derivative of Keggin structure or Wells Dawson structure, the AsO_4 tetrahedron were located in the inner side. The Na^+ ions were found directly bonded to the cluster through $\text{O}-\text{Na}-\text{O}$ and provided linkages between clusters (POMs) into a three-dimensional structure.



Representation of the heteropolyanion $[\text{As}_4\text{Mo}_{12}\text{O}_{50}]^{8-}$

Key Words: Arsenomolybdate, heteropolyoxometalate, IR spectroscopy, UV-visible, Cyclic Voltammetry.

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STRUCTURE AND CHARACTERIZATION OF THE ORGANIC–INORGANIC HYBRID MATERIAL (C₂H₈N₂)Zn(Br_{1.41}Cl_{0.59})₂

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The crystal structure of the organic–inorganic hybrid material (C₂H₈N₂)Zn(Br_{1.41}Cl_{0.59})₂ has been investigated. The title compound crystallizes at room temperature in the orthorhombic Ima2 space group with the following unit-cell parameters $a = 19.2178(15) \text{ \AA}$, $b = 7.1660(5) \text{ \AA}$, $c = 9.9160(7) \text{ \AA}$ and $V = 1365.58(17) \text{ \AA}^3$. Raman scattering confirms the presence of both Bromine and chlorine which are linked to the zinc(II) cation in this hybrid material.

The 1D structure is made up of infinite $-\text{Zn}(\text{Br}/\text{Cl})_2 - (\text{En}) - \text{Zn}(\text{Br}/\text{Cl})_2 - (\text{En}) -$ zigzag chains running along the a -axis. Only one equivalent position is assigned to both bromine and chlorine atoms with an occupancy rate of 1.41 for bromine and 0.59 for chlorine. Each Zn atom is linked to two Br/Cl atoms and two nitrogen atoms belonging to two different ethylenediamine molecules. The structure cohesion is ensured via N-H...Br/Cl hydrogen bonds. The optical study reveals that the title compound undergoes two optical absorption bands at 240 and 289 nm respectively which are attributed to electron charge transfer from ligand to metal (Zn) usually named as LMCT but no d-d absorption bands are observed in this spectrum.

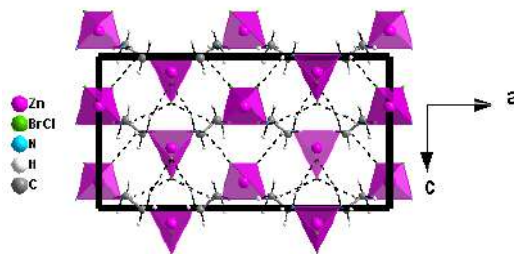


Figure: Projection of the structure along the b -axis.

Key words: Hybrid material, 1D structure, IR spectroscopy, Raman scattering, thermogravimetric measurement.

The anxiolytic-like activity of *Mitragyna Speciosa* korth.

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Mitragyna Speciosa (MS) has been shown to have central pharmacological activities. However, the mechanism of these properties is quiet unknown. One of the alkaloids in the methanoic leaf extract of *Mitragyna Speciosa* (mitragynine) has structure similarity to serotonin, which is an important neurotransmitter in both anxiety and depression. It is believed that serotonin may be involved in anxiety because, in general, stimulation of this system causes anxiety, whilst a reduction in serotonergic neuronal activity (e.g. by benzodiazepines) reduces anxiety this would tend to suggest some activities of *Mitragyna Speciosa* at the brain serotonergic system. Chronic administration of the *Mitragyna Speciosa* leaf extract 50, 100, 200, 400 mg/kg, orally for 14 days on rats were tested in the elevated plus-maze, 24h after the last administration. At the time of testing the exploratory behaviour of rats, the levels of different monoamines in four brain areas (the substantia nigra, the nucleus accumbus, the locus coeruleus and the raphe nuclei) were also assayed using HPLC-EC. The results of the present study found that *Mitragyna Speciosa* produce anxiolytic-like effect at doses 100, 200 and 400mg/kg and the levels of brain monoamines were significantly increased at doses 100, 200 and 400mg/kg. This will suggest that the central anxiolytic-like activity of *Mitragyna Speciosa* is probably mediated mainly through the enhancement of the central neurotransmitters levels.

Key words: *Mitragyna Speciosa*, Serotonin, brain monoamines, Anxiety.

Integrating hybrid materials into electrode via layer by layer deposition

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The modification of surfaces and interfaces by assembling porous materials is a topic of pronounced technological importance because this approach paves a way to the crystals with potential application such as chemical sensors, gas storage and separation, chemical sensing and catalysis [1]. In particular, Metal-Organic Frameworks (MOFs) are a reassuring class of porous materials resulting from the reaction between inorganic and organic species [2]. Owing to their uniform pores and high designability in the frameworks, while efforts continue on the combination of these hybrids compounds with electrode surfaces. In fact, several ways to deposit thin films of MOFs have been reported [3]. Layer by layer deposition is one of the most powerful techniques [4].

In this study, we report the elaboration of the indium tin oxide (ITO) glass electrode modified with ZIF-8, a representative MOF Material via layer by layer deposition. The structural and morphological studies of ITO-ZIF-8 electrode were characterized using ATR-FTIR(IR), Fourier X-ray diffraction (XRD) and optical microscopy

Key words : metal–organic framework, modified electrode, layer by layer deposition

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Adsorption of methylene blue from aqueous solutions by mud sediments of the Ghrib Algeria dam.

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Muddy sediments of a dam Algeria were used as an adsorbent of a cationic dye, methylene blue, in order to test their ability to fix organic contaminants. The adsorbent material is characterized by X-ray diffraction (PANALYTICAL PW-3710). The results show that the vessel contains a clay fraction which consists in proportion Halloysite -7A and impurities. The chemical composition of the mud is determined, it indicates that the mud contains mainly SiO₂ (39.64 %) and Al₂O₃ (14.39%wt). The morphological structure of the mud is analyzed by scanning electron microscope (SEM) and the total chemical composition is determined by (EDX), this latter analysis confirmed the results of the chemical composition found by XRF. The mud has a raw capacity cations exchange (CEC) low. In order to compare the measurement results of the specific surface area of the mud, it is determined according to different methods. The study shows that the adsorption of methylene blue can be attached to the vessel by electrostatic bonds. The adsorption kinetics is very rapid search for solutions of low methylene blue concentrations. Adsorption can be characterized by a two -order kinetics. The adsorption isotherm is the one characterizing the Langmuir for aqueous solutions of low concentrations and high concentrations of the solutions may be characterized by the Freundlich. The influence of pH and temperature of the harsh environment of adsorption of methylene blue by the mud is examined in this study.

Key word: Muddy, sediments, adsorbent, methylene blue

STRUCTURE AND CHARGE DELOCALIZATION OF PENTAVALENT HALOSILICONATE: A THEORETICAL STUDY

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Structures of pentavalent halo-siliconate $R-O-Si(CH_3)_3X^-$ ($X = F; Cl; Br$) and ($R = CH_3; CH_3-CH_2-; -CH(CH_3)_2; -C(CH_3)_3; -CH-CH_2; -C_6H_5$) are investigated using density functional theory (DFT) calculations at b3lyp-6-31G(d) level to understand their structure bonding characteristics and delocalization of electronic density. Our results indicate that pentavalent fluoro-siliconate $R-O-Si(CH_3)_3F^-$ are stable intermediates for all substitutions with a trigonal bipyramidal geometry, the substituents prefer the axial position and the loss of alkoxy group is observed and detected via electron charge transfer. In the case of $X = Cl; Br$ intermediates adopt a structure in which the alkoxy group is nearly double bonding with silicon atom. The loss of Cl^- and Br^- detected by their negative charge (-0,941) and distance of (3,89). GIAO method permits to calculate ^{29}Si NMR shifts for the $R-O-Si(CH_3)_3X^-$ systems as a function of (Si-X) distance and Si-O-C angle.

Keywords: DFT, pentavalent halo-siliconate, charge delocalization, GIAO, ^{29}Si NMR shifts.

Crystal structure of a New Bonding of (C₇H₁₁N₂)₄(H₄N)₂[Mo₇O₂₄]-6(H₂O)

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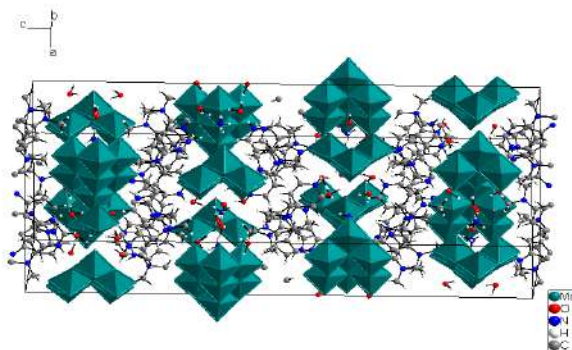
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Heptametalate polyoxomolybdates and polyoxotungstates ^{1,4} of general formula [M₇O₂₄]⁶⁻ (M = Mo^{VI} or W^{VI}, can both be isolated in the solid state. The heptamolybdate anions can be crystallized following acidification of aqueous molybdate solution. The structure of the heptamolybdate ion was solved by crystal-structure analysis, The compound crystallizes in the orthorhombic system with space group *Pbcn* and Z = 8 (R = 0.0314). The unit cell dimensions are *a* = 17.0366 (2) *b* = 14.0691 (2), *c* = 44.3305 (5) and *V* = 10625.6 (2) Å³. The planar cations, the water molecules and NH₄⁺ cation are positioned so as to be able to form hydrogen bonds with either molybdate oxygen atoms or water oxygen atoms. Four different types of hydrogen bonds have been found: N-H... O, N-H... Ow, Ow-Hw... O and Ow-Hw...Ow.

Theoretical and experimental studies was reported in this work; thermal, electrochemical and spectral analysis also Hirshfeld surface study



View perspective of the compound (1)

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Molecular Modeling Analysis of Atorvastatin Drug Enantiomers

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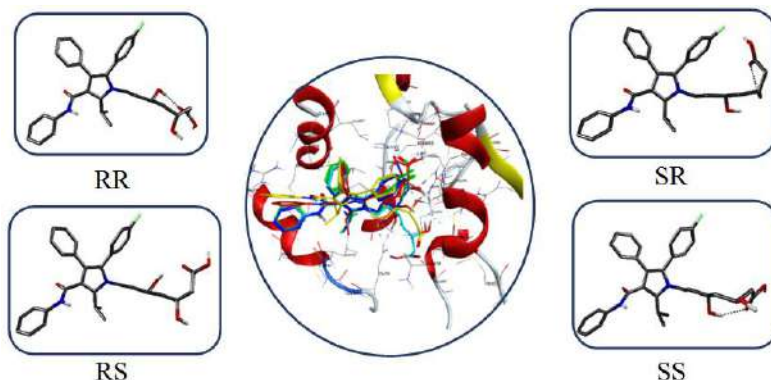
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The density functional theory (DFT) calculations were carried out on the four optical enantiomers (SS, SR, RS, RR) of Atorvastatin drug at B3LYP/6-31+G* level in the gas phase. The spectroscopic profiling (¹H and ¹³C NMR chemical shifts, UV and IR spectra), frontier molecular orbital (FMO), thermodynamic properties, the molecular electrostatic potential (MEP), NBO analysis and total density of states (DOS) of the four enantiomers were reported and investigated by theoretical calculations. E_{HOMO} , E_{LUMO} and HOMO-LUMO energy gap, Electron affinity (A), Ionization Potential (I), the electronic chemical potential (μ), chemical hardness (η), and electrophilicity (ω) also obtained. The four enantiomers were docked into HMG-CoA reductase active site, their interactions and binding energies were reported and analyzed.



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Synthesis, characterization and study chemical-physical properties of Mn₃O₄ nanometric

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The synthesis of uniformly sized and shape-controlled transition metal oxides has attracted a growing interest. This interest originated not only in novel chemical and physical properties of the nanoparticles [1], but also in many applications. However, Mn₃O₄ is one of the most stable oxides of manganese that found wide range of applications in molecular adsorption, electrochemistry and solar energy transformation [2-4].

In this context, Synthesis of Mn₃O₄ nanocrystals were achieved through a simple hydrothermal route, followed by the calcination at 300 °C using PEG, SDS and Triton as surfactants. The morphology and structural of the obtained products were characterized using X-ray diffraction and scanning electron microscopy. The effect of the surfactant nature on the optical and electrochemical properties of Mn₃O₄ was reported. UV-vis spectroscopic study showed a change in the energy band gap of Mn₃O₄ with the surfactant nature. The electrochemical properties of Mn₃O₄ based electrodes were systematically studied using cyclic voltammetry. The Results obtained reveal that the Mn₃O₄/SDS nanomaterial displays much higher specific capacitance and better cyclic stability. Specifically, it exhibits a specific discharge capacitance of 80 F.g⁻¹ and remains stable after 1000 charge/discharge cycles.

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Electrochemical sensors for determination of Cr(III) and Cr(VI)

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The implementation of environmental protection standards and the growing increase in potentially hazardous pollutants require the development of analytical techniques, which are specific, fast and robust. Beside the chemical methods for analysis of contaminants, biosensors and biological tools are widely used for the assessment of toxicity in the environment.

A biosensor is an analytical tool, which combines a bioreceptor with a physical transducer to detect specific components of a sample.

In this conference, we discuss the experimental results obtained with biosensors developed in our laboratory for the detection of phenols, pesticides (organophosphates and carbamates), heavy metals, cyanides, sulfides and viruses. Detection of emerging pollutants including drugs such as sulphonamides and endocrine disruptors such as bisphenol A in various environmental matrices at trace level will be presented.

Synthesis and characterization of fluoride containing carbonated hydroxyapatite.

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Fluoride substituted carbonated hydroxyapatite were synthesized by double decomposition method. The obtained powders were investigated by X-ray diffraction, infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy. The apatite phases were sintered between 1050°C and 1200°C. DRX results indicated that all peaks belonged to the apatite structure and no secondary phase has been detected. The insertion of the fluoride ions caused an increase in the crystallinity of the powders. The parameters a and c decreased with the increase of the content of F⁻. The density has also been studied. It increased with the increase of the temperature. The as prepared powders treated at 1000°C revealed a partial decomposition of the carbonated hydroxyapatite phase with a formation of CaO.

Synthesis of 1,2,3-triazolium-based polyfumarates from bio-based fumaric acid precursor

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Poly(ionic liquid)s (PILs), i.e. macromolecular analogues of ionic liquids (ILs), ideally combine the best features of ionic liquids (ILs) (e.g. tunable solubility as well as high thermal, chemical, electro-chemical and ion conducting properties...) with those of polymeric materials (e.g. processability, viscoelasticity, adhesion, film-forming properties, and microstructural design).^[1] Rapid advances in the chemistry, physics, and macromolecular architecture of PILs have prompted the development of new polyelectrolytes that have found applications in many fields, such as batteries, supercapacitors, solar cells, environment (water treatment), gas separation, catalysis, microelectronics (transistors, OLEDs), bio-related applications and so on...^[2] 1,2,3-Triazolium-based PILs (TPILs) have recently contributed to the development of this new family of polyelectrolytes.^[3,4] Their synthesis merges the versatility of step growth polymerization methods with the functional tolerance of CuAAC, the efficient N-alkylation of 1,2,3-triazole rings and the optional ion metathesis.

This work reports the synthesis of a new series of poly (fumarate-triazolium)s via the post-polymerization modification of their precursor. These materials can be considered as new candidates of polymer resins.

Key words: Poly(ionic liquid), CuAAC, poly(fumarate-triazole), poly(fumarate-triazolium).

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**Study the behavior of XC38 steel in sulfuric acid solution
(H₂SO₄, 1M, 97%) in presence of extracted natural inhibitor
using electrochemical technique**

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Our work aims to study the electrochemical behavior of XC38 steel in sulfuric acid solution (H₂SO₄, 1M, 97%) using electrochemical techniques in presence of the natural inhibitor obtained by the drying and grinding the red onion skin and then stirring with methanol, the resulting mixture was filtered and then dried in the oven. The extract was used at different concentrations 0 ppm; 1000ppm; 2000ppm; 3000 ppm in sulfuric acid solution (H₂SO₄, 1M, 97%). The results showed that the corrosion inhibiting effect of XC38 steel increases with increasing concentrations of the green inhibitor.

This work allowed us to deduce that the behavior of steel with respect to corrosion was optimal by adding the inhibitor to the concentration of 2000 PPM. This study will pave the way for further research on natural inhibitors due to non-toxicity of these natural products and also they are not expensive.

Key words: corrosion, inhibitor, polarization, XC38 steel.

AN EFFICIENT SYNTHESIS OF POLYSUBSTITUTED VINYL ETHERS

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Vinyl ethers have attracted considerable attention for their potential applications as monomers for the synthesis of functional polymer materials [1] and as precursors for synthesis of pharmaceuticals. [2] In this context, we describe in this communication, an efficient approach for the synthesis of difunctionalized vinyl ethers **2** through successive *O*-alkylation-isomerization reaction from the coupling reaction of ethyl 2-(bromomethyl)-3-cyanoacrylate **1** [3] with a series of alcohols as nucleophiles. A mixture of two regioisomers has been formed after being stirred for 5 min which allyl ethers [4] disappeared in favor of vinyl ethers by spontaneous isomerization. The coupling reaction was activated by the use of triethylamine leading to the formation of vinyl ethers **2** with total stereoselectivity in favor of *E*-isomer with good yields.



Key words: Ethyl 2-(bromomethyl)-3-cyanoacrylate, alcohols nucleophiles, triethylamine, vinyl ethers.

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Effect of preparation method in copper containing BaCeO₃ perovskites for CO-PROX reaction.

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Increased attention now turned to the development of fuel cell powered systems, because of their expectedly low environmental impact. The proton-exchange membrane fuel cell (PEMFC) is fueled with clean, CO-free hydrogen, which can be produced by steam reforming, autothermal reforming or partial oxidation of natural gas, light-oil fractions, and alcohols.

Unfortunately, significant amounts (ca. 5–15%) of CO are formed together with H₂, H₂O, CO₂, and CH₄ [1,2]. The concentration of carbon monoxide in the hydrogen feed must be kept below 1–100 ppm for the proper operation of PEMFC because the Pt anode of PEMFCs is highly sensitive to CO poisoning [3]. One of the most straight forward and cost effective methods to decrease the CO concentration down is the preferential catalytic oxidation of CO (CO-PROX).

Various oxides and supported metal catalysts have been reported to be effective for this process. Among them perovskite is one that has been intensively studied [4] with BaCeO₃ being one of the promising system. Perovskite ABO₃ can, in fact, tolerate significant partial nonstoichiometric substitution, without losing the characteristic structure [5].

In this work, BaCeO₃ prepared by citrate and microemulsion methods were thermally treated at various temperatures in order to modify their crystal size and surface area over a wide range. This allowed us to show the particle size effect on the perovskite catalytic performance.

Since the properties of the perovskite can be modified by changing cations A and B and their stoichiometry, the aim in this study was to examine the effects of adding Cu to the BaCeO₃ structure to form BaCe_{1-x}Cu_xO₃, on the properties and catalytic performance in CO-PROX. All samples have been characterized by XRD (Fig.1a and 1b), S_{BET} measurement, XPS and TPR(Fig.1c) and tested under CO-PROX conditions in combination with *operando*-DRIFTS in order to establish main structural and catalytic properties for this type of materials.

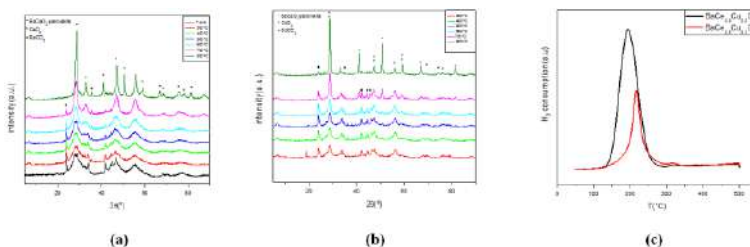


Figure 1. XRD profiles of BaCeO₃ prepared by citrate (a) and microemulsion (b) method and TPR profiles (c) for induced samples.

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Synthesis of Fe (0)@GA and its application as Green Catalyst in the Suzuki cross coupling reaction under ultrasound irradiation

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A novel and green procedure for synthesis of Iron (0) supported on gum acacia, as a reductant and ligand is described and characterised by UV-vis, IR, XRD, TEM, and TGA. The synthesized was examined as catalyst in the Suzuki cross coupling reaction with various substituted aryls in different conditions under ultrasound irradiation. The products were obtained in highly short reaction times with excellent yields.

The catalyst can be recovered and recycled by a simple filtration after the addition of methanol in the reaction solution with low decrease in catalytic activity.

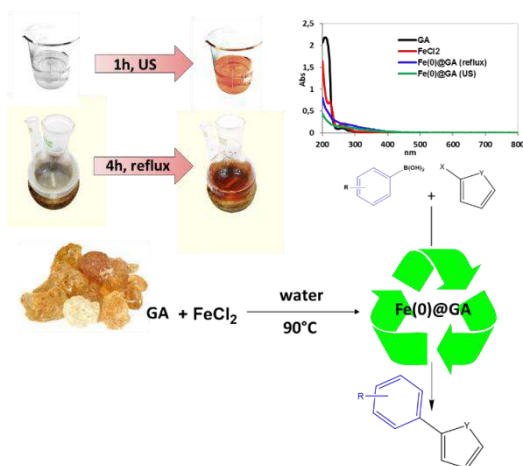


Fig. Synthesis of Fe (0)@GA and its application as Green Catalyst in the Suzuki cross coupling reaction

Key words: ultrason, gum acacia, catalyst, coupling reaction, green chemistry.

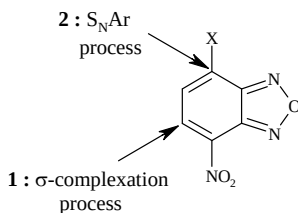
AMBIDENT REACTIVITIES OF 7-CHLORO-4-NITROBENZOFURAZAN

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Quantification of the ambident nucleophilicities and the factors which control the relative reactivities of the different nucleophilic centers has been considered by numerous authors. However, up to that time only a few papers have reported concerning the quantification of the ambident electrophilicities.

We now report our findings on the reactivity of ambident benzofurazan with various nitroalkaly anion in aqueous solution at 20 °C. Competitive between σ -complexation and S_NAr processes have been identified which lead, respectively to the formation of the Meisenheimer-type complex **1** and substituted product **2** (Scheme 1). On the other hand, the effect of basicity on reactivity is also discussed.



Scheme 1

Key words: Benzofurazan, Nitroalkaly Anions, Equation of Mayr, Ambident, Reactivity.

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Adsorption and photodegradation of anionic dye on polyaniline synthesized by two different pathways under simulated solar light

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The development of visible-light responsive photocatalysts would permit more efficient use of solar energy, and thus would bring sustainable solutions to many environmental issues. Conjugated polymers with extended π -electron systems act as a p-type semi-conductors with a band gap absorption border that can extend into the range of visible light. Conducting polyaniline (PANI) exhibits high absorption coefficient in the visible part of the spectrum, high mobility of charge carriers and good environmental stability and hence could have potential as photocatalyst. In the present investigation, we demonstrate that pure conducting PANI can increase the photocatalytic activity towards the decomposition of organic molecules under simulated solar light irradiation.

The first objective of this work is to synthesize PANI by two different polymerization pathways: Solid Based Polymerization (PSBP) and Aqueous Based Polymerization (PABP). Structural, morphological and optical properties were characterized by XRD, SEM coupled to EDX, TEM, UV-Vis DRS and BET. The influence is explored by the type of polymerization synthesis on the removal of anionic dye such as methyl orange (MO) from aqueous media.

The second objective is to compare the obtained powders in terms of the adsorption and photodegradation kinetics.

The effects of some influential parameters such as pH, catalyst dosage are evaluated. The results show that Polyaniline obtained by Aqueous based polymerization (PABP) exhibit higher photocatalytic efficiency than the latter obtained by Solid-Based polymerization (PSBP).

In fact, almost 98% of Methyl Orange removal was achieved at ambient temperature with 0.5 g/L of the adsorbent (PABP) within 120 min related to the effects of doping degree, band gap and surface area of the considered matrix.

Finally, this study reveals the potential of PANI for the removal of dyes from waste water.

Keywords: Polyaniline, Methyl orange, Solar light, Adsorption, Photodegradation.

Characterization of hydrological parameters and study of the metal content in algae taken at the coastal level of the city of bizerte

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Industrial effluents are loaded with pollutants of different types : organic, mineral, etc... which causes an aggressive and harmful to the receiving environment. Moreover, algae play an important role in the equilibrium of the aquatic ecosystem [1,2]. The Bizerte Lagoon has several industrial and domestic wastewater discharges. In addition, it contains a large and natural deposit of benthic marine algae.

Our work is to use some of these algae (*Ulva lactuca*) as a bio-indicator of metallic pollution (Cr, Ni and Cu). Moreover to studying the water quality of these discharges by the measurement of hydrological parameters (ions: phosphates, nitrites, nitrates, etc.). The study of the metal content in algae harvested from the industrial waste station shows significant variations related to the correlation of hydrological parameters and the sampling seasons.

Key words: *Ulva lactuca*, algae, metals, Bizerte coast.

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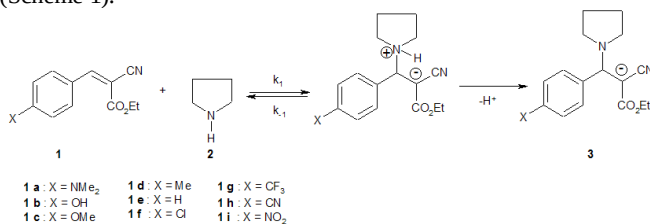
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NONLINEAR HAMMETT CORRELATION ASSOCIATED TO REACTIONS OF MICHAEL ACCEPTORS WITH PYRROLIDINE IN AQUEOUS SOLUTION

Kamilia AZAIEZ and Taoufik BOUBAKER

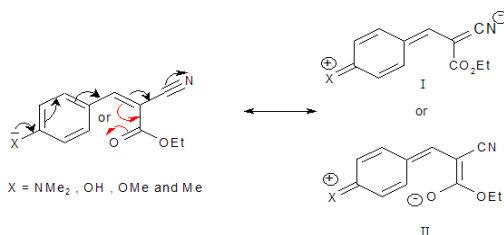
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Second-order rate constants (k_1) have been measured spectrophotometrically for the reactions of Micheal acceptors **1a-i** with pyrrolidine in aqueous solution at 20 °C (Scheme 1).



Scheme 1

These values have been analysed in terms of the electronic effect of the substituent X on reactivity and found that the stucture-reactivity relationship shows clear evidence of nonlinear behaviors. As will be seen, the biphasic-type Hammett plot has been interpreted as anground state stabilization through resonance interactions between the electron-donating substituent and the CN or COEt groups as illustrated by resonance structures I-II.



Key words: Michael Acceptors, Structure–Reactivity Relationships, Kinetics, Hammett’s Equation, Correlation of Yukawa-Tsuno, Substituent Effects.

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Pd-catalyzed arylation and Cu-catalyzed arylation of 5-vinyl-1,2,4-triazoles

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Mohamed Lotfi Efrit,^a Damien Prim^b

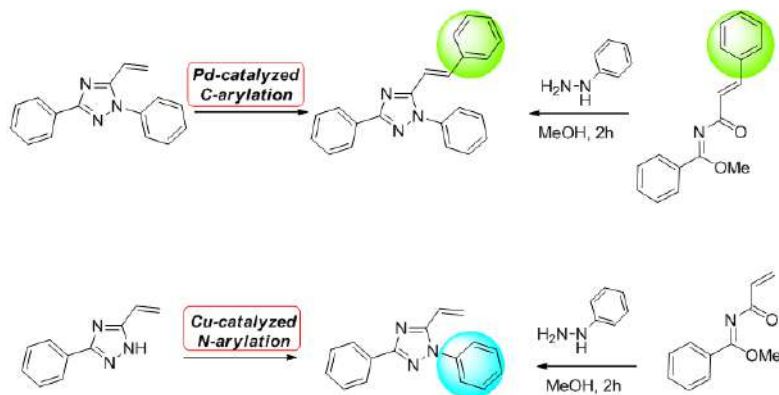
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Triazole compounds have paying strong interest due to their pharmacological^[1] and agricultural activities^[1,2].

The construction of the triazole ring allows the installation of variety of substituent combination at the N(1), C(3) and C(5) positions of the five-membered heterocycle in good to high yields. The method reveals selective towards 5-vinyl-1,2,4-triazoles avoiding the potential formation of seven- and five-membered side products as supported by theoretical calculations and NMR experiments. First lines of Pd-catalyzed arylation of the vinyl fragment towards 5-styryl-1,2,4-triazoles and Cu-catalyzed arylation^[3] at the N(1) site are described.



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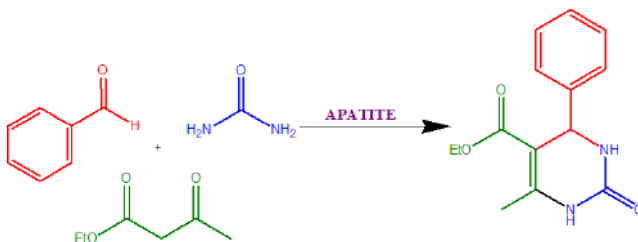
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Britholites: A new family of catalysts in organic synthesis

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Substituted hydroxyapatites of general formula $\text{Ca}_9\text{Bi}_x(\text{PO}_4)_5(\text{SiO}_4)\text{F}_2$ were synthesized by the thermal method and characterized by powder X-ray diffraction, Fourier transform infrared spectroscopy, transmission electron microscopy. The catalytic activity of these compounds were tested on one pot multicomponent reaction for the synthesis of 3,4-dihydropyrimidin-2(1H)-one and its derivatives [1-3]. The compound was confirmed by spectroscopic techniques and melting point [4]. An enhanced yield was observed with these catalysts for the condensation of ethyl acetoacetate, urea and benzaldehyde compared to unsubstituted hydroxyapatite.



Key words: Britholite, Biginellireaction, catalysis.

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Synthesis and characterization of chitosan film using as packaging materials

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In this study, we determined the effect of different ionic strengths on Zeta potential and pH zero charge point (pH_{PCN}) of chitosan. The results obtained show an important decrease in pH_{PCN} (from 8.3 to 6.7) of chitosan with a high concentration of NaCl under air atmosphere. The effect of the nature of plasticizer has been studied. The characteristics of the chitosan films were investigated by Differential Scanning Calorimeter (DSC), UV-vis, FT-IR and Water vapor transmission rate of materials (Q). Tensile tests were performed according to ISO 527 to measure the Young's modulus, tensile strength and elongation at break. The addition of 5% of glycerol (Gly), sorbitol (Sorb) or polyethylene-glycol (PEG) shows good mechanical properties of bio-films. Using a small amount of NaOH (0.3 mmol) revealed that from the different films prepared important physico-mechanical properties. The conditions food analysis (overall and specific migration) was determined using the European Regulation N°10/2011. The results exhibited the potential utilization in producing environmentally packaging chitosan films with high performance properties.

Keywords: Chitosan, bio-films, mechanical properties, food packaging

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

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The work developed in my study focuses on elaboration and characterization of a new class of polymers..Blends polypropylene / ethylene-diene-monomer have been studied for many years. Mixes polypropylene matrix have attracted the attention of academic and industrial researchers, because of the commercial interest is improving the impact resistance of the polymer at low temperatures.

To this end, the way which comprises mixing the polypropylene with a compound of lower glass transition temperature or higher ductility(elastomer, PE.....). in our case it is particles elastomeric EPDM to remedy the incompatibility problem between PP and EPDM, two compatibilizers were used: block copolymer 'PEP' and copolymer 'PP-g-MAH' to improve the interfacial adhesion between the two phase, and to improve the rigidity of the material, inorganic particles of silica has been added. These lead to materials with high mechanical properties both in terms of rigidity in terms of ductility and impact resistance. The study of mechanical properties such as tensile strength and impact strength show typical as hybrid materials. The introduction of the modified and not modified filler has allowed to improve rigidity of composites. In addition, the use of compatibilisants has allowed to improve interfacial adhesion of the phases in presence by giving mechanical properties higher than those of the pure mixtures.

Key words: Blend, elastomer, compatibilizer, interfacial adhesion

Effect of incorporation of EPDM elastomeric particles on mechanical properties of blend polymer PP and PA

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The work developed in my study focuses on improving the mechanical properties and of a new class of polymers..Blends polypropylene / polyethylene have been studied for many years. Mixes polypropylene matrix have attracted the attention of academic and industrial researchers, because of the commercial interest is improving the impact resistance of the polymer at low temperatures.

To this end, the way which comprises mixing the polypropylene with a compound of lower glass transition temperature or higher ductility(elastomer, PE.....). in our case it is particles elastomeric EPDM to remedy the incompatibility problem between PP and EPDM, two compatibilizers were used: block copolymer 'PEP' and copolymer 'PP-g-MAH' to improve the interfacial adhesion between the two phase, and to improve the rigidity of the material, inorganic particles of silica has been added. These lead to materials with high mechanical properties both in terms of rigidity in terms of ductility and impact resistance. The study of mechanical properties such as tensile strength and impact strength show typical as hybrid materials. The introduction of the modified and not modified filler has allowed to improve rigidity of composites. In addition, the use of compatibilisants has allowed to improve interfacial adhesion of the phases in presence by giving mechanical properties higher than those of the pure mixtures.

Key words: Blend, elastomer, compatibilizer, interfacial adhesion.

**Synthesis, Crystal Structure,
Physico-chemical Properties and Theoretical Study
of a new Organic-Inorganic Hybrid Material
($C_9H_{11}N_2O_5$)₂($SnCl_6$)**

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Chemical preparation, X-ray single-crystal diffraction, IR, UV-visible spectroscopic and theoretical calculations of a novel organic–inorganic hybrid material ($C_9H_{11}N_2O_5$)₂($SnCl_6$) are described. The 2-ammoniumbenzamide hexachlorostannate crystallize in the triclinic system with P-1 space group. Its unit cell dimensions are $a = 7.0859$ (7) Å, $b = 9.0553$ (9) Å, $c = 9.1442$ (8) Å, $a = 81.152(8)^\circ$, $b = 87.126(8)^\circ$, $c = 67.977(10)^\circ$ with $V = 537,43(25)$ and $Z = 2$.

In the compound in study, hydrogen bonds interactions $N-H\cdots Cl$, $C-H\cdots Cl$ and $N-H\cdots O$ contribute to the stability of the crystal. IR and uv-visible spectra are reported and discussed. The Hirshfeld surface and associated fingerprint plots of the compound are presented to explore the nature of intermolecular interactions and their relative contributions in building the solid-state architecture.

The optimized molecular structure, the theoretical IR vibrational frequencies and uv-visible absorption have been performed, using the density functional theory (DFT) method, at B3LYP/6-31G (d,p). The molecular HOMO–LUMO compositions and their respective energy gaps are also drawn to explain the activity of our compound.

Key words: Hybrid; X-ray diffraction; infrared spectroscopy; uv-visible; Hirshfeld surface; DFT calculus.

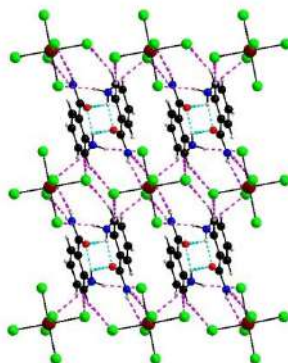


Fig.1. Projection along the b-axis of the atomic arrangement in ($C_9H_{11}N_2O_5$)₂($SnCl_6$)

**Synthesis and Physico-Chemical Characterization
of A New Member of β -Octamolybdate's Family:
[Na₄ (C₄H₁₁NO₃)₄]{[Mo₈O₂₈(C₄H₁₁NO₂)₂][Mo₈O₂₈(C₄H₁₁NO₂)₂]}·9H₂O**

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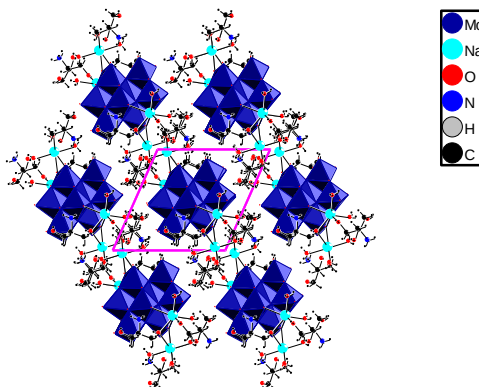
The new polyoxomolybdate [Na₄ (C₄H₁₁NO₃)₄]{[Mo₈O₂₈(C₄H₁₁NO₂)₂][Mo₈O₂₈(C₄H₁₁NO₂)₂]}·9H₂O was synthesized by conventional solution method at room temperature. Then, it was characterized by single crystal X-ray diffraction, IR, UV and thermogravimetric analysis.

The title compound crystallizes in the triclinic system, space group P-1 with $a = 12.3390(5)\text{Å}$, $b = 12.6766(5)\text{Å}$, $c = 18.9156(8)\text{Å}$, $\alpha = 72.293(2)^\circ$, $\beta = 87.153(2)^\circ$, $\gamma = 66.243(1)^\circ$.

This new compound consists of an assembly of two octamolybdates functionalized with trishydroxymethylaminomethane (TRIS). four sodium cations and four trishydroxymethylammoniummethane cations as well as nine water molecules.

The clusters are connected by organic cations and water molecules via hydrogen bonds.

The refinement of the structure led to a residual factor $R = 0.023$.



The packing view of the compound [Na₄ (C₄H₁₁NO₃)₄]
{[Mo₈O₂₈(C₄H₁₁NO₂)₂][Mo₈O₂₈(C₄H₁₁NO₂)₂]}·9H₂O along the c axis

Keywords: polyoxometalate, octamolybdate polyanions, Crystal Structure.

Evaluation of the impact of commingling two different waters in a Tunisian oilfield

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In oilfields, the produced waters may be mixed to enhance the production during improving oil recovery operations (IOR). At the mixing of different waters, the change of solubility of certain salts can lead to scale deposition, which is one of the serious problems experienced in the oil production industry. Therefore, a prediction study is recommended to assess the scaling risks.

The purpose of this study is to evaluate the impact of commingling two different waters, to predict mineral scale formation in a tunisian oilfield.

Two samples collected from both formation water and injected water were analysed, using Inductively Coupled Plasma- Atomic Emission Spectroscopy and Ion chromatography. The results of complete waters analysis were the typical input parameters, to determine scaling tendency. A computerized scale prediction model was developed to calculate the Saturation indices values related to CaCO_3 and BaSO_4 scales for the water mixtures at different shares, and under various conditions of temperature.

The future scale inhibition and removal strategies to be implemented in the concerned oilfield are being derived in a large part from the results of the present water compatibility study.

Key Words: Produced water, scaling, mineral deposit, compatibility.

Investigation of the interaction between sodium dodecylsulfate and cationic polymer

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The effect of additives such as salt or polyelectrolyte on the properties of aqueous surfactant solutions has been a subject of intense research due to their extensive commercial applications and researcher viewpoints. An important reason for this interest is that the complex formation between surfactant and polyelectrolyte showed widespread applications in fields like foods, paints, drug delivery, coatings and laundry products. Hence, the interaction of oppositely charged polymers with ionic surfactant is more convoluted comparing with nonionic polymerssurfactants. Poly (diallyldimethylammonium chloride) (PDAC), an important commercial water-soluble cationic functional polymer, is useful in water treatment as a flocculant or coagulant for the removal of organic and mineral contaminants such as arsenic, etc. We investigated the interactions between PDAC and SDS for determining the influence by varying the concentration of polyelectrolyte and temperature on the characteristics of PDAC/SDS complexes by using conductance, density & speed of sound and zeta potential. Because of hydrophobic interactions present in all the studied systems there is an increase in cmc with the increase in the concentration of PDAC and also increases with the increase in temperature except the values obtained at concentration of polyelectrolyte around 2.0 g/L. Density and speeds of sound data for SDS in aqueous solutions of PDADMAC at different temperatures have been reported in the present study. The apparent molar volume, partial molar volume and molar adiabatic compressibility have been obtained. These results show that V_{ϕ}^0 values increase with increase of temperature. This trend is due to hydrophobic interactions or caging effect of water molecules. Zeta potential measurements exhibited noticeable differences between surfactant and polyelectrolyte in wide range of surfactant concentration. The reason for the differences was explained by the differences in molecular structure and bulk properties on SDS/PDAC complexes.

Synthesis, crystal structure and physicochemical Characterization of a new copper (II)-orotate coordination compound

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Orotic acid (H₃Or, vitamin B13) and its metal complexes continue to attract attention because of its multidentate functionality and its ability to play differently hydrogen bond and π - π interaction in supramolecular architectures due to their proton donating and accepting ¹.

As a part of our ongoing research on the study of supramolecular metal–organic architectures, we have been engineered and synthesized a new supramolecular single crystals of metal-orotate complex of formula (nBu₄N)₂[Cu(orotate)₂].2H₂O. Although, this compound crystallizes in the monoclinic system, space group P2₁/n with the following unit cell parameters a= 23.2179(10) Å, b=8.3932(4) Å, c=25.5570(12) Å, β =99.420(4)°, Z=4, V=4913.2(4). This compound was synthesized by the slow evaporation method at room temperature and characterized by X-ray diffraction, FTIR, UV spectroscopy, and TGA analysis. The X-ray powder was used to check the purity of this compound.

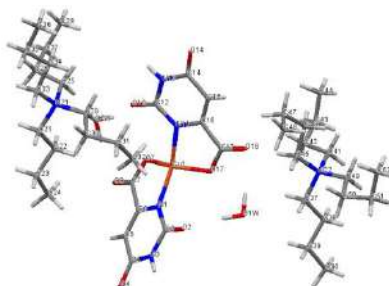


Fig. Asymmetric unit of the title compound

Key words: X-Ray Diffraction, Hybrid Compound, Copper Complex, metal-orotate, FTIR, UV, TGA

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Synthesis, Structural Study and Physico-Chemical Characterization of a new Nitrate ($C_8H_{12}NO$).[NO₃]

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Benzylamine and its derivatives have been widely studied as precursors in organic synthesis. They are also used in the industrial production of many pharmaceuticals including alniditan, lacosamide, moxifloxacin, and neбиволol [1-3]. In order to enhance the varieties of materials and to examine the influence of hydrogen bonds on the chemical and structural features, we report herein the chemical preparation and crystal structure of new organic salts, ($C_8H_{12}NO$).[NO₃].

The unit formula of ($4-(OCH_3)C_6H_4CH_2NH_3$).[NO₃], contains one inorganic nitrate anion and one 4-methoxybenzylammonium cation (Fig. 1). This compound crystallizes in the orthorhombic space group Pnma ($Z = 4$). The atomic arrangement of this compound consists of layers built from the NO₃⁻ anions and the -NH₃⁺ groups, interconnected by N-H...O hydrogen bonds, extending parallel to the (*b*, *c*) and located at $x = 1/4$ and $x = 3/4$ (Fig. 2). The organic entities are anchored between these layers and connect them via C-H...O and C-H...N interactions to form an infinite three-dimensional network (Fig. 2). This compound is also investigated by FT-IR and solid-state ¹³C and ¹⁵N CP-MAS NMR spectroscopy..

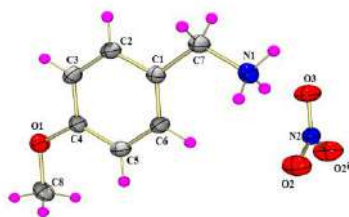


Fig. 1: Asymmetric unit of ($C_8H_{12}NO$).[NO₃]

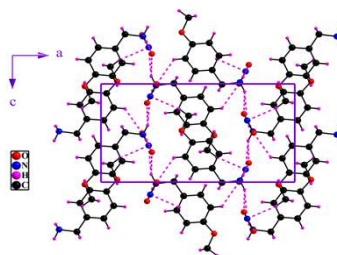


Fig. 2: The crystal packing of ($C_8H_{12}NO$).[NO₃] viewed along the *b* axis.

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Synthesis, crystal structure of the new arsenate compound $\text{Na}_3\text{Al}_3(\text{AsO}_4)_4$

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During the investigation of the $\text{Na}_2\text{O}-\text{Al}_2\text{O}_3-\text{As}_2\text{O}_5$ system, in which we previously highlighted the arsenates $\text{Na}_3\text{Al}(\text{AsO}_4)_2$ [1] et $\text{Na}_7\text{Al}_3(\text{As}_2\text{O}_7)_4$ [2], a new phase $\text{Na}_3\text{Al}_3(\text{AsO}_4)_4$ has been isolated. Single crystals have been synthesized by solid state reaction and their crystal structure has been determined by X-ray diffraction. This compound, isostructural to $\text{Na}_3\text{Fe}_3(\text{PO}_4)_4$ [3], crystallizes in the monoclinic space group C2/c with $a=19.8327(8)$ Å; $b=6.448(2)$ Å; $c=10.437(3)$ Å, $\beta=91.986(3)^\circ$ and $Z=4$. The structure of $\text{Na}_3\text{Al}_3(\text{AsO}_4)_4$ can be described as a two-dimensional layered structure. The layers, parallel to the bc plane, consist of corner-sharing AlO_6 octahedra that are further connected by AsO_4 tetrahedra through corner and edge sharing. The sodium ions are located in the interlayer space in two different fully occupied crystallographic sites. The layers are not compact and exhibit cavities along the [110] and [1-10] directions. The obtained structural model was confirmed by both Bond Valence Sum (BVS) and the Charge Distribution (CHARDI) methods.

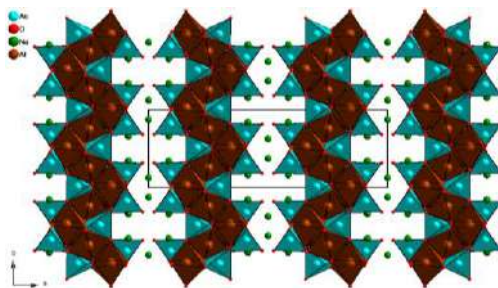


Figure: Projection of $\text{Na}_3\text{Al}_3(\text{AsO}_4)_4$ structure along [001] direction.

Key words: XRD, Single crystal, Crystal structure, BVS, CHARDI.

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$\text{Na}_6\text{Mg}_{1-x}\text{Co}_x(\text{SO}_4)_4$ a new cathode materials for Na-ion battery

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$\text{Na}_6\text{Mg}_{1-x}\text{Co}_x(\text{SO}_4)_4$ ceramics denoted as NMCoSx ($x=0.1, 0.3, 0.5, 0.7$ and 1) were obtained via the solid state reaction method. Refinement of structural parameters confirmed that the Co^{2+} dopant can replace the magnesium in this structure with a slight increase of the lattice parameters. The spectroscopic studies by means of infrared (IR) and visible (Vis) spectroscopies revealed the vibrational mode of sulfate groups and verified the amount of cobalt inserted in the host lattice. Electrical conductivity was studied by impedance spectroscopy in the [553–733 K] temperature range and results show that the materials present a semiconductor ionic character and the conductivity increases when the Co^{2+} dopant content x increases. Results also show that at low temperatures, NMCoSx ($x = 0.5$) has the highest electrical conductivity representing a candidate that may be used as an electrode in sodium-ion batteries.

Crystal structure of (Tris (2, 2'-bipyridine) cobalt (II) bis (1, 1, 3, 3-tetracyano-2-ethoxypropenide))

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Organic polynitrile ligands are known for their ability to build varied and original structural architectures and for their extensive electronic delocalization. Here we report the structural study of $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)_3](\text{C}_9\text{H}_5\text{N}_4\text{O})_2$. The single crystal diffraction proves that this compound crystallizes in the C2/c monoclinic space group with $a=22.335(4)\text{\AA}$, $b=10.9454(17)\text{\AA}$, $c=18.721(3)\text{\AA}$ and $\beta=110.691(5)^\circ$. The cation lies across twofold rotation axes. The nitrogens of three bipyridines are located on the vertices of a distorted octahedral coordination of the cobalt as shown on figure 1. In the polynitrile anion, the C-N and C-C bond lengths reveal huge electronic delocalization. The structure of the crystal is composed by infinite blocks of the cations running along the [100] direction. These blocks are connected to the polynitrile anions through weak C-H...N hydrogen bonds and anion... Π interaction to form a three dimensional framework.

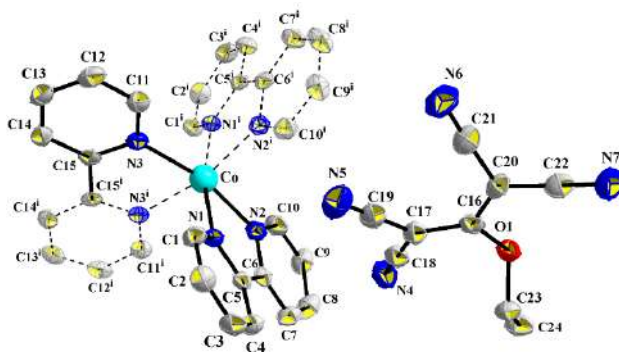


Figure 1. Atom numbering scheme of the structural unit in the studied structure.

The atomic displacement ellipsoids are drawn at 50% probability level.

The hydrogen atoms are omitted for clarity. [Symmetry codes : (i) 1-x, y, 0.5-z]

Keywords: single crystal X-ray diffraction, polynitrile anion, cobalt complexes, hydrogen bonds, anion... Π interaction

Development and validation of colorimetric method for the quantitative analysis of thioamides derivatives

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Thioamides (Thm) have diverse biological activities such as antibacterial, anti-HIV, anti-hyperthyroid, antituberculous and anti-tumor. The study of their pharmacokinetics and the clinical follow-up of thioamides are not elucidated in the bibliography. As a result, work has been done to develop and validate a simple, rapid and accurate spectrophotometric method for the analysis of Thm derivatives in pure form and in plasma. This spectrophotometric method has not been used before for determination of Thm. Reviewing the literature revealed that the monitoring of S⁻ group assay is based on the reaction with DTNB according to the Ellman method to form a yellow complex which absorbs at 412 nm. To assay the thioamides according to this method it is necessary to make the basic medium have S- to react with the DTNB. Experimental conditions affecting the color development were studied and optimized. The proposed spectrophotometric procedures were effectively validated with respect to linearity, ranges, precision, accuracy, specificity, robustness, detection and quantification limits. Calibration curves of the formed color product with DTNB showed good linear relationships over the concentration ranges (0, 50, 100, 500, 1000, 1500 mg/L). The proposed method was successfully applied to the assay of Thm dosage with good accuracy and precision. The principal advantages of the proposed method were rapidity, small cost and suitability for the routine quality control assay of the drug alone and in dosage form without interference.

**Synthesis, crystal structure, vibrational properties, thermal analysis and optical properties of a new organic–inorganic material:
[C₄H₈N₅]₃BiCl₆·H₂O**

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Single crystal of a new organic–inorganic hybrid compound [C₄H₈N₅]₃BiCl₆·H₂O has been synthesized by slow evaporation at room temperature and characterized by X-ray single crystal diffraction, infrared absorption, Raman spectroscopy scattering, thermal analysis, optical absorption and photoluminescence measurements.

The single X-ray diffraction results revealed that the compound crystallizes in the triclinic system with P-1 space group with the following parameters $a = 9.3143(2) \text{ \AA}$, $b = 12.6548(4) \text{ \AA}$, $c = 12.8962(4) \text{ \AA}$, $\alpha = 65.7230(18)^\circ$, $\beta = 86.6300(19)^\circ$, $\gamma = 76.2350(19)^\circ$, $Z = 2$ and $V = 1344.55(7) \text{ \AA}^3$. Its structure consists of [BiCl₆]³⁻ anions, showing the distorted octahedral geometry, surrounded by three crystallographically independent 2,4-diamino-6-methyl-1,3,5-triazin-1-ium cations and a water molecule. The crystal packing is governed by the formation of N–H...Cl, N–H...N and N–H...OW hydrogen bonds arranged in a three-dimensional network. ATG coupled to DSC analysis were carried out to study the thermal behavior of the prepared materials. Finally, The optical properties of [C₄H₈N₅]₃BiCl₆·H₂O were investigated by UV-Vis and luminescence spectroscopy.

Keywords: Crystal structure, Vibrational studies, thermal analysis, Absorption, Photoluminescence.

Phytochemical Analysis and Identification of Flavonoids and Phenolic Acids in ethanol extract from Tunisian Sea Cucumber *Holothuria Tubulosa* using LC-ESI-MS

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Sea cucumbers belonging to echinoderm family are traditionally used as tonic foods in China and other Asian countries. Sea cucumbers, referred sometimes as marine ginseng, they have potential sources of active ingredients for agricultural, nutraceutical, pharmaceutical and cosmeceutical products. Produced compounds are characterized by diverse activities and effects. High-performance liquid chromatography coupled with electrospray ionization mass spectrometry (LC/ESI-MS/MS) analysis in the negative ion mode was used for the separation and identification of flavonoids and phenolic acids derivatives detected in ethanolic extract from *H.Tubulosa*. One flavonoid glycoside (apigenin-7-O-glucoside), four flavonoids (naringin, quercetin, kampherol, cirsilineol) and three phenolic acids (trans ferulic acid, quinic acid, salviolinic acid) were identified. In this study, the antioxidant activity, phenolic and flavonoid contents related to the ethanolic extract were evaluated.

The results showed that the ethanolic extract had a power radical scavenging property with IC₅₀=0.010 mg/mL. Moreover, this extract present significant phenolic content (55.61 mg gallic acid equivalents/g extract).

Keywords: Sea cucumbers, *Holothuria Tubulosa*, LC/ESI/MS, flavonoid, phenolic acid

ADSORPTION OF CATIONIC DYE ON SODIUM DODECYL SULFATE FUNCTIONALIZED REED PARTICLES:

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The present investigation reports whether reed particles (RP) surface modification using sodium dodecyl sulfate (SDS) can affect a toxic triphenylmethane dye removal from water. To the best of our knowledge, SDS modified-RP - referred to as SDS-RP - has not been explored toward cationic dyes uptake so far. The impact of key parameters such as solutions pH, dye initial concentration, sorbent concentration, contact time and temperature on malachite green (MG) dye uptake by SDS-RP was evaluated for the first time in a batch mode.

To further understand the MG adsorption progress onto RP and SDS-RP, we evaluated kinetic data by chemical reaction based kinetic models and diffusion-based kinetic models and isotherm data by Langmuir, Freundlich, Temkin, and Dubinin–Radushkevich models [1]. Furthermore, we calculated thermodynamic parameters (ΔG° , ΔH° and ΔS°) and explored the recycling of MG from RP and SDS-RP.

Key words: Biosorption, Reed, Sodium dodecyl sulfate, Malachite green

Acknowledgments

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Novel phenoxazine and phenothiazine derivatives for OLED applications

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Luminescent materials for organic light-emitting diodes (OLEDs) have been an important subject of both academic and industrial research in recent years [1]. Although OLEDs that employed fluorescent materials have been progressively replaced by metal-based phosphorescent materials, the latter exhibit certain disadvantages, such as cost and the need to use heavy metals. Recently, organic emitters displaying thermally-activated delayed fluorescence (TADF) have become relevant in this field, leading to remarkable results [2,3].

Phenoxazine and phenothiazine are potentially good electron donors and hence have been used extensively as fluorescent emitters for OLEDs, dye sensitized solar cells and laser dyes. However, because these materials are conventional fluorescent emitters rather than TADF ones, the EQEs obtained for their devices are less than those of phosphorescent OLEDs. In these fluorescent compounds, the large overlap between HOMO and LUMO is probably a major factor preventing the generation of TADF. In general, strong electron donors and acceptors tend to localize the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) on them.

In this communication are presented four novel phenoxazine and phenothiazine luminescent derivatives, which were designed having in mind their ability to display TADF, in order to explore their potential application in OLEDs.

Keywords: High external quantum efficiencies, Thermally Activated Delayed Fluorescence, luminescent, Organic Light Emitting Diodes

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Aminoquinuclidinediium tetrachlorocuprate(II)-complex: crystal packing, phase transitions, optical studies and electrical properties

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Single crystals of a new organic–inorganic compound $[\text{C}_7\text{H}_{16}\text{N}_2][\text{CuCl}_4]$ were grown by hydrothermal technique and characterized by X-ray diffraction, infrared absorption, Raman spectroscopy, optical and differential scanning calorimetry (DSC) analysis as well as electrical studies. The compound $[\text{C}_7\text{H}_{16}\text{N}_2][\text{CuCl}_4]$ is crystallized in the monoclinic space group $P2_1/c$. In crystal structure, the tetrachlorocuprate anions are linked to the organic cations through N–H $\cdots$ Cl hydrogen bonds. The theoretical results were obtained using density functional theory (DFT) with the B3LYP/LanL2DZ level of theory for studying the molecular structure and vibrational spectra of the title compound. UV-Vis spectrum reveals three bands at 287, 400 and 683 nm. The optical band gap energy was estimated to be 4.61 eV. The DSC measurements indicated that $[\text{C}_7\text{H}_{16}\text{N}_2][\text{CuCl}_4]$ underwent two sequential phase transitions at around 288 and 388 K. The modulus plots are characterized by the presence of two peaks associated with the grain and grain boundaries. The temperature dependence of the electrical conductivity confirmed the phase transitions that were well detected with differential scanning calorimetry. The present study reports our investigation on a new compound: 3-aminoquinuclidinediium tetrachlorocuprate (II) with the general chemical formula $[\text{C}_7\text{H}_{16}\text{N}_2][\text{CuCl}_4]$. It presents the structural characterization by X-ray diffraction, FT-IR, FT-Raman, optical properties, DSC analysis and dielectric measurements. Moreover, the behaviors of temperature-dependent dielectric and impedance spectroscopy were investigated. Finally, the electrical conduction mechanism of $[\text{C}_7\text{H}_{16}\text{N}_2][\text{CuCl}_4]$ was also discussed.

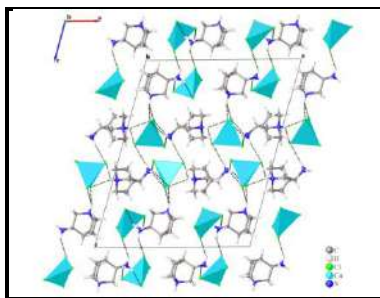


Figure. View of $[\text{C}_7\text{H}_{16}\text{N}_2][\text{CuCl}_4]$ along the b-axis. The dotted lines indicate hydrogen bonds.

Keywords: Metal complex; phase transitions, optical studies; electrical properties.

Particulate Polycyclic Aromatic Hydrocarbons (PAH) in the Atmosphere of Bizerte City, Tunisia

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The particle-phase concentrations of polycyclic aromatic hydrocarbons (PAH) were determined in 13 air samples collected in an urban area of Bizerte (Tunisia) during 2009–2010. Atmospheric particulate samples were extracted by ultrasonic bath and analyzed by high-performance liquid chromatography with fluorescence detection. PAH were found in all the analyzed air samples and the most abundant compounds were pyrene, fluoranthene, benzo[g,h,i]perylene, benzo[b]fluoranthene, chrysene and benzo[a]pyrene. $\Sigma 14$ -PAH concentrations ranging from 9.38 to 44.81 ng m⁻³ with mean value of 25.39 ng m⁻³. PAH diagnostic ratio source analysis revealed gasoline and diesel vehicular emissions as major sources. The mean total benzo[a]pyrene toxicity equivalent calculated for samples was 3.66 ng m⁻³ and the mean contribution of the carcinogenic potency of benzo[a]pyrene was determined to be 55.8 %. Concentrations of particulate PAH in Bizerte city atmosphere were approximately eight times greater than sampled at a nearby rural site.

Keywords; Particle-associated polycyclic aromatic hydrocarbons (PAH); HPLC-FLD analysis; Sources; Benzo(a)pyrene equivalent toxicity (BaP-TEQ); Diagnostic ratios; Tunisia

Chitosan-functionalized magnetic nanoparticles: Preparation for extraction and analysis of carbaryl in environmental water samples

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Composite materials based on the combination of nanoparticles (NPs) and polymers have attracted much attention in recent years thanks to their positive characteristics. In this study an easy, cheap and green procedure is proposed for the synthesis of magnetic nanocomposites. Magnetic Fe₃O₄-chitosan nanoparticles (Fe₃O₄-CNPs) were synthesized using co-precipitation method in the presence of Fe₃O₄ magnetic nanoparticles. The synthesized particles were, then, characterized using Fourier transform infrared spectroscopy (FTIR), Scanning electron microscopy (SEM), Thermogravimetric analysis (TGA), Energy dispersive X-Ray analysis (EDX) and X-Ray diffraction (XRD). Owing to the strong metal chelating ability of chitosan Fe₃O₄-C NPs exhibit adsorption capacity. Their application for the dispersive solid phase extraction of carbaryl from aqueous samples was studied. Several factors affecting the extraction efficiency were systematically optimized. The potential use of the composite for the isolation of the target from more complex samples has been outlined.

Structural and computational analysis of intermolecular interactions in new orthorhombic polymorph of dichloro-bis(4-dimethylaminopyridine) cobalt(II) complex, [Co(II)(C₇H₁₀N₂)₂Cl₂]

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The crystallization and characterization of a new polymorph of dichloro-bis(4-dimethylaminopyridine) cobalt(II) complex, [Co(II)(C₇H₁₀N₂)₂Cl₂] (I) by single - crystal X-ray diffraction, Hirshfeld surface analysis and density function theory (DFT) calculations are described. The previously published polymorph (A) [1] crystallizes in the monoclinic space group *P2/c*, while that described herein (B) crystallizes in the orthorhombic with the space group *Pccn*, *Z*=8, and unit cell parameters *a*=13.634(5) Å, *b*=14.394(5) Å, *c*=18.245(5) Å. The crystal structure of this new polymorph is built of discrete monomer molecules. The central cobalt(II) ion is coordinated by two Cl⁻ anions and two 4-dimethylaminopyridine ligands in C₂ symmetry, with the two-fold axis passing through the Co(II) ion and the mid-point of two Cl⁻ anions (**Fig**). Density functional theory (DFT) calculations of the structure, natural population analysis and the thermodynamic properties at different temperatures have been performed. The cobalt(II) ion is a distorted tetrahedron CoN₂Cl₂ and the pyridine rings with the dimethylamino group are fairly planar. The three-dimensional Hirshfeld surface (3D-HS) and the two-dimensional fingerprint plots (2D-FP) reveal that the structure is dominated by H...Cl/Cl...H (22.7%) and H...H (50.3%) contacts.

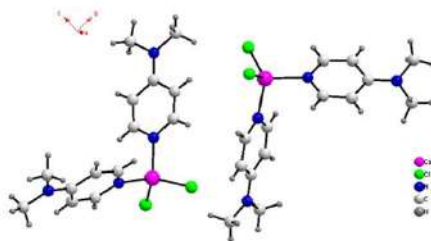


Fig. Molecular structure for the new polymorph (B).

Key words: Hirshfeld surface, polymorph, crystal structure, fingerprint plots.

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Synthesis, crystal structure and Hirshfeld surface analysis of bis(2,6-diamino-3-chloropyrinium) octachlorotricuprate, $(C_5H_7Cl_1N_3)_2[Cu_3Cl_8]$

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Crystals of bis(2,6-diamino-3-chloropyrinium) octachlorotricuprate (1) were grown by slow evaporation method. The single crystal X-ray diffraction results reveal that the newly-prepared compound crystallizes in the monoclinic system with $P2_1/n$ space group with the following parameters: $a = 3.8076(1)$ Å, $b = 22.7261(5)$ Å, $c = 12.8882(3)$ Å, $\beta = 95.759(2)^\circ$. The cohesion and stabilization of the structure are provided by N–H...Cl and C–H...Cl hydrogen bond between $(C_5H_7Cl_1N_3)_2^{2+}$ cations and $[Cu_3Cl_8]^{2-}$ anions (**Fig.1**). Moreover, the cations show a π - π interaction adding extra stability to the three-dimensional architecture. The prevalence of these interactions is illustrated by an analysis of the three-dimensional Hirshfeld surface (3D-HS) and by two-dimensional fingerprint plots (2D-FP). The relative contribution of different interactions to the 3D-HS indicates that the H...Cl/Cl...H account for 43.2% of the total 3D-HS area (**Fig.2**).

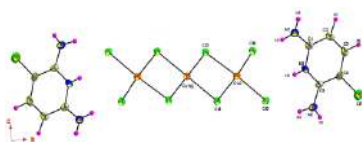


Fig. 1 The asymmetric unit of the crystal structure of (1)

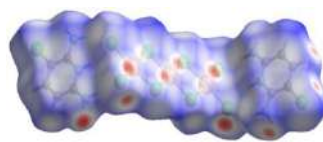


Fig.2 View of the 3D-HS of (1) mapped with d_{norm}

Key words: Octachlorotricuprate, crystal structure, Hirshfeld surface analysis.

Chemical profiling and evaluation of antioxidant, antiacetylcholinesterase, antidiabetic and antimicrobial properties of *Volutaria lippii*

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The total phenolic and flavonoid contents of *Volutaria lippii* fractions (hexane, dichloromethane, ethyl acetate, butanol and aqueous) and their in vitro antioxidant, anti-acetylcholinesterase, anti-diabetic and antibacterial activities were investigated [1,2]. The results indicated that the ethyl acetate and aqueous fractions have the highest levels in phenolic and flavonoid contents and showed remarkable antioxidant activities using three complementary assays (DPPH, total antioxidant capacity and reducing power). Also, the ethyl acetate and aqueous fractions exhibited powerful anti-acetylcholinesterase and anti-diabetic activities and a moderate antibacterial effect. Additionally, the HPLC-ESI-MS analyses of both fractions allowed the identification of 10 phenolic acids and 8 flavonoids. The quinic acid derivatives constituted the most abundant components in the two fractions. Overall, these results demonstrated, for the first time, that *Volutaria lippii* is a potent source of natural inhibitors of α -amylase and acetylcholinesterase enzymes with powerful antioxidant properties that might be used to prevent diabetes and Alzheimer complications as a complementary pharmacological drug.

Keywords: *Centaurea lippii*; antiacetylcholinesterase; antidiabetic; antioxidant; antibacterial; polyphenols.

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Essential Oil from *Rhanterium suaveolens* Growing Wild in Tunisia: A proposal for a novel natural antifungal and antimicrobial agent

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The intention of this study was to determine the chemical composition and to explore the antibacterial and antifungal properties of essential oil from the flowers of *Rhanterium suaveolens* Desf. growing in Tunisia [1]. The GC and GC-MS analyses of essential oil conducted to the identification of twenty-seven compounds representing 99.08% of the total oil. The main constituents were α -pinene (25.84%), β -pinene (17.57%), 1-octen-3-ol (16.23%), camphene (12.28%), limonene (8.03 %), β -myrcene (5.13 %), pinocarvone (2.98%) and p-cymene (2.51%). *Rhanterium suaveolens* essential oil was characterized by high contents in monoterpenes hydrocarbons (64.96 %) and oxygenated monoterpenes (23.62 %).

The antibacterial and antifungal activities of the volatile oil were screened *in vitro* using microdilution and disc diffusion methods [2]. Considerable antibacterial effect was recorded against both Gram-positive and Gram-negative bacteria with MIC values ranging from 23 to 230 $\mu\text{g/mL}$. A powerful antifungal activity was also observed against 5 human pathogenic fungi. The highest antifungal effect was revealed against *Candida albicans* and *Fusarium phylophylum* with less MIC values of 11.5 $\mu\text{g/mL}$. These results suggest the possibility to use of *Rhanterium suaveolens* essential oil as a promising antimicrobial and antifungal agent in drug and food preservation.

Key words: *Rhanterium suaveolens* Desf., essential oil, antibacterial activity, antifungal activity, GC-MS analysis.

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Design, synthesis of novel Triazolones and bis-Triazolones derivatives under ultrasound irradiation and evaluation as potent angiotensin converting enzyme (ACE) inhibitors

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The condensation of several primary amines and diamines with various *N*^l-ethoxycarbonyles *N*^l-tosylhydrazonates (**1a-b**), triazolones (**2**) and bis-triazolone (**3**) resulted in ethanol under ultrasound irradiation. Compared with the conventional methods, the main advantages of the present procedure are milder conditions, shorter reaction time and higher yields. The newly synthesized compounds were evaluated for angiotensin I-converting enzyme (ACE) inhibition. The results were compared to Captopril as a reference drug. Compounds **3b**, **2h**, **3a**, **2d**, and **2f** showed not only inhibition activity with IC₅₀ values of 0.162, 0.253, 0.253, 0.281 and 0.382 μM, respectively, but also minimal toxicity. The docking of chemical compounds in the ACE active site showed possible inhibitory effect of all compounds on the catalytic activity of the enzyme, which would satisfactorily explain the anti-hypertensive effect of these compounds.

Keywords: *N*^l-ethoxycarbonyles *N*^l-tosylhydrazonates, triazolones, bis-triazolones, ultrasound, angiotensin I-converting enzyme (ACE) inhibitory activity.

**First principal study of apatite structures
 $\text{Ca}_5(\text{PO}_4)_3\text{X}$ (X=OH, F, Cl, Br, I): Effect of X element on the
physical, chemical and structural properties of crystals**

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Usually, researcher use the total energy of the structure as parameter to select the best structure after the geometry optimization in the DFT calculation. In our case, we have used the charge distribution model (CHARDI) [1-2] to choose the best configuration and to select the best parameters for the DFT calculation of the apatite structure (best= compromise between calculation time and reliability of results). The obtained structure model was then used to determine the physical and chemical properties of the $\text{Ca}_5(\text{PO}_4)_3\text{X}$ (X=OH, F, Cl, Br, I) such as: Bond structure, density of state, IR and Raman theoretical spectra. The comparison between experimental and theoretical spectra of IR and RAMAN and the effect of X element on the structure and on the vibrational properties are the aim of this study. This comparison is the proof of our choice of CHARDI model as criterion to select the best configuration after a geometry optimization.

Keywords: DFT, Charge distribution model, apatite, geometry optimization

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Multiobjective optimization of wastewater treatment by electro-chemical process

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The aim of this study is to model and optimize the performance of a new electrocoagulation (E.C) process for the treatment of wastewater as well as the energy consumption in order to extrapolate it to the industrial scale. Through judicious application of an experimental design (DOE), it has been possible to evaluate the individual effects and interactions that have a significant influence on both objective functions (maximizing efficiency and minimizing energy consumption) by using aluminum electrodes as sacrificial anode. Preliminary experiments have shown that the pH of the medium, the applied potential and the treatment time with E.C are the main parameters. A factorial design 3^3 has been adopted to model performance and energy consumption. Under optimal conditions, the pollution reduction efficiency is 93%, combined with a minimum energy consumption of $2.60.10^{-3}$ kWh / mg-COD. The potential or current applied and the processing time and their interaction were the most influential parameters in the mathematical models obtained. The results of the modeling were also correlated with the experimental ones. The results offer promising opportunities to develop a clean process and inexpensive technology to eliminate or reduce wastewater

Key words: Electrocoagulation, green process, experimental design, modelling, optimization

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Characterization of stable concentrated colloidal silica dispersions as nanoparticles

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Two recent rather techniques have been implemented to characterize the properties of concentrated suspensions of nanoparticles in the process line (acoustic spectroscopy) and (light scattering). A commercial colloidal silica suspension was chosen for this study. The use of these techniques for the characterization of physico-chemical properties (stability, pH, zeta potential) and a rheological behavior was used to understand the properties of the initial suspension. Thus, the analysis of pH, zeta potential and especially the analyzes conducted by dynamic light scattering at Turbiscan MA 2000 have verified that the initial suspensions, a dilution range from 1% to 30 wt. %, remained stable and homogeneous. Changes in particle size distributions (PSD) function of time during the aggregation. Process in then followed in line under dense Ultrasizer acoustic spectroscopy.

Studies have shown that the results of particle size analysis by both methods are in good agreement, which proves that the silica aggregates formed under the conditions of experiments are not destroyed by dilution. PSD for monitoring the process of destabilization highlights the existence of two aggregation steps with different kinetics: slow aggregation first-kinetic small primary particles (up to one hundred nanometers) and more rapid aggregation second-kinetic large aggregates (up to a little more than ten micrometers).

Keywords: nanoparticles, dense suspensions, stability, aggregation, correlation photon spectroscopy, acoustic spectroscopy.

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The disinfection by-products (THMs) levels in drinking tap water at Mostaganem region (Northern West Algeria)-Algeria.

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Introduction: The use of chlorine to disinfect water produces various disinfection byproducts such as trihalomethanes (THMs). These compounds are formed when free available chlorine reacts with natural organic matter in raw water during water disinfection. Epidemiologic studies have shown an association between long-term exposure to THMs and an increased risk of cancer, all of them are suspected of having carcinogenic effects. The aim of this paper is to determine the presence of disinfection byproducts (THMs) in the drinking tap water of Mostaganem region (Algeria) during the year 2017.

Methods: This analytical study is based for collecting tap water samples from deferent area of Mostaganem region in order to analyse trihalomethanes. Primary, we have preceding a collect of 20 samples from different area of Mostaganem region which are marked a higher level of residual chlorine; secondly, we have utilised the HS-SPME method for determination of trihalomethanes in drinking tap water.

Results The results obtained have shown that the maximal concentration is 172.61 µg/l was in Achaacha region and 17.54 µg/l in Salamandre area. It was concluded that the drinking tap water distributed in Mostaganem region, contains a considerable amount of Trihalomethanes, chlorodibromomethane and bromoform are in majority, this could impact directly on consumer's health during a long period of time.

Conclusion: Our drinking tap water samples include a large quantity of THMs with different concentrations, where the dibromochloromethane and the bromoform constitute the major portion of THMs.

Key words: Analyse, drinking tap water, disinfection byproducts (THMs).

Molybdenum complex of the antibiotic sulfanilamide, the X-ray single crystal structure of $[\text{Mo}(\text{C}_{12}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2)] \cdot \text{NO}_3$

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Sulfanilamides were successfully employed as effective chemotherapeutic agents for the prevention and cure of bacterial infections in human biological systems. Moreover, sulfadruugs and their complexes, have applications as diuretic, antiglaucoma or antiepileptic drugs, antifungal, antiviral, antitumor, and anti-inflammatory ones among others.

The new complex of molybdenum of sulfanilamide formulated as $[\text{Mo}(\text{C}_{12}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2)] \cdot \text{NO}_3$ is synthesized by the hydrothermal route. The crystal structure of complex molybdenum was identified by X-ray. The complex of molybdenum crystallize in the orthorhombic space group Pbca with crystal data $a=13.904(5)$, $b=13.2572(7)$, $c=18.7436(8)$, $V=3455(3)$, $Z=4$, with sulfanilamide acting as bidentate ligand. Zolybdenum is coordinated to the nitrogen and oxygen from the sulfanilamide group. In the crystal structure of the title compound, $[\text{Mo}(\text{C}_{12}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2)]^+ \cdot \text{NO}_3^-$ the cations and anions are connected by $\text{N} \cdots \text{H} \cdots \text{O}$ hydrogen bonds into a three-dimensional network.

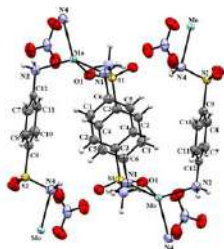


Fig. 1. Coordination mode of the complex $[\text{Mo}(\text{C}_{12}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2)] \cdot \text{NO}_3$

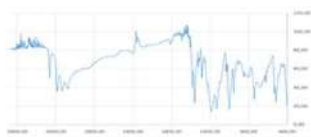


Fig.2. IR spectrum of nitro (4-aminobenzenesulfonamide) Molybdenum (II) in the range 3900-400cm⁻¹

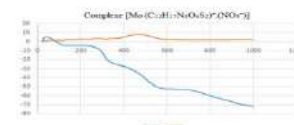


Fig.3. Thermogravimetric analysis (ATG) of the compound $[\text{Mo}(\text{C}_{12}\text{H}_{17}\text{N}_4\text{O}_4\text{S}_2)] \cdot \text{NO}_3$ with a heating rate of 10 °C / min

Key indicators: Single-crystal,X-ray study; Hydrothermal synthesis, Molybdenum sulfanilamid.

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Kinetics and thermodynamic studies of adsorption process of methylene blue using PANI/SiO₂ nanocomposite.

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Conducting Polymeric nanocomposites have attracted great attention over the last years because of their potential uses as chemical sensors, electronic and optical devices, and as catalysts as well as in adsorption processes. For adsorption applications, in particular, small and well dispersed nanoparticles are desired. We report in this work chemical synthesis of SiO₂-polyaniline (PANI) nanocomposite and their adsorptive performance in different mediums. In the present work, a polyaniline/SiO₂ composite was prepared and evaluated for its methylene blue (MB) dye adsorption characteristics from aqueous solution. Adsorption equilibrium kinetic and thermodynamic experiments of MB onto PANI/SiO₂ were studied with two different pH values. The effects of solution pH, initial dye concentration, contact time and temperature on the adsorption capacity of PANI/SiO₂ for MB have been investigated. The pseudo-first order and pseudo-second order kinetic models were used to describe the kinetic data. It was found that adsorption kinetics followed the pseudo-second order kinetic model at all of the studied temperatures. The Langmuir, Freundlich and Dubinin Raduschkevich adsorption models were used for the mathematical description of adsorption equilibrium data and the fit obtained using the Dubinin Raduschkevich isotherm has an R² value of 0.73. The properties of the synthesized polyaniline were investigated by FTIR analysis, and X-ray diffraction (XRD).

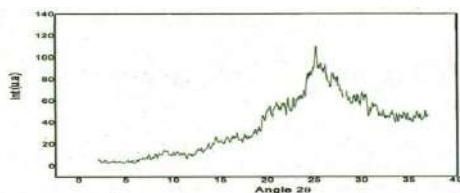


Figure 1: XRD diagram of synthesized polyaniline (PANI)

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**New quaternized poly(4-vinylpyridine-co-divinylbenzene) material containing nickel(II) Schiff base complex:
Synthesis, thermogravimetry, and application for heterogeneous electrooxidation of ethanol**

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Poly(4-vinylpyridine) crosslinked by 2 % divinylbenzene was partially quaternized (20 % monomer equivalents) by a bidentate Schiff base nickel complex containing C–Br function in its molecular structure using dioxane as solvent. The resulting poly(4-vinylpyridine-co-divinylbenzene)-Ni(II) Schiff base complex (PVP-coDVB-Ni(II)-L2) was characterized using various techniques such as elemental analysis and Fourier-transform infrared (FT-IR) spectroscopy. Thermogravimetric (TG)/differential thermogravimetry (DTG) analysis of the nonmodified copolymer, free complex, and the copolymer modified with the nickel complex was carried out to elucidate the thermal behavior. The synthesized copolymer covalently grafted with the nickel(II) complex was mixed with carbon black paste to prepare a new modified electrode material. This electrode was characterized by wide-angle X-ray diffraction analysis, scanning electron microscopy/energy-dispersive X-ray spectroscopy, and cyclic voltammetry. The electrochemical properties of the resulting modified electrode, recorded in alkaline solution, were investigated by cyclic voltammetry, revealing a well-defined redox process corresponding to the Ni(III)/Ni(II) redox couple. The effects of parameters such as the scan rate and ethanol concentration were explored for electrooxidation of ethanol using this modified electrode. A mechanism for the electrooxidation of ethanol is suggested based on the cyclic voltammetry results.

Keywords : Poly(4-vinylpyridine) Divinylbenzene, Ni(II) Schiff base complex, Thermogravimetry, Cyclic voltammetry, Ethanol electrooxidation

Synthesis of novel fluorinated pyrazolo[4,3-*e*]pyrimido[1,2-*c*]pyrimidin-2(8*H*)-one derivatives

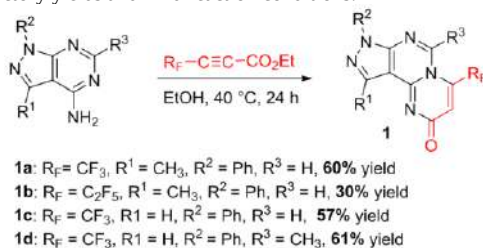
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Pyrazolopyrimidine derivatives represent an important class of heterocycles possessing diverse biological properties including antimicrobial, antiviral, anti-inflammatory, cardiovascular and anticancer activities.¹ The introduction of a fluoroalkyl group on such heterocyclic pattern may be very interesting for the enhancement of the biological properties of these molecules, in a similar way to that reported for other pharmaceuticals.² Indeed, the role of fluorine in drug design and development is expanding rapidly and the judicious introduction of fluorine into a molecule can productively influence conformation, intrinsic potency, membrane permeability, metabolic pathways, and pharmacokinetic properties.²

With this in mind, and in the continuation of our interest to develop efficient protocols for the synthesis of novel heterocyclic compounds with possible biological properties,³ we now report an efficient regioselective and catalyst-free synthesis of unprecedented fluorinated pyrazolo [4,3-*e*]pyrimido[1,2-*c*]pyrimidin-2(8*H*)-ones, through the reaction of 4-amino-1*H*-pyrazolo[3,4-*d*]pyrimidines with fluorinated ethylpropiolates, in ethanol, at 40 °C (Scheme 1). This protocol is endowed with several advantages such as easy operation, generality, satisfactory yields and mild reaction conditions.



Scheme 1

Keywords: Fluorinated heterocycles, fused heterocycles, pyrazolopyrimidines, pyrazolo[4,3-*e*]pyrimido[1,2-*c*]pyrimidin-2(8*H*)-ones.

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Removal of emerging pharmaceutical contaminants by adsorption

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Each year, thousands of tons of pharmaceutical compounds are used in human and veterinary medicine to treat symptoms, diseases and infections. These molecules detected in ground and drinking water have a harmful effect on human health and environment. Thereby, they are considered as emerging contaminants. To face this worrying situation, many works are oriented for the elimination of these emerging pharmaceutical contaminants by several processes (physicochemical and biological treatments). In this context we will focus on the study of the elimination of this type of organic pollutants in water by adsorption on a bio-adsorbent thereby valorize highlighting food processing waste.

This work has been carried out in order, to use the prepared bio-adsorbent in a beneficial manner in the treatment of pharmaceutical industrial effluents. Bio-adsorbent was prepared using pomegranate peels. Structural and physicochemical characterizations were carried out by different analytical techniques such as: IR spectroscopy, Zeta potential, Boehm titration, SEM... The adsorption study of emerging pharmaceutical contaminant on this bio-adsorbent was initiated by a preliminary optimization of the experimental parameters (stirring speed, mass ratio of bio adsorbent / volume....) in order to determine the optimal conditions of adsorption. This study has led to yielded encouraging results to eliminate this type of pollutants.

Synthesis, crystal structure and Characterization of a new hybrid compound based on heptamolybdate isopolyanion

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The class of compounds known as POMs is based upon metal-oxide building blocks. The polycondensation that takes place between the same type of metal atoms results structures structured only by the metal element and oxygen atoms called Isopolyanions (IPAs)[1]. The Heptamettallate is the dominant species in an aqueous medium with a pH range between 3 and 5.5 [3]. These frameworks are consisting of molybdenum (VI) or tungsten (VI) grouped under the general formulas: heptamolybdate $[\text{Mo}_7\text{O}_{24}]^{6-}$ and heptatungstate $[\text{W}_7\text{O}_{24}]^{6-}$ Anions. It is described by the association of seven distorted octahedra sharing edges. [2]

A hybrid organic-inorganic material based on heptamolybdate anions and the 2-aminopyridine as an organic cation was prepared by conventional method in an aqueous solution. The compound crystallizes in the orthorhombic system and Pbcm space group with $a = 17,079(1)\text{\AA}$, $b = 14,813(1)\text{\AA}$, $c = 39,562(1)\text{\AA}$, $V = 10009.1(1)\text{\AA}^3$, $Z = 8$. It is characterized by IR spectroscopy, UV spectroscopy, single crystal X-ray diffraction elemental analysis...

The Hirshfeld surface analyses indicate the important role of the hydrogen bonds to stabilize the structure.

Key word: Polyoxometalates, X-ray diffraction, crystal structures, characterization

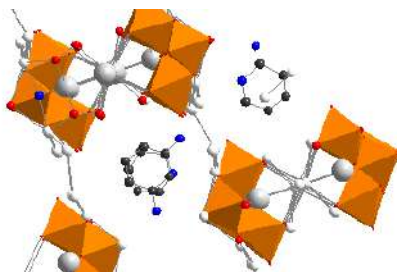


Fig. Projection along a axis of the new organic-inorganic hybrid material

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Manufacturing of thermal insulating foams from glass bottles waste

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Foam glass is a well-known insulating material due to its unique combination of insulating and functional characteristics. Materials recycling are nowadays well implanted in worldwide quotidian lives. The recycling of glass is a main objective for environmental protection. It allow saving energy, raw materials and CO₂ emissions. It also allows the manufacture of high value-added materials such as cellular glass. The objective of our work is to develop foam glass samples from glass waste used for packaging bottles, and to value them as an insulating material in the habitat sector, or as filters for the purification of waste water. Several materials and different techniques can be used to produce cellular materials. One of the techniques widely used for the production of glass foams, is the addition of foaming agent to the powdered glass, followed by a heat treatment to form a cellular structure. The aim of this work is to elaborate and characterize glass foam samples obtained from ordinary glass bottles waste with the objective to be used as thermal insulating or water filters.

In this study, packaging glass bottles were used as raw materials. This type of glass has a relatively high level of Fe₂O₃, Al₂O₃ and Na₂O. These oxides are an important factor for the foaming process. The selected glass bottles were washed and dried. The glass was crushed and finely ground until reaching a particle size less than 100 µm. Then, it is mixed with a variable content of calcium carbonate (0.5, 1.0 and 1.5) % for 2 hours in a hammer crusher. The carbonate is used in form of fine powder with a particles size less than 70 µm. The prepared mixtures were uniaxially pressed (80 MPa, 5 min) to obtain cylindrical samples. Then the samples are heat treated at (800-950) °C during 15 minutes, and finally cooled naturally to room temperature.

The results show that the best porosity in terms of thermal and acoustic insulation is obtained for the content 1% CaCO₃. The initial volume expansion of the samples passes up to about 10 times. The mean mechanical strength reaches 0.8 MPa, which was estimated not important enough. To increase this strength value, a variable content of fine kaolin (1 - 25)% are added in the same conditions than above. In this case, the porosity level remains nearly constant (88.7%), while the fracture strength increases 3 times and reaches 2.6 MPa. With the variation of the kaolin content, it has been possible to obtain samples intended not only for thermal and sound insulation, but samples with fine and open porosity, which can be used in the manufacture of water filters for domestic or industrial uses..

Key words: Glass foams, carbonate calcium, kaolin, insulation, water filter.

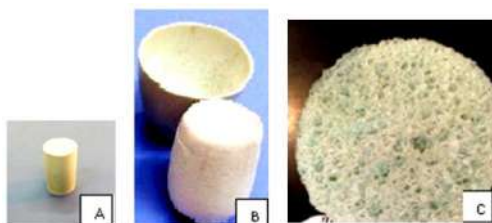


Fig. 1 : Sample containing 99% glass + 1% CaCO₃ :

A: before foaming

B: after foaming

C: Porous structure

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Intermolecular antiferromagnetic interactions in dinuclear Copper(II) complex with 2-Thiopheneacetic acid

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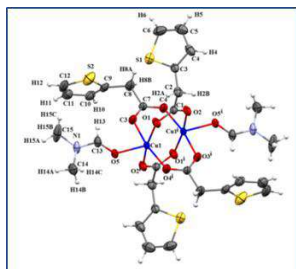
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Complexes containing two or more metal ions are of considerable interest not only because they offer high aesthetics in their structures but mainly because they offer new patterns in reactivity, magnetic exchange phenomena and the transfer of energy between their centers.

One dimeric copper carboxylate of formula $[Cu(taa)_2(dmf)]_2$ (where taa denotes 2-thiopheneacetate anion) have been synthesized, structurally characterized, and its magnetic properties have been studied. The crystal structure of the complex belongs to monoclinic system with space group P2(1)/c, it consists of centrosymmetric dimers where the bidentate 2-thiopheneacetate anions form *syn, syn* bridges between copper (II) ions. The coordination polyhedron of each metal ion is completed by the dmf molecule, with a Cu ... Cu distance of 2.632(6) Å.

The variable temperature magnetic susceptibilities of the complex have been measured in the range 2 – 400 K under external fields of 0.1 T. The X_mT product at room temperature is close to the expected one for two isolated Cu(II) with $S=1/2$, when the T is lowered, X_mT decreases indicating the presence of a strong antiferromagnetic coupling between neighboring Cu(II) centers. The model leads to the following values, g (Landé factor) = 2.240, J (exchange coupling) = -321 cm^{-1} .



Interpretation in terms of Dielectric friction of the Abnormal Kohlrausch behavior of the Variation of the Equivalent Conductivity of PDDPX Polyelectrolytes with the Nature of the Counterions X⁻

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It is well known that according to Kohlrausch law, the equivalent conductivity Λ_{MX} of a simple electrolyte MX, is equal to the sum ($\lambda_M + \lambda_X$) of their ionic conductivities. In general, λ_M and λ_X decreases of the same order with the ionic force due to the electrophoretic and ionic friction processes.

As a consequence of this principle of additivity, for electrolytes MX with a common ion M and different counterions X, and for any given concentration C, Λ_{MX} increases (or decreases) when the ionic conductivity at infinite dilution λ_X° increases (or decreases) with the nature of the counterion X. (I.e. $\forall C$, $\Lambda_{MX} > \Lambda_{MX'}$ if $\lambda_X^\circ > \lambda_{X'}^\circ$).

This normal Kohlrausch behavior is generally also observed in the case of polyelectrolyte solutions despite the great complex interdependence between λ_p and λ_X [1].

However, for some polyelectrolytes PX like PDDPX, *poly(1,1-dimethyl-3,5-dimethylene piperidinium, X)*, experiments show an inversion in the Kohlrausch behavior (I.e. $\forall C$, $\Lambda_{PX} < \Lambda_{PX'}$ if $\lambda_X^\circ > \lambda_{X'}^\circ$).

Note that hydrodynamic, electrophoretic and ionic frictions on polyions cannot completely explain this abnormal behavior of the variation of the equivalent conductivity Λ_{PX} of some polyelectrolytes with the nature of their counter-ions X, which seems in complete contradiction with the usual Kohlrausch law. Moreover, the degree of condensation of the counterions X is practically independent on their nature.

In fact, this anomaly occurs for polyions having a stretched conformation for which the dielectric friction effect becomes very important [2, 3].

In this Poster, we represent the conformation of polyions by a chain of charged spheres. Each spherical group is surrounded by a dielectric medium characterized by a local permittivity ϵ which depends greatly on the nature of the counterions X. Calculations show that the dielectric friction and therefore the conductivity λ_p of the polyion are very sensitive to ϵ .

Keywords: stretched polyion; dielectric friction; conductivity; Kohlrausch law

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DFT AND EXPERIMENTAL STUDIES ON COPPER (II) AND IRON (II)-ADRIALYCIN INTERACTIONS.

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Adriamycin (ADR) is an anticancer agent that has been used successfully [1,2] in chemotherapy since 1963. Nevertheless, this molecule displays a cardiotoxicity as a side effect which is caused by the radical reactions in which the ADR molecule is involved [3].

Also, it has been reported also that the presence of Fe (III) and Cu (II) ions catalyzes the reaction of ADR with free radicals. This finding prompted researchers to investigate the interaction of these ions with ADR and its role in radical reactions[4,5]. The objective of the present work is to carry out a spectroscopic and thermodynamic study of

of Fe (III) and Cu (II) –ADR interactions. Distribution diagrams of different formed chemical species were plotted, stability constants of 1:1 and 1:2 complexes then the thermodynamic quantities (ΔH^0 , ΔS^0 , ΔG^0) were computed.

The solid state complexes were prepared in methanol solution under ultrasonic conditions at 20 kHz frequency, and characterized.

On the other hand, these ion-ADR interactions were investigated by molecular modeling studies using DFT / B3LYP / 6.311++g (d, p) and DFT / B3LYP / 6.311++g (d,p) Empirical Dispersion = GD3BJ (taking into account the Grimme dispersion).The obtained results were compared and discussed with respect to bonds lengths, angles and dihedrals.

The FTIR (DFT) and UV-vis spectra (TD-DFT) obtained theoretically are in good agreement with those obtained experimentally. Also, the TD-DFT allowed to acquire the description of the frontier orbitals properties namely the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO), and to compute the corresponding electronic properties such as: Energy Gap, hardness, electrophilicity etc...

The NBO analysis were carried out to elucidate intermolecular interactions between ADR molecules and metallic ions.

Keywords: Adriamycin, metallic ions, complexes, interaction, DFT,TD-DFT,NBO

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Elements investigation of Opuntia Ficus Indica using PIXE analysis

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Particle induced X-ray emission (PIXE) technique was used to determine various trace-element concentrations in two part of Opuntia Ficus Indica (OFI): cladode and seed planted in different regions of Tunisia. PIXE is non-destructive analytical method which relies on the spectrometry of characteristic X-rays emitted by the target elements due to the irradiation of a high energy ion beam (typically 1-2 MeV of H or He) [1]. PIXE has been successfully applied to solving problems in many different fields including the detection of elements in very low concentrations used in medicine drug, in medicinal plants and some others vegetables [2,3]. The objective of this study is to provide some informations of heavy and light elements concentrations between these two compartments. Opuntia cladode juice was extracted by a mechanically press system for each sample and lyophilized; the Opuntia mucilage was grinded in a blender until obtaining a fine powder. The seed of OFI were extracted from fruits, dried and grinded until fine powder. Borax powder was added to the OFI powder to prepare the pellet following by carbon pulverization and then analyzed by PIXE system. Eleven elements concentrations were measured in cladodes and seed of Opuntia Ficus Indica. Al, Fe, K and Cl are founded in high concentrations in all parts of OFI. It has shown that Ca, K and S have higher concentration comparing to others elements in the seed. Furthermore, the Ti, Mn, Br and Cu have lower concentration in cladodes than seed but still in feeble concentration. It's clear that the variation of concentrations of elements in the different samples of OFI depends on the soil, water and air pollution.

Key words: PIXE, trace elements, Opuntia Ficus Indica, seed, cladode.

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Synthesis, crystal structure, characterizations and magnetic study of a novel two-dimensional iron fluoride

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A new hybrid compound formulated as $[\text{Fe}_3\text{F}_8(\text{H}_2\text{O})_2](\text{Am}_2\text{TAZ})_2$ (Am_2TAZ = 3,5-diamino-1,2,4-triazole) was prepared under hydrothermal conditions. The crystal structure was solved by single-crystal X-ray diffraction and the bulk was characterized by thermal analyses (TG-MS), vibrational spectroscopy (FTIR, Raman), Ultraviolet-visible spectroscopy (UV-Vis), and scanning electron microscopy (SEM-EDX). It crystallizes in the triclinic system space group P 1. The studied X-ray crystal structure shows the two oxidation states for iron atoms (Fe^{2+} , Fe^{3+}) and generates a 2D inorganic network, built up of inorganic layers constructed from infinite inorganic chains running along aaxis. In fact, these chains are connected via $(\text{Fe}^{3+}(3)\text{F}_6)$ octahedral. OW-H...F and N-H...F hydrogen bonds, making up the whole 3D network, are strongly linked in the layers. Thermal analysis (TG, MS) of the title compound shows that the decomposition introduces three steps between 25–993 °C. IR and Raman spectroscopic studies confirm the presence of coordinating (Am_2TAZ) organic molecules. Magnetization measurements were performed, exhibiting the paramagnetic feature of the studied compound above 150 K.

Keywords: Fluoride, Iron, Hydrothermal synthesis, Thermal analysis, Vibrational spectroscopy, Magnetic.

Synthesis, crystal structure, and characterization of a new Bi(III) halide complex: $(\text{C}_6\text{H}_{16}\text{N}_2)_2[\text{BiCl}_6]\text{NO}_3$

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Bismuth complex chemistry has attracted significant interest not only because of the low cost and high abundance of bismuth resources on Earth, but also due to their practical applications in pharmaceuticals and medicine, catalysis, superconductors and semiconductors, etc. [1]. We report in the present work, the synthesis and the characterization of a new hexachlorobismuthate compound: $(\text{C}_6\text{H}_{16}\text{N}_2)_2[\text{BiCl}_6]\text{NO}_3$. Single-crystal X-ray diffraction analysis revealed that the complex crystallizes in the monoclinic system $C 2/c$ space group. Its crystal structure consists of protonated ethyl piperazine cations, $[\text{BiCl}_6]^{3-}$ and nitrate anions. These components are connected into a three-dimensional network via hydrogen bonds $\text{N}\cdots\text{H}\cdots\text{Cl}$, $\text{N}\cdots\text{H}\cdots\text{O}$, $\text{C}\cdots\text{H}\cdots\text{Cl}$, $\text{C}\cdots\text{H}\cdots\text{O}$ (**Figure 1**), the significant intermolecular interactions in the crystal structure are identified and analyzed using the Hirshfeld surface (**Figure 2**). This compound is also characterized by infrared spectroscopy, UV-Vis and antioxidant activity.

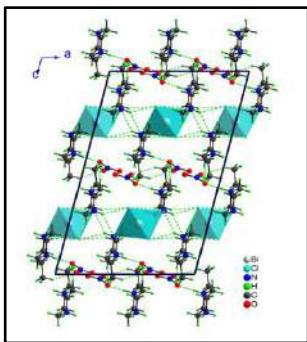


Figure 1: Projection along the b-axis of the atomic arrangement of $(\text{C}_6\text{H}_{16}\text{N}_2)_2[\text{BiCl}_6]\text{NO}_3$

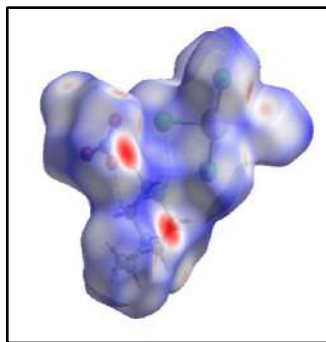


Figure 2: hirshfeld surface mapped over d_{norm} of $(\text{C}_6\text{H}_{16}\text{N}_2)_2[\text{BiCl}_6]\text{NO}_3$

Keywords: Hexachlorobismuthate; Crystal structure; Hirshfeld, Vibrational spectrum.

Reference:

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Synthesis and characterization of a plant-based inhibitor: Corrosion application of structural steel

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One of the major problems encountered in industry is the degradation of certain machinery parts under the effect of corrosion. The present manuscript focuses on the effect of addition of the rosemary extract and chimec 1839 and the effect of applying a nickel-based coating and a cobalt-based coating made under high energy beam on corrosion of XC38 steel in 3% NaCl medium. The stationary and non-stationary electrochemical methods constituted the tool for experimental realization of this research. The results we found confirm that the optimal concentration is 2% for the first inhibitor (inhibitor1) which gives good efficacy 84.93% and 0.05% with the second inhibitor (inhibitor 2) which gives an efficiency 89.64% and also showed that the nickel-based metal coating with high efficiency ($E = 98.12\%$), much better than that of cobalt-based metal coating ($E = 83.22\%$).

Key words: corrosion; XC38 steel; 3% NaCl; electrochemical methods; coating; Inhibitor.

Access to 9,10-diheteroarylated phenanthrenes via successive Pd-catalyzed direct hétéroarylations

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The reactivity of positions C9 and C10 of 9- or 10-bromophenanthrenes in palladium-catalyzed direct heteroarylations was investigated¹. A wide variety of heteroarenes such as thiazoles, (benzo)thiophenes, (benzo)furans, pyrroles, selenophenes or imidazopyridazines was successfully introduced at phenanthrene C9-position *via* palladium-catalyzed direct arylations, using 0.5-0.1 mol% of phosphine-free Pd(OAc)₂ catalyst. Then, C10-bromination of the 9-heteroarylated phenanthrenes, followed by a second palladium-catalyzed direct heteroarylation gives access to symmetrical and non-symmetrical 9,10-di(heteroaryl)phenanthrenes (Scheme 1).²

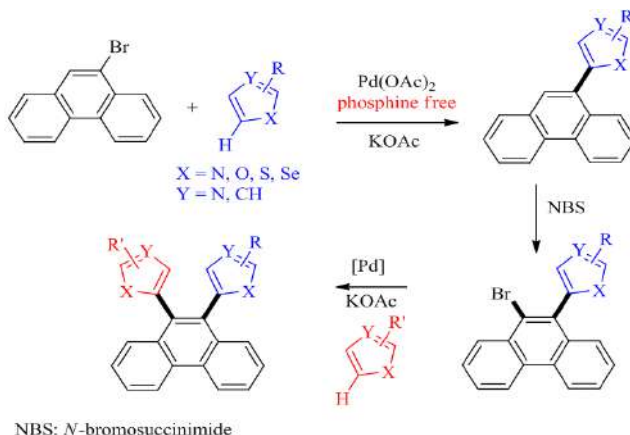


Fig. Access to 9,10-diheteroarylated phenanthrenes
via successive Pd-catalyzed direct heteroarylations

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Synthesis of Novel Biosourced Polytriazoles by CuAAC for the Pollutants Extraction from Wastewater

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Since two decades ago, a considerable attention has been given to the use of natural resources instead of the fossil fuels. Among the important biosourced precursors, the dianhydrohexitols (DAH) that obtained industrially from sugar have been the subject of several works over the years.^[1] In polymer science these attractive diols have been used in the synthesis of various materials such as polyesters,^[2] polyethersulfones,^[3] poly(ether ketone)s,^[4] polyamides^[5]

In this work, we describe the synthesis of novel polytriazoles by copper(I)-catalyzed alkyne-azide cycloaddition (CuAAC) of several DAH-diazides with dialkynes monomers. The backbone structures of the obtained polymers should have interesting properties especially for pollutants extraction from wastewater.

Moreover, the non-covalent interactions can take place between the triazole units and polar molecules based pollutants (polyphenols, pesticides...) which make these polytriazoles a powerful tool for the reversible pollutants and metals adsorption from wastewater and sediment.

Key words: Dianhydrohexitols, CuAAC, polytriazoles, reversible adsorption

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Removal of heavy divalent metal ion using a novel synthetic bis(2-pyridylmethyl)amino-chloroacetyl chloride- ethylenediamine-grafted GO sheets combined with magnetic nanoparticles.

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In this research, the functionalization of graphene oxide sheets by ethylenediamine (EDA) was accomplished followed by the grafting of bis(2-pyridylmethyl)amino group (BPEN) onto the activated graphene oxide sheets in the presence of chloroacetyl chloride (CAC) when combined with magnetic nanoparticles ($\text{Fe}_3\text{O}_4\text{NPs}$) to produce a magnetic graphene-based composite $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$. The physic-chemical properties of $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ composites were investigated by Fourier transform infrared (FT-IR) Vibrating sample magnetometer (VSM), Scanning electron microscopy (SEM), X-ray diffraction (XRD), Thermogravimetric analysis (TGA). $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ was of a narrow size distribution, and exhibited ferromagnetic behaviors with saturation magnetization 24.63 emu.g^{-1} . Additionally, the catalysts can be easily recycled within ten seconds by using an external magnetic field (Fig.1). Moreover, $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ was used for removing Cu(II) ions from aqueous solutions using a batch process. The effect of pH, contact time and temperature were investigated, however weakly dependent on ionic strength. The chemical adsorption involving the strong surface complexation of metal ions with the nitrogen and oxygen containing groups on the surface of graphene oxide (Fig.2). The maximum adsorption capacity values of Cu(II) on the $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ at the pH of 6 is 3.46 mmol.g^{-1} . To examine the underlying mechanism of the adsorption process, pseudo-first, pseudo-second-order and intraparticle diffusion models were fitted to experimental kinetic data. Results showed that the pseudo-second-order equation was appropriate to describe the Cu (II) adsorption by $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$. Adsorption data were further analyzed by the Langmuir, Freundlich and Jossens adsorption approaches (Fig.3). Additionally, the adsorption properties of the $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$, their reusability (more than 10 cycles) and durability in the aqueous solutions open the path to removal of Cu(II) from water solution. Based on the results obtained, we conclude that $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ can be an effective and potential adsorbent for removing Cu(II) ions from an aqueous solution.

Keywords: Graphene, bis(2-pyridylmethyl)amino, magnetic nanoparticles, adsorption kinetics, isotherms.



Figure.1

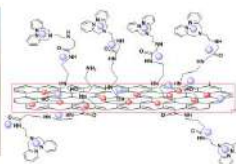


Figure.2

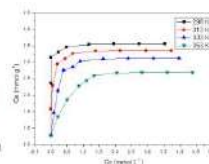


Figure.3

Fig.1 Illustration of the interaction between $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ and Cu(II).

Fig.2 Digital images of aqueous suspensions ($c=0.35 \text{ mg/mL}$) of (A) GO-EDA (B) GO-EDA-CAC and (C) $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$.

Fig. 3 Effects of temperature on the maximum adsorption capacity (q_m) of the $[(\text{Go-EDA-CAC})@ \text{Fe}_3\text{O}_4\text{NPs-BPEN}]$ for adsorption of studied metal ions.

Removal of organic micropollutants from water by a new Glux-based polymers

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Recently, numerous approaches have been studied for the development of adsorbents containing natural polymers. Among these polysaccharides, starch and their derivatives deserve particular attention.

These by-products of biomass represent an interesting and attractive alternative as adsorbents because of their particular structure, chemical stability, physico-chemical characteristics, high reactivity and excellent selectivity towards aromatic compounds and metals. All these characteristics are due to the presence of chemical reactive groups (hydroxyl, acetamido or amino functions) in polymer chains.

We currently investigated the use of 2,4:3,5-di-O-methylene-D-glucitol or Glux, for the synthesis of various polymers (polyether PE-Glux and Polyester PEs-Glux). This bio-based diol is a bicyclic diacetalized that may be prepared from available 1,5-D-gluconolactone by acetalization and subsequent reduction.

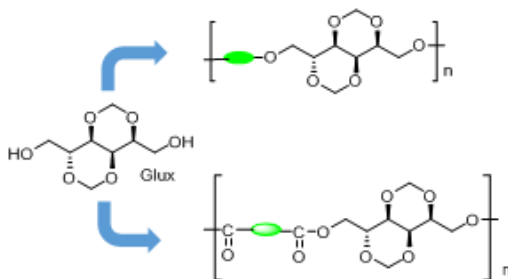


Figure 1: Chemical structures of PE and PEs based on Glux

In order to extend the potential application field of the sorption properties of bio-based polymers, we evaluated the uptake behavior of our new polymeric adsorbent phase based on Glux in aqueous media for several organic micropollutants (polyphenols and pesticides) of different polarity.

The analysis of the targeted polar pollutants was successfully carried out by high performance liquid chromatography analysis meanwhile gas chromatography was used for the detection of the non polar pollutants. Polar and non polar pollutants demonstrate a good adsorption for PE-Glux, (80-100% of the adsorbed quantity reached after one hour of contact) whereas a low adsorption capacity was noticed for PEs-Glux.

Chemical composition and anticancer activities of *Eucalyptus* leaves extracted by Supercritical CO₂

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Recently, research upon natural products such as aromatic and medicinal plants has concentrated on two primary areas: identification of their biological activity (such as cytotoxic activity) and development of novel extraction methods insuring better quality, cleaner and less energy-intensive operation. In the present study, the *Eucalyptus diversifolia* will be investigated in respect to both these aspects.

Extracts were obtained by supercritical CO₂ from *Eucalyptus diversifolia* originating from southern of Tunisia and analyzed by GC-FID and GC-MS. Among 60 compounds identified in these extracts, the main were butylated hydroxytoluene (40 %), alpha-cadinol (6 %), 8-cedren-13-ol (4%) and umbelliferone (2.1%).

Extracts were evaluated for their cytotoxic activities against three cancer cell lines: human colon cancer line (HCT-116), breast cancer cell line (MCF-7) and ovary cell line (AA8). The strongest cytotoxic activity against HCT-116 cells, was obtained for the ethanol extract (IC₅₀ = 3 mg/l). Moreover, the best cytotoxic activity against MCF-7 cells was obtained for extract at 120 bar (IC₅₀ = 30 mg/l). However, leaves showed moderate inhibitory activities against AA8 cells.

These important biological activities showed that extract obtained from *Eucalyptus diversifolia* by Supercritical CO₂ could be a potential source of the active molecules intended for applications in pharmaceutical industry.

Key words: *Eucalyptus*, extract, supercritical CO₂, cytotoxic.

Copper Mediated Acetoxylation with Diaryliodonium Salts

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The acetoxy group acts as a functional group modifier while imparting polar nature to a molecule. It is ubiquitous in a plethora of prodrugs, natural products, antimicrobial agents, and herbicidal materials. [1]

Newer methods of regiospecifically introducing this group in organic molecules continues therefore to be of relevance.

In this work we present a new method of copper mediated aryl acetoxylation under mild conditions with the diaryliodonium salts as aryl source for the first time.

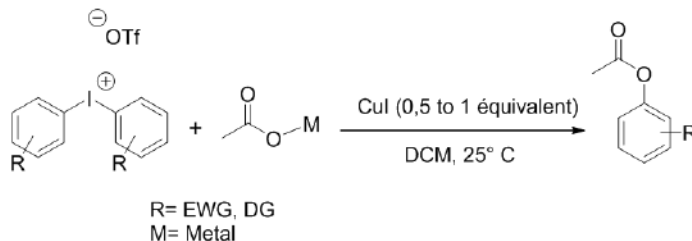


Figure1: general procedure aryl acetoxylation

Keywords: Copper, diaryliodonium, acetoxylation

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Synthesis and characterization of nanostructured composite materials with metallic matrices

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Depending on the nature of their matrix we can classify composite materials. In this study, the focus is on aluminum matrix composites, which are the most widely used and marketed by virtue of their favorable price, ease of production and mechanical properties.

Since the size of the grain is inversely proportional to the mechanical strength, the reinforcements used in the present work were nanoscale powders (Al-Co-Nb) produced by mechanical milling using a planetary mill (P7) and the matrix was also a powder of a Al-Si alloy (Hermillon powder). High energy mechanical milling has reduced the particle size of the reinforced powders and consequently reduce the amount of pores in the sintered composites. After having optimized the consolidation conditions, the whole (reinforcement powder + matrix powder) were mixed for 2 hours in the Turbula WAB (Willy A. Bachofen Maschinenfabrik). Then they were compacting in a cylindrical graphite mold by hot pressing.

The relative density of the composite material was measured using the Archimedes principle, its value is close to 1. And the hardness (HV) of the new composite is twice that of matrix.

Keywords: Mechanical alloying, Sintring, Composite material, Mechanical properties.

Biodiesel from *P. lentiscus* seed oil (PLO)

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Pistacia lentiscus L., an evergreen shrub of the family Anacardiaceae, can reach 3 m in height, grows wild in arid areas and is characteristic of Mediterranean countries [1]. In this work, *P. lentiscus* seed oil (PLO) was evaluated for the first time as a potential biodiesel feedstock, which contains 19 % oil (w/w) whereas the acidity of the oil was 10%. PLO has a high content of linoleic acid (50.82%) followed by oleic acid (19.74%), and palmitic acid (10.5%).

In this context, a high content of non-edible by product from *P. lentiscus* seed oil was chosen as the test oil for production of fatty acid methyl ester (FAME) or known as biodiesel. Biodiesel can be derived from vegetable oils or animal fats by simple transesterification and esterification processes [2], the most important factors for choosing the technology to be employed for biodiesel production is quality of the oil; consisting with different amount of free fatty acid (FFA), moisture and saturation level of vegetable oils and animal fats. There are two main types of catalysts which were normally used in the biodiesel production process; homogeneous and heterogeneous catalyst. Homogeneous catalyst is the catalyst that has the same phase with the reactant or the sample feedstock. Meanwhile, the heterogeneous catalyst is the catalyst which has a different phase from the reactants [3]. *P. lentiscus* methyl esters (PLME) were prepared by an acid-catalyzed esterification reaction. The maximum yield of FAME was about 98, 95% in about 60min for the molar ratio of 18:1.

A sequence of experiments were carried out in order to assess the influence of reaction parameters as follows: catalyst concentration (1.5–3.0 wt %), reaction time (0.5–5 h), methanol to oil molar ratio (9:1–18:1) and reaction temperature (75–150 °C) for methyl ester production. Structural, physicochemical, thermal, and morphological properties of the synthesized catalysts were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), ammonia temperature programmed desorption (NH₃-TPD), thermogravimetric analysis (TGA), and transmission electron microscopy (TEM).

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Tyrosinase Biosensor Used for the Determination of phenolic content in olive oil (*Olea europaea* L. cv. Chemlali Sfax)

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Olive oil is one of the richest antioxidant oils, containing more particularly phenols such as hydroxytyrosol, tyrosol and secoiridoides as oleuropein. It's well-known that the treatment of olive pastes can influence properties and antioxidant composition of oil. In this study, the global phenolic content of local virgin olive oils resulting from different treatments has been monitored using an amperometric biosensor based on tyrosinase. This enzyme was immobilized in a polyvinyl alcohol matrix on a carbon screen-printed electrode modified with cobalt-phtalocyanide (CoPC) as mediator. Under optimized conditions, the chronoamperometric response of different oil extracts has been evaluated and expressed as equivalent tyrosol content. The developed biosensor exhibits sensitive bioelectrocatalytic response at a working potential of -0.05 V vs. pseudo Ag/AgCl reference allowing the comparison of different treatments and the selection of the best one for further investigations.

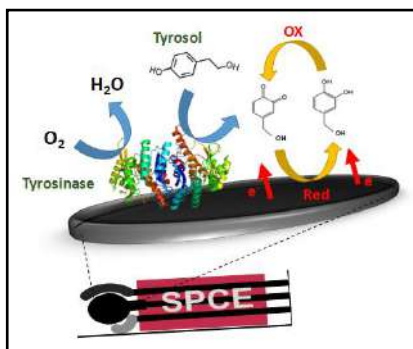


Fig. Principle of the tyrosinase-based biosensor

Key words: olive oil, phenol content, tyrosinase, amperometric biosensor

Synthesis of molecularly imprinted polymer – Mn-doped ZnS quantum dots QDs for fluorescent screening of aflatoxins in non-dairy beverages

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Aflatoxins (AFs) are a class of structure related mycotoxins produced as secondary metabolites by fungi belonging to several *Aspergillus* species, particularly *Aspergillus flavus* and *Aspergillus parasiticus* [1]. Currently, there are over 18 aflatoxins identified, the most famous being AFB1, AFB2, AFG1 and AFG2 [2]. Among AFs, AFB1 is considered the most toxic [3], and has therefore been classified as a group I human carcinogen by the IARC [4]. Thus, control of these substances is necessary. Molecularly imprinted polymers (MIPs) can be useful tools for screening of AFs in complex samples as the foodstuff.

Therefore, Synthesized molecularly imprinted polymer (MIP) materials have been anchored on the surface of PEG-Mn-doped ZnS quantum dots (QDs) to develop a fluorescence probe for aflatoxins (AFs) recognition/determination in non-dairy beverages (milk substitutes), mainly prepared from almonds, soy, and other nuts. MIP synthesis used 5,7-dimethoxycoumarin (DMC) as a dummy template, and methacrylic acid (MAA) as a functional monomer. Under optimized conditions (1.25 mL of 5 mg L⁻¹ MIP-PEG-ZnS QDs solution, pH 6.0, and 12 min delay time before scanning), the prepared MIP-QDs composite was found to offer high affinity and selectivity for AFs (AFB1, AFB2, AFG1 and AFG2). A fast fluorimetric screening method (total AFs assessment) was therefore feasible. The limits of detection (LOD) and quantification (LOQ) were 0.016 and 0.053 mg L⁻¹, respectively. Analytical recoveries (inter- and intra-day assays) were from 99±4% to 107±5%, with RSD (intra-day assay) lower than 13, and RSD (inter-day) lower than 7%. The optimized method was applied for total AFs assessment in several non-dairy beverage samples.

Keywords: Aflatoxins, quantum dots, molecularly imprinted polymer, fluorescence probe, non-dairy beverages.

Reference:

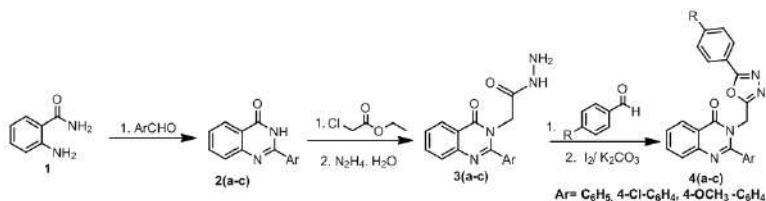
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Design and synthesis of novel hybrid compounds incorporating pyrimidinone and 1,3,4-oxadiazole moieties

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Heterocyclic compounds have drawn special attention in organic chemistry because of their abundance in natural products and their diverse biological properties.¹ On the other hand, oxadiazole and its derivatives have been recognized as important heterocyclic compounds due to their biological activities such as anticancer,² antitubercular,³ anti-inflammatory⁴ and analgesic.⁵ Keeping in view the above, we wish to report herein the synthesis of some new hybrid compounds **4** combining the pyrimidinone and 1,3,4-oxadiazole rings, in three steps, starting from the 2-amino-benzamide **1** (Scheme 1). The structures of the prepared products were confirmed by spectroscopic means.



Scheme 1

Keywords: 2-amino-benzamide, pyrimidinone, 1,3,4-oxadiazole

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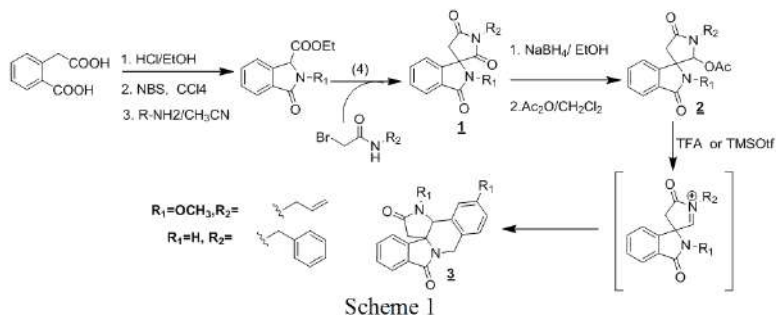
Access to novel polycyclic systems fused isoindole via *N*-Acyliminium ion aromatic cyclization

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Isoindolinone and C3 isoindolinone-derived heterocycles [1] are prevalent structural motifs in numerous synthetic and natural products, which exhibit important biological activities. Many of them have been prepared and examined as antihypertensive [2], antipsychotic [3] and antiinflammatory agents [4]. We report herein a novel approach to diversely spirocyclic isoindoles **3** has been developed by using *N*-acyliminium. Spirocyclization precursors and π -cationic cyclization have been obtained by a regioselective reduction of the spiro-imide compounds **1**, followed by the aromatic cyclisation of the *N*-acyliminium intermediates (generated from the acetoxylactam compounds **2**) (Scheme 1).



Keywords: *N*-Acyliminium, spiro-imide, regioselective reduction

References:

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Influence of lewis acid catalysts on structural of lignins

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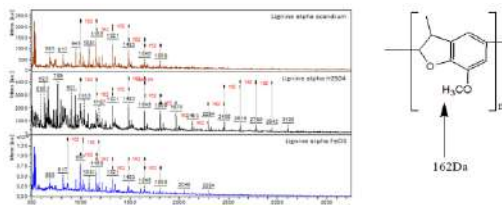
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After cellulose, lignin is the second macromolecular structure present in plants. It is a crosslinked in situ polymer having a very complex structure that varies more depending on the plant species, the age of the plant, the prevailing climatic conditions, etc. According to the structure proposed by Freudenberg, the phenylpropane unit of lignin are interconnected by a variety of carbon-carbon bonds and ether¹. In this context that this characterization and use of lignin as a main source of aromatic nuclei.

The aim of this work is to evaluate the effect of the catalyst on the lignin structure of alpha. Lewis acids have been used in the first time at. 2012 as catalyst in the fractionation of lignin wheat straw². In this regard, the lignin studied have been extracted from the plant of alpha by an organosolv method, this method comprises to use water and ethanol ratio of 65/35 as the solvent and sulfuric acid, iron trichloride and scandium triflate as a catalyst.

Several techniques (FTIR, SEC, MALDI -TOF and NMR) were used to establish a general structure of the alpha lignin and show the various reactive functions that it possessed and the impact of its structure on catalysis.

Molecular weight distributions of lignins were analysed by SEC. The average molecular masses of the lignin were in the range 4000-12000 g mol⁻¹ which is higher than masses, found in other organosolv lignins³. The lowest masses were observed from treatment with scandium triflate but the higher masses with sulfuric acids, we can compare the impact of acid on the masses of lignin. Scandium triflate □ iron chloride(III) □ sulfuric acid. Indeed, the hardest acid can reduce the size of polymer lignin. This observation is in agreement with result by MALDI-TOF method. The MALDI-TOF Spectrum shows that the alfa lignin extracted with 3 different catalysts has some structural similarity. For the sample prepared with the H₂SO₄, the masses are detected up to 3100 Da, in contrast to samples prepared with acids Sc(OTf)₃ and FeCl₃ detected weights of less than 2100 Da. As presented in these spectra, treatment with the latter two acids can reduce the size of the polymer lignin Alpha compared to treatment with acid H₂SO₄. A High mass about 1000 Da, we notice the repetitions of a pattern mass of 162 Da which could have been the following structure based on the work of Banoub and all⁴.



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⁴ J. Banoub, B. Benjelloun-Mlayeh, F. Ziarelli, N. Joly, Elucidation of the complex molecular structure of wheat straw lignin polymer by atmospheric pressure photoionization quadrupole time-of-flight tandem mass spectrometry, Rapid Commun. Mass Spectrom. 2007 ; 21: 2867–2888.

SYNTHESIS OF NEW 4-ARYLAMINO-7-PHENYLPYRIMIDO[4,5-d]PYRIMIDINE

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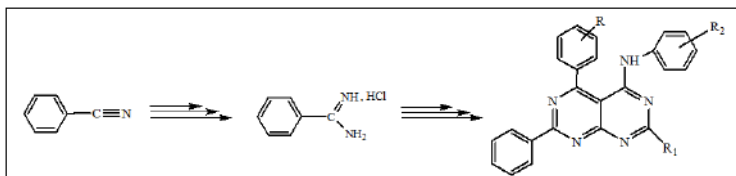
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In the present work, it is proposed to describe the synthesis of 2-alkyl-4-arylamino-5-aryl-7-phenylpyrimido[4,5-d]pyrimidine via several steps.

In the first, the benzonitrile is converted to benzamidinehydrochloride. After that, the reactivity of this product with different arylidene offered the 4-amino-5-cyanopyrimidine derivatives. Then, the action of these compounds with different orthoester via irradiation with microwave (MWI) (45 min, 110 °C, 300 W) gives the imidate correspondent.

Finally, we transformed these imitates into new heterocyclic compounds via treatment with the derivatives of anilines.



All the structures obtained are identified and characterized by ¹H NMR spectroscopic techniques, ¹³C NMR and FTIR.

Key words: Benzamidine hydrochloride, Imidate, Microwave irradiation

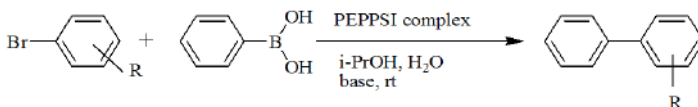
New Sterically Bulky NHC Pd(PEPSSI) Complexes Catalyzed Suzuki- Miyaura Cross-Coupling Reactions in aqueous medium

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Palladium-catalyzed cross-coupling reactions are a popular method of forming C–C bonds and have become a standard synthetic assembly tool in organic and organometallic chemistry.[1] Among these, the Suzuki–Miyaura reaction represents a preferred methodology. In an effort to reduce the generation of hazardous substances, variations of the Suzuki–Miyaura cross-couplings have been developed using *green* solvents,[2] particularly water.[3] These variations are especially attractive as water is nontoxic, non-flammable, inexpensive, and can be easily separated from organic products. In this study, we have been synthesized a new series of air and moisture-stable N-heterocyclic carbene precursors and their Palladium (II)-pyridine (PEPSSI) complexes. With the development of a more efficient catalytic system for the cross-coupling of aryl halides in mind, the catalytic performance of the NHC-PdCl₂-pyridine complexes for Suzuki cross-coupling under mild conditions in green solvents at room temperature was investigated.



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

Keywords: Suzuki cross-coupling reaction, N-heterocyclic carbene –Pd complex

References:

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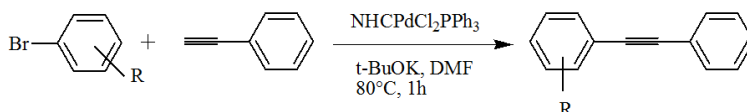
Sonogashira Coupling Reaction catalyzed by benzyladamantyl substituted N-Heterocyclic carbene-Pd(II)-PPh₃ complex

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The Sonogashira cross-coupling reaction is one of the most straightforward methods for the production of internal alkynes and enynes.[1–3] This cross-coupling reaction is definitely a fast-growing research field with enormous academic and industrial interest due to extensive use of products in the synthesis of pharmaceuticals, natural products, biologically active molecules and conducting polymers and in nonlinear optics and liquid crystal materials.[4–8] In this work we used new NHC-Pd-PPh₃ complexes and various aryl bromides were coupled with alkynes to afford sonogashira products in DMF at 100°C.



Sonogashira coupling reaction of phenylacetylene with different aryl halides catalyzed by NHC-Pd-PPh₃ Complexes

Keywords: Sonogashira coupling reaction, NHC-Pd-PPh₃.

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Investigations on a new Copper(II) complex: Structure, thermal behavior and Magnetic Properties.

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A new binuclear Copper(II) compound with mono-atomic bridging ligands has been synthesized. The crystal structure, thermal behavior and magnetic susceptibility of the complex are reported. The complex crystallizes in the triclinic space group $P\bar{1}$ with two molecules in the unit cell. The inorganic layer, built up by independent anionic binuclear moiety is connected to the organic layers through hydrogen bonding to build a three-dimensional network. Thermal analysis shows endothermic phenomena that may mark interesting structural phase transitions. The magnetic susceptibility data (1.8-300 K) show a maximum in χ near 8 K with a significant decrease in susceptibility at lower temperatures.

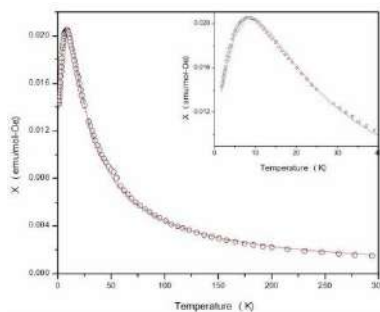


Fig: Susceptibility data for the Copper(II) compound.

Key words: Crystal structure, intermolecular interactions, thermal behavior, Magnetic susceptibility.

STRUCTURAL, ELECTRIC MODULUS AND COMPLEX IMPEDANCE ANALYSIS OF Zn DOPED TiO₂ NANOPARTICLES

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Zn doped TiO₂ nano-powder is prepared by sol-gel technique at 500°C. The samples are characterized by SEM, XRD, UV-VIS, FTIR, and dielectrical measurements. The X-ray diffraction results reveal the formation of polycrystalline secondary phases referred to hexagonal anatase-rutile. The complex modulus (M) and electric impedance of the samples are investigated by broadband dielectric spectroscopy in frequency range from 40 Hz to 1 MHz and temperature from 400K to 600K. The Nyquist plots (M', M'') illustrate the presence of non-Debye relaxations attributed to the effects of interfacial and dipolar polarizations. The real and imaginary parts of the impedance are well fitted to equivalent circuit models. From the obtained results, we can conclude that the electrical properties are sensitively Zn doping dependent.

Keywords: Impedance spectroscopy, modulus, titanium oxide, XRD.

A PRACTICAL SYNTHESIS OF NEW 2-BENZYLAMINO-8-METHOXY-4H-CHROMEN-3-CARBONITRILE DERIVATIVES

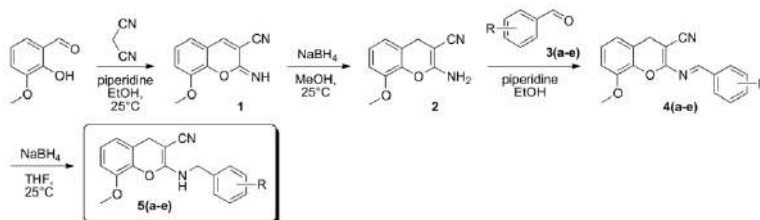
Marwa DHIABI^a, Ali BOUATTOUT^a, Mehdi FAKHFAKH^a, Souhir ABID^{a,b},
Ludovic PAQUIN^c, Jean-Pierre BAZUREAU^c and Houcine AMMAR^a

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Since the two last decades, the interest for 4H-chromenes and their derivatives increased because in this family of compounds are components of natural products which were subjected to structural modifications for potential medicinal properties.



In this context we report here a practical and efficient four steps synthesis of new 2-benzylamino-8-methoxy-4H-chromen-3-carbonitrile derivatives **5(a-e)** in good overall yields (55-81%) using the starting 3-cyano-8-methoxy-iminocoumarine **1** which was prepared by cyclocondensation from malonodinitrile and 3-methoxy-2-hydroxy benzaldehyde. Then, the building block **1** was easily reduced by NaBH₄ and afforded the corresponding 2-amino-3-cyano-8-methoxy-4H-chromene **2** (A. Bouattout et al., *Arkivoc* **2017**, iv, 291-302; *Synthesis* **2017**, 49, 3768-3774). Introduction of molecular diversity was possible on the amino function of **2** by reductive amination by using various aromatic aldehydes. This involved condensation of **2** with aldehydes **3(a-e)** and produced the desired 2-benzylidene amino-8-methoxy-4H-chromen-3-carbonitrile derivatives **4(a-e)** followed by reduction of the imino function in the presence of NaBH₄ in THF solution. For this communication, we shall detail the complete synthesis.

Keywords: 3-cyano-8-méthoxy-iminocoumarine, 2-amino-3-cyano-8-methoxy-4H-chromen

Structural, Physico Chemical Studies and Biological Analyses of a Cadmium Cluster Complex

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The decachlorocadmate (II) cluster templated with homopiperazinium cations ($(C_5H_{14}N_2)_2[Cd_3Cl_{10}].4H_2O$), has been grown using the slow evaporation method and characterized by X-ray diffraction, FTIR, Raman, ^1H and ^{13}C -NMR spectroscopies. Thermal investigations have also been made for the title compound. The X-ray structural analysis has elucidated the different inter-contacts in the crystal structure between the $[Cd_3Cl_{10}]^{4-}$ clusters, the water molecules and homopiperazinium entities stabilizing the 3D-supramolecular structure (Figure 1). The thermal investigations revealed a double dehydration phenomenon at around 96 and 125°C. The TG curve shows that the compound is stable up to the decomposition temperature of around 317°C (Figure 2). The title compound has been tested for its in vitro antioxidant and antibacterial activities. The 1,1-diphenyl-2-picrylhydrazil (DPPH) and 2,2'-azinobis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) tests have shown that the title complex is characterized by a significant antioxidant activity when compared to ascorbic acid and that it is active against all the tested bacteria. Nevertheless, bacteria sensitivity depends on the bacterial membrane structure. Indeed gram-negative bacteria are more sensitive to the compound tested than the gram-positive ones.

Keywords: decachlorocadmate, crystal structure, thermal investigation, antioxidant activity, antibacterial activity.

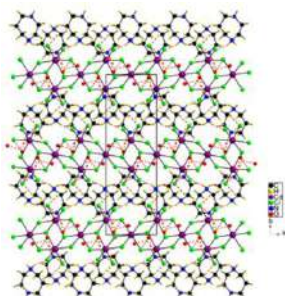


Fig. 1: Projection of the structure of $(C_5H_{14}N_2)_2[Cd_3Cl_{10}].4H_2O$ in (a) and (b) plan

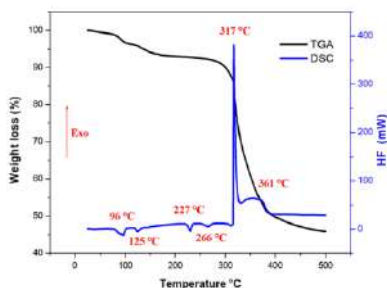


Fig. 2: TGA and DSC curves of $(C_5H_{14}N_2)_2[Cd_3Cl_{10}].4H_2O$ between room temperature and 500°C

A 3D supramolecular architecture built from an Organic–Inorganic Hybrid Arsenotungstates: Synthesis, Characterization

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A new polyoxometallate $(C_7H_{11}N_2)_7 [As^V Sb^{III} As^{III} W_{10} O_{39}] \cdot 4H_2O$ (**1**) have been isolated by conventional solution method and characterized by single-crystal diffraction, IR, UV–visible spectroscopies, Thermogravimetric analysis and cyclic voltammetry.

This compound crystallizes in the monoclinic space group $P2(1)/n$, with cell parameters: $a=11.5548$, $b=30.3707$, $c=22.2552$, $V=7787.35$, $Z=4$, $\beta=94.3650$. Crystal structure of this compound is built up of anions $[As^V Sb^{III} As^{III} W_{10} O_{39}]^{7-}$ clusters, protonated $[C_7H_{11}N_2]^+$, $[C_7H_{11}N_2]^{2+}$, and water molecules. In $[As^V Sb^{III} As^{III} W_{10} O_{39}]^{7-}$. Clusters are linked to each other's by organic cations by hydrogen bond interactions between N atoms of the organic molecules and the O atoms of the polyanions as well as between the O atoms of the water molecules and N atoms of organic cations. They hydrogen bonds play an important role in the stabilization of the three-dimensional supramolecular network.

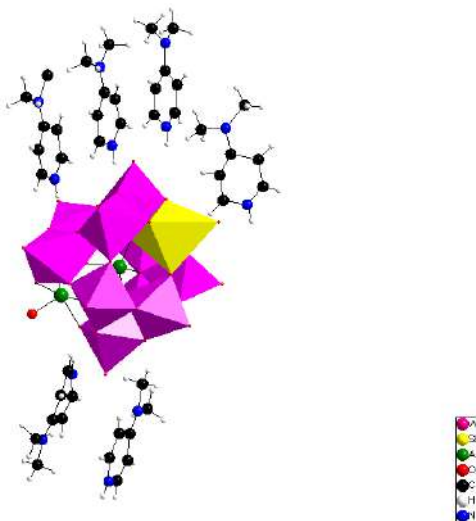


Figure: unit cell of compound 1

Linear model for the prediction of boiling temperatures of different classes of solvents

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A Quantitative Structure-Property Study (QSPR) was applied for modeling and predicting the boiling temperatures of different solvent classes, using multiple linear regression (MLR).

The multiple linear regression approach was applied on a mixture of different classes of solvents. The studied compounds were separated using the CADEX algorithm into 2 subsets: one set for calibration and the other for the model test.

The linear model of 5 descriptors was obtained by maximizing the difference $K_{xy}-K_{xx}$ and having the least outliers compared to other models with sizes between 2 and 10 (descriptors).

The robustness and predictive capacity of the models were verified using the internal validation statistics parameters (cross validation Q^2_{LOO} and Q^2_{LMO}) and the external validation Q^2_{ext} .

Key Words: Solvents - Quantitative Structure Property Relationship - Multiple Linear Regression.

Synthesis, crystal structure of $K_3Na((Mo_{1.33}Cr_{0.67})O_4)_2$ adopting glaserite structure-type

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A new rare Cr^{6+} compound of $K_3Na((Mo_{1.33}Cr_{0.67})O_4)_2$ formulation was prepared by form melt and characterized by single-crystal X-ray and qualitative energy dispersive X-ray spectroscopy (EDS) analysis. It crystallizes in the trigonal system space group P-3 and its unit cell has the following parameters: $a = 5.9600(5)$ Å, $c = 7.5224(9)$ Å, $V = 231.41(6)$ Å³, $Z = 1$. The $R1$ [$I > 2s(I)$] and $wR2$ (all data) values are 0.034 and 0.084, respectively, for all 344 independent reflections. $K_3Na((Mo_{1.33}Cr_{0.67})O_4)_2$ can be considered as a new member of the glaserite family. The mixed 2D framework of this structure is built of (Mo/Cr)O₄ tetrahedra sharing corners with NaO₆ octahedra. This arrangement allows the appearance of additional cationic positions X and Y which characterize the structures of glaserite type. The Mo^{6+} and Cr^{6+} cations are located at the same general site with occupancies of 0.67 and 0.37 respectively. O1 atom is split into two separate positions O11 and O12 with occupancies of 0.275 and 0.725 respectively. The proposed structure model is supported by bond-valence-sum BVS and charge-distribution CHARDI methods.

Key words: X-ray diffraction; Bond valence analysis; Structure; Charge Distribution

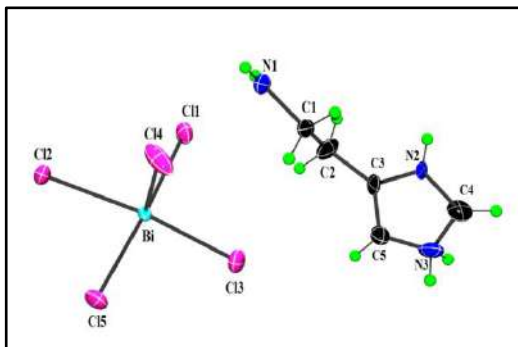
Crystal Structure, Hirshfeld Surface and Spectroscopic Studies of a new Bi (III) complex (C₅H₁₁N₃) BiCl₅

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Single crystals of a novel bismuth complex (C₅H₁₁N₃) BiCl₅ were synthesized and characterized by X-ray diffraction at room temperature. This compound crystallizes in the non-centrosymmetric space group P2₂1₂ of the orthorhombic system with the unit cell parameters: *a*=7.758(4), *b*= 12.275(7), *c*= 13.949(9) Å, *V*=1682.4(15) Å³ and *Z* = 4. The crystal structure consists of one-dimensional [Bi₂Cl₅]⁻²ⁿ polyanionic zig-zag chains and histaminium dications. The crystal packing is governed by the formation of a number of N–H...Cl hydrogen bonds arranged in a three dimensional network. Crystal structure analysis was supported with the Hirshfeld surface and fingerprint plots enabled the identification of the significant intermolecular interactions. This material was characterized too by IR spectroscopy, UV–Vis spectrum, photoluminescence and thermal analysis.

Key words: Bi(III) complex; Crystal structure; X-ray diffraction; Optical properties.



ORTEP drawing of (C₅H₁₁N₃) BiCl₅

A Hirshfeld surface analysis, crystal structure and spectroscopic properties of new Cd(II) complex with 1-(3,4-dichlorophenyl)piperazine ligand

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A new organic-inorganic hybrid material, [1-(3,4-dichlorophenyl)piperazine-1,4-diium] tetrachloridocadmate (II) hydrate, (C₁₀H₁₄N₂Cl₂)[CdCl₄].H₂O, has been synthesized and characterized by various physicochemical techniques including Infra-Red (IR) and NMR spectroscopy. The compound crystallizes in the triclinic system and $P\bar{1}$ space group with $Z = 2$ and the following unit cell dimensions: $a = 7.4350$ (2), $b = 8.1737$ (2), $c = 14.8057$ (3) Å, $\alpha = 87.0320$ (14), $\beta = 89.4100$ (12), $\gamma = 83.0150$ (13)° and $V = 891.88$ (4) Å³.

In this structure, the Cd²⁺ ion, surrounded by four chlorides, adopts a distorted tetrahedral coordination geometry. The structure of this compound consists of 1-(3,4-dichlorophenyl)piperazine-1,4-diium dications, [CdCl₄]²⁻ anions and water molecules. These entities are interconnected by means of hydrogen bonding contacts [N-H...Cl, N-H...O, O-H...Cl and C-H...Cl], forming a three-dimensional network. Intermolecular interactions were investigated by Hirshfeld surfaces. More than three quarters of the interaction surface in the crystal packing is constituted by attractive and favored H...Cl hydrogen bonds. The ¹³C and ¹⁵N CP-MAS NMR spectra are discussed and the vibrational absorption bands were identified by infrared spectroscopy.

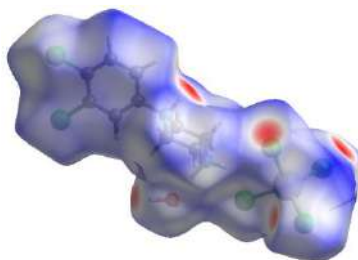


Fig. Hirshfeld surfaces mapped around the asymmetric unit for the compound (C₁₀H₁₄N₂Cl₂)[CdCl₄].H₂O with d_{norm} , the surface is shown as transparent to allow visualization of the orientation of subgroups of the asymmetric unit.

Key words: Cd(II) complex; X-ray diffraction; NMR spectroscopy, IR spectroscopy, Hirshfeld surface analysis, Coordination compound.

Synthesis, crystal structure and physico-chemical characterization of Bis(2-methoxybenzylammonium) diaqua bis(dihydrogen diphosphato)-cobaltate(II) dehydrate

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As a part of our interest in diphosphate materials, we report here the preparation and the structural study of the title compound, $(C_8H_{12}NO)_2[Co(H_2P_2O_7)_2(H_2O)_2] \cdot 2H_2O$, (I). The asymmetric unit of (I) consists of a Co(II) atom, one $H_2P_2O_7^{2-}$ anion, one organic cation and two water molecules (one coordinating to Co(II) and the other a lattice water molecule). The Co(II) ion lies on an inversion centre, hence the complete formula unit is generated by this element of symmetry (Fig. 1). The crystal structure of (I) it is built up from centrosymmetric $[Co(H_2P_2O_7)_2(H_2O)_2]^{2-}$ complex anions arranged in layers parallel to (100). These layers are interconnected by a set of $O-H \cdots O$ and $N-H \cdots O$ hydrogen bonds between the components.

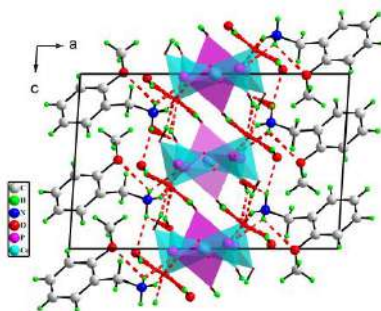


Figure.1: Perspective view of the crystal packing of (I) in a projection along the b-axis.

Electrical properties, phase transitions and conduction mechanisms of $\text{Ti}_{1.90}\text{Rb}_{0.10}(\text{SO}_4)_{0.92}(\text{SeO}_4)_{0.08}\cdot\text{Te}(\text{OH})_6$

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The compound $\text{Ti}_{1.90}\text{Rb}_{0.10}(\text{SO}_4)_{0.92}(\text{SeO}_4)_{0.08}\cdot\text{Te}(\text{OH})_6$ (TlRbSSeTe) has been synthesized in order to determine the temperature transitions and to study the electrical properties as well as the conduction mechanism. It is obtained by slow evaporation at room temperature and found to crystallize in the monoclinic system with P2₁/c space group using X-ray diffractometer data.

Thermal analysis (DSC, DTA and TG) of the title compound confirms the presence of the phase transitions and the temperature of the decomposition of the studied salt. In order to characterize the phase transitions, Raman spectra have been recorded at various temperatures in the wavenumber range from 50–1200 cm⁻¹. Detailed dielectric and electrical properties of the material have been analyzed as a function of frequency (100 Hz–10 MHz) and temperature (383–518 K). Besides, the analysis of Nyquist plots were well fitted to an equivalent circuit consisting of a series of combination of grains and grain boundary elements.

The variation of the DC and AC conductivity confirms all the transitions of our sample. Furthermore, the frequency dependence of alternative current (AC) conductivity is interpreted in terms of Jonscher's law (developed). The alternative current (AC) electrical conduction in TlRbSSeTe material is accounted for in terms of two processes that can be attributed to a hopping transport mechanism. These processes are the correlated barrier hopping (CBH) model in some regions, as well as the non-overlapping small polaron tunneling (NSPT) model in the other regions. The conduction mechanism for each phase is determined with the help of Elliot's theory.

Key words: Structure study; Thermal analysis; AC conductivity; Dielectric properties.

NiCoFe₂O₄ Nanocomposites: Synthesis, Characterization and electro-chemical Properties

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The development of low-cost and high-performance, energy storage systems is critical to meeting the growing demand for electrochemical storage devices such as portable electronic and hybrid electric vehicles. Supercapacitors (SCs) with high power density and long cycle life have attracted great attention [1-2].

In this context, the oxide NiCoFe₂O₄ nanoparticles were prepared by with different method: so-gel, hydrothermal and auto-combustion method [2]

Characterization was performed by a number of physicochemical techniques commonly used in materials science. We mainly used X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy. The FTIR and XRD techniques were used to confirm the formation of NiCoFe₂O₄ nanocomposites.

The morphology and structure of the obtained products were characterized using X-ray diffraction and scanning electron microscopy.

UV-vis spectroscopic study was used in order to estimate the failure of energy band gap of NiCoFe₂O₄.

The preparation protocols have dominated influence on structural, morphological, optical, and electrochemical.

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How the interaction of phenanthroline affects the structure, Energetics, and bonds properties of DNA base pairs : Theoretical study

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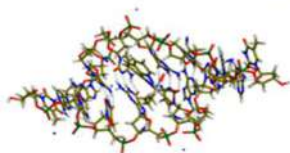
Intercalation of metal complexes containing flat ligands with DNA has been shown to be a clinically relevant process due to its potential to inhibit the growth and survival of tumor cells.

The interaction of the $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ metal complex synthesized in our group with DNA has been studied at computational level by docking, semiempirical methods including dispersion, QM/MM and DFT. The $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ metal complex exists as two main isomers in solution. Indeed in one isomer phenanthroline (phen) is coordinated in the equatorial plane (EqEq), whereas in the other one N of phen is coordinated in an equatorial position and the other N in an axial one (EqAx). Although the EqEq structure is more stable, there is not a great difference between the energy of the isomers and we studied both systems, EqEq and EqAx, interacting with DNA to explain the experimentally found cytotoxicity. We also took into account two different modes of interaction with DNA, that is, groove binding and intercalation, since such competition has been recently described in the bibliography for metal complexes with flat ligands interacting with DNA. PM6-DH2 hamiltonian and QM/MM methods by using M11L/6-31+G(d,p): AMBER were calibrated with the intercalated 1n37 structure of PDB and were observed to perform excellently. On the other hand, for the $[\text{Mo}(\eta^3\text{-C}_3\text{H}_5)\text{Br}(\text{CO})_2(\text{phen})]$ metal complex [4], it is observed that the system prefers the intercalation via minor groove than through the major groove. Moreover, once the bases experimented the rise movement to allocate the metal complex, the groove binding mode became unstable and the intercalation more likely.

Keywords

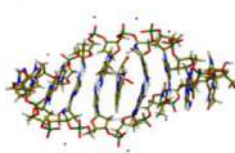
Intercalation; DNA; Tumor cells; metal complexes.

Geometry optimised (PM6-DH2(Mopac) Complex EqEq



Intercalation : minor groove

$$\Delta H_f = -425,81$$



Intercalation : major groove

$$\Delta H_f = -328,466$$

Performance study of CeO₂/CuCr₂O₄ catalysts in CO-PROX with H₂-rich stream

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The CO preferential oxidation in H₂-rich stream (CO-PROX) is an important step for the purification of the hydrogen produced from hydrocarbons or biomass-derived molecules. Basically three types of catalysts show activity for such process: i) platinum group metals; ii) gold-based ones; and iii) base metal ones. Among the latter, catalysts based on combination of copper and cerium oxides can apparently compete with noble metal ones while they are economically more interesting. CuCr₂O₄ is a mixture of copper and chromite oxide employed in gas masks due to its high activity for CO oxidation. However, studies concerning performance of copper-chromite and related materials in the CO-PROX are scarce. In the present work, the CO-PROX performance of CeO₂/CuCr₂O₄ sample, prepared by micro-emulsion method, is studied. The catalysts, with different amounts of CeO₂, have been characterized by XRD, HREM-EDX, N₂ adsorption manometry, XPS and TPR techniques in order to establish structure/activity relationships in combination with catalytic activity testing complemented with operando-DRIFTS analysis.

Most active sites for the process are shown to be related to the interfaces formed between the spinel phase (CuCr₂O₄) support and relatively large supported CeO₂ crystals.

Keywords: CuCr₂O₄, CO-PROX; catalytic activity, DRIFTS.

HOW NECKLACE PEARLS EVOLVE IN HYDROPHOBIC POLYELECTROLYTE CHAINS UNDER GOOD SOLVENT ADDITION: A SANS STUDY OF THE CONFORMATION

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The chain conformation in sulfonated polystyrene PSSNa of a sulfonation rate $0.34 \leq f \leq 1$, i.e. of various hydrophobicity, is followed in mixtures of water and increasing content of TetraHydroFuran (THF), a good solvent of the hydrophobic polystyrene moieties (which improves the solvent quality of the mixture). This is achieved by measuring the chain form factor by small-angle neutron scattering using the Zero Average Contrast method (ZAC) [1]. Polyelectrolyte concentrations were 0.17 M and 0.34 M, correspond in our case to the semi dilute regime.

The main result is the monitoring with added THF of the pearl necklace conformation. This heterogeneous structure made of wormlike chain parts (strings) and pearls was observed formerly in water [2]: when f decreases, the string contribution decreases, and the pearls size increases. Here we see that in presence of increasing content of added THF, (i) the pearls contribution decreases, as expected, but (ii) their size distribution does not change, which was unexpected. Hence our observations are slightly off the Dobrynin-Rubinstein description [3].

A second result, important in practice, is that the modelization of the signal establishes that THF addition makes vanish an excess of low q scattering due to large compact spheres present in water. The rest of the signal addresses accurately the signal from strings plus pearls enabling to determine their size and polydispersity. The Guinier regime enables to determine the radius of gyration in agreement with this description.

A third result is obtained after a "THF treatment" procedure, where THF is added and then removed (i), the spherical aggregates are washed out (ii), the pearl necklace conformation of the chain returns to the one in water solution before treatment. So, the pearl necklace conformation of the hydrophobic polyelectrolyte in aqueous solution appears to be in an annealed equilibrium state resulting from hydrophobic attraction and electrostatic repulsion.

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Stability of Synthesized mixed fatty-acid anhydrides

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Mixed anhydrides are appreciated in organic chemistry because of their high reactivity. They are finding an increasing interest in the chemical industry. Most of the mixed anhydrides are unstable molecules, not easy to handle, not reusable or else need lengthy workup and particularly difficult to isolate. They are generated rapidly to disproportionate into two kinds of symmetrical anhydrides. That is why no standards are commercially available. Despite the importance of organic anhydrides, the separation and quantification of mixtures containing several symmetric anhydrides, mixed anhydrides, and the corresponding carboxylic acids are difficult, also very little analytical methods have been reported for their direct determination. We propose in this work to prepare mixed carboxylic fatty anhydrides in organic solvent and in the presence of triethylamine as acid acceptor. These mixed anhydrides were prepared from palmitic acid and aliphatic or aromatic carboxylic acid chloride. This anhydride must be stable (no disproportionation) and reactive as acylating agent.

Analysis of anionic surfactants in environmental samples

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A spectrophotometric method was adapted for the determination of anionic surfactants using the Crystal Violet. Anionic surfactant gives an ion pair with the dye which is extracted with an organic solvent. The developed method has been studied and optimized for various parameters, such as the effect of the buffer solution on the extraction of the ion pair (pH= 8,1) and the volume of solvent extraction (15 ml). Determination of anionic surfactants in distilled water gives good precision and a significant detection limit up to $2, 5 \cdot 10^{-6}$ M. Interferences have been eliminated by determining anionic surfactants in sea water.

An application part of this method was carried out in the determination of anionic surfactants in an estuary treatment plant in Algiers city. Many results have been obtained and some interesting observations are done. For this, the optimized method for anionic surfactant determination gives significant and reproducible results

Synthesis and characterization of new β -chloro- α,β -unsaturated *N*-acylhydrazones

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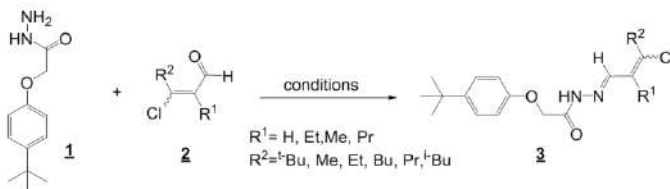
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N-Acylhydrazones (NAHs) are an important class among biologically active compounds and are widely used in many fields [1-4]. They have attracted increasing interest due to their pharmacological properties as anticancer and anti-inflammatory agents [5]. More specifically, they have been described as potential inhibitors of cyclooxygenase (COX) [6], inducible nitric oxide synthase (iNOS) [7] and phosphodiesterases [8]. In this work, we describe the synthesis of new *N*-acylhydrazones starting from β -chloro- α,β -unsaturated aldehydes. The new adducts **3** were fully characterized by (¹H, ¹³C) NMR, IR, and UV-Vis spectroscopies.



Keywords: β -Chlorovinylaldehydes, β -chloro- α,β -unsaturated *N*-acylhydrazones, NMR

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Adsorption of dyes by HDPy⁺-clay: Mechanism studies.

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Tunisian surfactant-modified (HDPy⁺-clay) clay was investigated for the availability of three dyes (indigo carmin IC, phenol red RP and methyl orange MO) removal from aqueous solution. Batch sorption experiments were carried to evaluate the influence of pH, contact time, initial dye concentration, and temperature. Pseudo-first-order and pseudo-second-order, were considered to evaluate the kinetic parameters. To understand the interaction of dye with adsorbent, Langmuir and Freundlich isotherms were applied. Thermodynamic studies were conducted to calculate the changes in free energy ($\Delta^{\circ}G$), enthalpy ($\Delta^{\circ}H$) and entropy ($\Delta^{\circ}S$). The changes in the surfaces and structures of the modified-clay after dye removal were characterized using XRD, FTIR and DSC. These pH results suggested that dye adsorption onto modified clay should be mainly controlled by hydrophobic interaction mechanism, along with a considerable contribution of the anionic exchange mechanism. The dye adsorption equilibria were rapidly attained within 120 min. The adsorption kinetic followed the pseudo-second order kinetic model. The monolayer adsorption capacity of the adsorbent, predicted by the Langmuir model, was 227.27, 326.40 and 344.82 mg/g for MO, IC and RP, respectively. Thermodynamic parameters indicate the feasibility and spontaneity of the adsorption process. The results indicate that HDPy⁺-clay could be employed as low-cost material for the removal of dyes from wastewater.

Keywords: dyes, modified-clay, equilibrium isotherms, thermodynamic studies.

Synthesis and investigations of $(C_6H_9N_2)_2[CuCl_4]$ complex using Hirshfeld surface analysis and spectroscopic features

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More particularly, the hybrid compounds based on halogen of the general formula $R_2[MX_4]$ where **M** transition metal, **X**: Cl, Br, I and **R** is an organic cation, attract the interests of chemists because of their structural flexibility and their interesting properties in various fields namely in magnetism, photoluminescence, biological, photocatalysis, nonlinear optics, electric and ferroelectric. In the title salt complex $(C_6H_9N_2)_2[CuCl_4]$, the Cu^{2+} cation is coordinated to four Cl atoms and adopts a distorted tetrahedral geometry. This compound crystallizes in the monoclinic space group C2/c and the following parameters $a = 13.0244(19)$ Å, $b = 8.3149(11)$ Å, $c = 16.001(2)$ Å, $\beta = 93.730(6)^\circ$, $Z = 4$, $V = 1729.2(4)$ Å³ at 150 K. In the crystal structure the atomic arrangement consists of isolated tetrahedral entities connected to the organic groups by weak hydrogen bonds N-H ... Cl and C-H ... Cl forming a three-dimensional network. Consequently, the present paper reports the chemical preparation of the $(C_6H_9N_2)_2[CuCl_4]$ complex, as well as their characterization by various experimental and theoretical techniques such as X-ray diffraction, this is the main technique that we used to determine in a first step the crystallographic characteristics of our structure and in a second stage their atomic arrangement. Hirshfeld surfaces analysis, reduced density gradient (RDG), Molecular electrical potential surface and spectroscopic measurements (FTIR, UV-visible) are also studied.

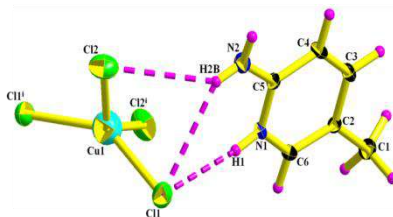


Fig. 1. ORTEP drawing of $(C_6H_9N_2)_2[CuCl_4]$ with the atom-labeling scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii (i: -x, y, -z+1/2).

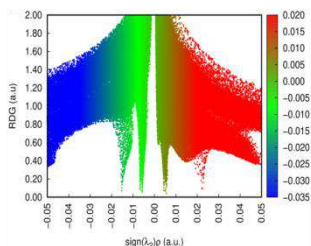


Fig. 2. Reduced density gradient plot along with the color filled scale bar defining interaction limits for the $(C_6H_9N_2)_2[CuCl_4]$ compound.

Keywords: Complex, 3D network, Hirshfeld surface, RDG, FTIR, UV-visible.

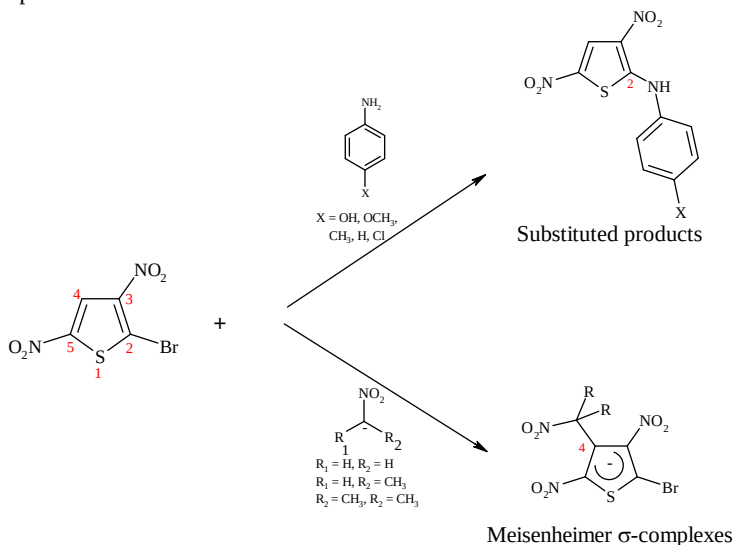
AMBIDENT ELECTROPHILIC BEHAVIOR OF 2-BROMO-3,5-DINITROTHIOPHENE

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Kinetics of the reactions of 2-bromo-3,5-dinitrothiophene with a series of para-substituted anilines and various nitroalkyl anions have been investigated at 20°C. Two electrophilic centers C-2 and C-4 of this thiophene have been identified and discussed.

According, to the free energy relationship $\log k(20\text{ }^{\circ}\text{C}) = s(E+N)$, the electrophilicity parameters E of C-2 and C-4 positions of the electrophile have been determined and compared with the reactivities of other ambident compounds.



Keywords: Ambident Reactivity, Kinetics, Mary's approach, Electrophilicity

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Enhanced figure of merit in nanostructured (Bi,Sb)₂Te₃

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Sb-doped Bi₂Te₃ is known since the 1950s as the best thermoelectric material for near-room temperature operation. Improvements in material performance are expected from nanostructuring procedures. We present a straightforward and fast method to synthesize already nanostructured pellets that show an enhanced ZT due to a remarkably low thermal conductivity and unusually high Seebeck coefficient for a nominal composition optimized for arc-melting: Bi_{0.35}Sb_{1.65}Te₃. We provide a detailed structural analysis of the Bi_{2-x}Sb_xTe₃ series ($0 \leq x \leq 2$) based on neutron powder diffraction as a function of composition and temperature that reveals the important role played by atomic vibrations.

Arc-melting produces layered platelets with less than 50 nm-thick sheets. The low thermal conductivity is attributed to the phonon scattering at the grain boundaries of the nanosheets. This is a fast and costeffective production method of highly efficient thermoelectric materials.

Keywords : thermoelectrics, nanostructuration, lattice thermal conductivity, thermopower.

Adsorption of Strontium into magnesium phosphate cement.

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Water pollution is one of the most serious ecological threats we face today. Especially radioactive pollution results of nuclear waste which produced from industrial, medical and scientific processes that use radioactive material. In this work we study the Sr water pollution because of its half-life about 18 years in the human body also its chemical similarity to calcium it accumulates in bones and irradiates the bone marrow, causing its high radio-toxicity. The technique used for the retention of Sr in this work is the adsorption by lamellar manganate type birnessite, which is characterized by a very large specific surface area, high reactivity and its adsorption and ion exchange capacity due to negatively charged layers and the coexistence of heterovalent Mn cations. The problem is how to recover the adsorbent after the adsorption process? So, we have thought of a material that can be alloyed with this compound while keeping their performance, this material is the phosphate magnesium cement (MPC) which was prepared with magnesia oxide (MgO), potassium dihydrogen phosphate (KH₂PO₄) and some retarders. This new material retains the advantages of cement: fast setting, low permeability, accelerated resistance development, excellent adhesion on almost all clean and dry surfaces. The obtained composite material and its performance were examined and analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), BET and atomic adsorption.

Keywords: Magnesium phosphate cements (MPC), birnessite, adsorption, strontium.

ADSORPTION OF ANIONIC DYE ON CETRIMONIUM BROMIDE FUNCTIONALIZED ALMOND SHELL POWDER: OPTIMIZATION, KINETICS, ISOTHERMS

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With respect to all methods, adsorption is a common and effective method for heavy metal ions removal because of low cost, high efficiency, and good operational conditions [1]. The present investigation focuses on the removal of methyl orange (MO) by cetyltrimethylammonium bromide (CTAB) functionalized almond shell powder. Various process parameters such as effect of adsorbent/chemical dose, reaction temperature and contact time were experimented through batch study and statistical method to study the effect of these parameters on dye removal efficiency. The optimized condition was achieved statistically using CCD in response surface methodology (Fig. 1). The optimized condition was considered further to study the combined effect of adsorbent with chemical treatment for the treatment of MO containing solution.

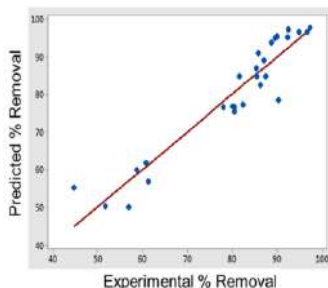


Fig. 1 Comparison of predicted and experimental % removal MO dye

Key words: Biosorption, Almond shell, Cetyltrimethylammonium bromide, Methyl orange

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Synthesis, characterization and biological activity of new β -fluoro- α,β -unsaturated aldehydes

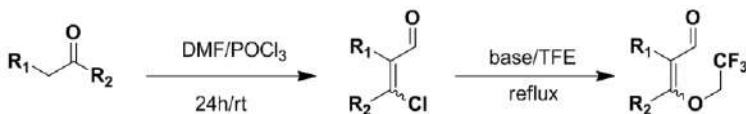
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The incorporation of good leaving groups (chloro or alkoxy) at the β -position of the α - β -Unsaturated carbonyl derivatives serve as convenient building blocks for the synthesis of different classes of acyclic, carbocyclic, and heterocyclic compounds [1,2]. In another hand, an increasing interest has been paid to the chemistry of fluoroalkyl compounds, not only due to their potential biological applications [3,4] but also for their specific chemical reactivity. Therefore, considerable attention has been given to the development of new procedures for the synthesis of fluoro- α,β -unsaturated carbonyl compounds. In this work, we report the synthesis and the characterization of a new series of β -fluoro- α,β -unsaturated aldehydes. They have been characterized in solution using multinuclear NMR (^1H , ^{13}C , ^{19}F), IR spectroscopies and GC-MS. The biological activity of β -fluoro- α,β -unsaturated aldehydes and their β -chlorovinylaldehyde homologues will be also discussed.



Keywords: Vilsmeier-Haack, β -chlorovinylaldehydes, β -fluorovinylaldehydes, NMR characterization, biological activity.

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Synthesis and Characterization of Novel Biobased Poly (ether-pyridine) s Used for the Removal of Organic Pollutants and Metal Ions From Water

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In recent decades, many efforts have been made to create structurally modified aromatic polymers having increased chemical resistance, thermal stability, low flammability, and good mechanical performance. It is recognized that these proprieties are often improved when flexible bonds, large pendent groups, or polar substituents are incorporated in the polymer backbone. For instance, pyridine is well known by its remarkable proprieties that are provided by the aromatic heterocycle. These advanced properties include high polarity, hydrophilicity [1], excellent thermo-mechanical resistance [2] and specially an elevated adsorption capacity of metal ions [3].

The present work aims to study the effect of introducing a pyridine unit to a bio-based diol: the 1,4:3,6-dianhydrohexitol to obtain a bio-based monomers. This kind of diols has a combination of excellent properties such as amorphous transparent character, high glass transition temperatures ($T_g > 190^\circ\text{C}$), high hydrolytic stability, low sensitivity to oxidation, chirality, rigidity and high adsorption capacity [4].

The current investigation deals with the synthesis and characterization of various biosourced A-A type monomers derived from the 1,4:3,6-dianhydrohexitol bearing halogenated pyridine units and creating new linear aromatic poly(ether-pyridine)s by combination with several diols. In addition, the high performance of the developed polymers for the adsorption of organic polar pollutants and metal ions from aquatic environment was performed.

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Compatibility study between acebutolol and pharmaceutical excipients used in solid dosage forms

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The study of compatibility of active pharmaceutical ingredient (API) with excipient is an important stage in the development of pharmaceutical dosage forms. In a dosage form, an API comes in direct contact with one or more excipients of the formulation that facilitate the administration and release of an active component as well as protect it from the environment. Although excipients are pharmacologically inert, they can interact with API that lead to changes in the chemical, physical, therapeutic properties of the pharmaceutical dosage form are termed as incompatibilities. This incompatibility in a formulation can alter the stability and/or bioavailability behaviour of the API, thereby affecting its safety and/or efficacy. The changes can be both physical and chemical.

The purpose of this work is to study the stability of β -blockers as acebutolol, with common pharmaceutical usual excipients (lactose monohydrate, magnesium stearate, polyvinylpyrrolidone) and antioxidants (ascorbic acid, citric acid, butylhydroxyanisole), used in the solid dosage form, by IR spectroscopy (FTIR), differential scanning calorimetry (DSC) and HPLC. In a first part, analyses were performed on the binary mixtures of API-excipient (1:1, w/w). One serie of samples was analysed directly after preparation and the other samples were stored during one month at 40°C/75 % RH.

In the presense of antioxidants, there are significant shifts in melting temperature of acebutolol. No melting peak appears in the DSC curve for the acebutolol / PVP mixture placed in a humidity-saturated atmosphere (75%).

The samples showing a remarkable shift of melting point compared to the active principle alone, were analyzed by HPLC. Thanks to this technique, the degradation of acebutolol mixed with PVP, citric and ascorbic acids is also demonstrated. Additional studies using infrared spectroscopy confirm the interaction of Aceputolol with these antioxydants, it was possible to observe the modification of C = O and N-H bonds of acebutolol, as being the most concerned by the establishment of hydrogen bonds in physical mixtures.

This study could offer the drug formulator a scientific support in his strategy of developing finished products, especially generic, and help him to optimize his process and his composition.

Keywords: Acebutolol, Excipients, Interactions, DSC, FTIR.

Synthesis and characterization of a novel organic-inorganic hybrid material $C_8H_{14}N_2(H_2PO_4)_2$

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A novel organic-inorganic hybrid material $C_8H_{14}N_2(H_2PO_4)_2$ formed has been synthesized and structurally determined by X-ray diffraction method, Hirshfeld surface analysis, IR, UV visible spectroscopy and Thermal analysis. This compound crystallizes in the orthorhombic system, space group Pnna, with $a = 9.1291(14)$, $b = 21.109(3)$, $c = 7.1519(8)$ Å, $V = 1378.2(3)$ Å³ and $Z = 4$. The atomic arrangement shows an alternation of organic and inorganic entities. The cohesion between these entities is performed via N–H...O, O–H...O and C–H...O hydrogen bonds, forming a three-dimensional network. The Hirshfeld surface analysis and the two-dimensional fingerprint maps indicate that the packing is dominated by H...O/O...H and H...H contacts.

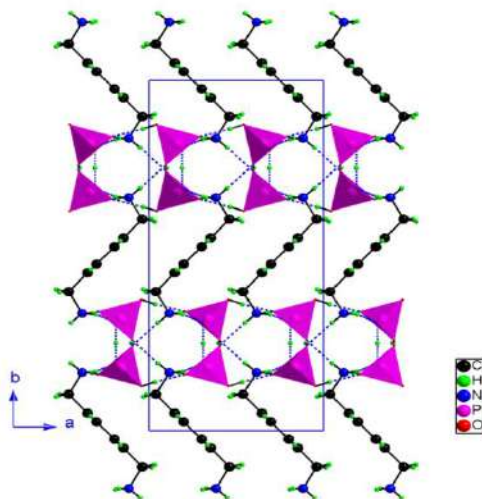


Fig. Projection of $C_8H_{14}N_2(H_2PO_4)_2$ along the c-axis.

Keywords: crystal structure, p-xylylenediaminium, Hirshfeld surface analysis, fingerprint maps.

Quantitative and Qualitative Characterization of some Active Pharmaceutical Ingredients and their Commercial Formulations

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A generic drug is a copy of brand-name drug (original), it must have the same pharmacological effects as its brand-name. It has exactly the same therapeutic, safety, and performance characteristics, same qualitative and quantitative composition in active pharmaceutical ingredient (API), same dosage form, same bioequivalence and bioavailability as the reference product.

In fact, it is important to compare some of pharmaceutical equivalent drug products in order to control the stability of the pharmaceutical formulations.

During manufacturing, many physical transformations of the solid state form of an API (polymorphism, solvation, dehydration, crystalline/amorphous conversion) can occur due to milling, granulation, compression and storage. However this degradation can affect the solubility, dissolution rate, stability and bioavailability of a pharmaceutical formulation. Therefore identification of the crystal phase of an API has to be investigated.

In the present study, a quantitative comparison of two tablets A and B of acebutolol (400 mg) was carried out by DSC, PXRD and ¹³C CP/MAS NMR. A higher content of API for B tablet was established and physical chemical stability of API was shown despite the variety in terms of excipients contained in the two tablets.

In the case of carvedilol (25 mg), ¹³C CP/MAS NMR showed sufficient sensitivity to monitor the neat drug substance in the drug product.

Keywords: XRD, DSC, ¹³C CP/MAS NMR, solid state analysis,

**Synthesis, crystal structure, photoluminescence
of a new organic–inorganic compound:
 $\text{FeF}_3(\text{H}_2\text{O}) \cdot [\text{C}_{12}\text{H}_8\text{N}_2]$**

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A new hybrid compound was synthesized under hydrothermal reaction, by a mixture of $\text{FeF}_2/\text{FeF}_3$, 1,10-phenantroline, and hydrofluoric acid solution (HF 4%) in ethanol absolute solvent. The crystal structure of $\text{FeF}_3(\text{H}_2\text{O}) \cdot [1,10\text{-phen}]$ crystallizes in monoclinic system with $P2_1/c$ space group and cell parameters $a = 8.458(5) \text{ \AA}$, $b = 7.289(2) \text{ \AA}$, $c = 22.3607(5) \text{ \AA}$, $\beta = 122.492(9)^\circ$ and $Z = 4$.

The asymmetric unit cell of $\text{FeF}_3(\text{H}_2\text{O}) \cdot [\text{C}_{12}\text{H}_8\text{N}_2]$ is built up from $\text{FeF}_3\text{N}_2\text{O}$ octahedra coordinated by two nitrogen atoms of the 2,2'-bipyridine molecules, and three fluorine atoms as well as coordinated H_2O molecules.

Thermal analysis of the title compound showed that the decomposition introduced four steps. Furthermore, the room temperature infrared (IR) spectrum of the title compound was recorded and analyzed on the basis of data found in the literature. The photoluminescence properties of the compound were also investigated in the solid state at room temperature.

Keywords: structure, hybrid, fluoride, thermal, spectroscopic

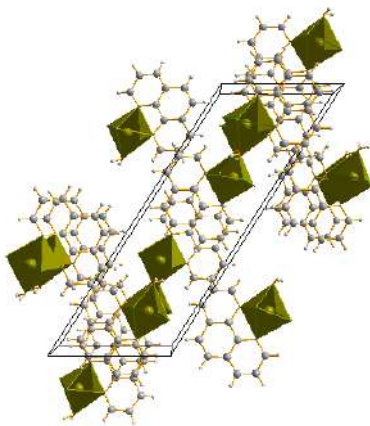


Figure 1: representation of $\text{FeF}_3(\text{H}_2\text{O}) \cdot (1,10\text{-phenantroline})$ crystal structure

Crystal structure, spectroscopic and biological study of a new hybrid compound inorganic-organics $[\text{Cd}_4\text{Cl}_{12}(\text{H}_2\text{O})_2]_n(\text{C}_{10}\text{N}_4\text{H}_{28})_n$

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The objective of this work consists in synthesizing a new organics-inorganic hybrid compound $[\text{Cd}_4\text{Cl}_{12}(\text{H}_2\text{O})_2]_n(\text{C}_{10}\text{N}_4\text{H}_{28})_n$ with [1,4-Bis(3-amino-propyl)piperazine = $\text{C}_{10}\text{N}_4\text{H}_{28}$] was prepared. It was characterized by single crystal X-ray diffraction, spectroscopy measurement, DTA-TG measurement, photoluminescence properties, and biological analysis. It crystallizes in the monoclinic system with the space group of P21/n with the following unit cell parameters: $a = 9.5808(17)$, $b = 9.8438(18)$, $c = 16.050(3)$ Å, $\beta = 93.142(6)$, $V = 1511.4(5)$ and $Z = 2$. The atomic arrangement can be described as an infinite one-dimensional coordination polymeric double-chain running along the crystallographic b-axis, those chains are interconnected by water molecules via O-H...Cl hydrogen bonds to form layers parallel to (101) plane, between those layer interconnected the organic cations to performed an infinities three dimensional network. The nature and proportion of contacts in the crystal packing were studied by the Hirshfeld surfaces. The vibrational properties were investigated experimentally by means of IR spectroscopy and theoretically by DFT calculations on the organic cation. Furthermore the optical absorption and photoluminescence properties of the compound were achieved at room temperature in the solid state and illustrated two absorption bands and three emissions peaks. The antioxidant properties were determined via the DPPH radical scavenging, the ABTS radical scavenging. The bioassay results showed that the structure exhibits significant antibacterial activity. The thermal analysis shows that this compound is stable until 250 C°.

Synthesis, Crystal structure, spectroscopic properties of trans 2,5-dimethyl-piperazinium tetrachloridocuprate(II)

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This work reports the preparation and structural characterization of a new complex $[\text{CuCl}_4](\text{C}_6\text{H}_{16}\text{N}_2)$ were grown by slow evaporation technique in aqueous solution and characterized by X-ray diffraction, spectroscopy measurement, DTA-TG analysis, photoluminescence properties. The crystal structure determination shows that the title compound crystallizes in the C 2/c space group of the monoclinic system. The unit cell dimensions are as follows: $a = 14.500(5) \text{ \AA}$, $b = 14.619(5) \text{ \AA}$, $c = 5.9173(17) \text{ \AA}$, $\beta = 107.419(11)^\circ$, $V = 1196.8(7) \text{ \AA}^3$ and $Z = 4$. The atomic arrangement can be described by thick layers of inorganic entities, made up from CuCl_4 anions and NH_3 groups, developed parallel to the (a, c) planes at $y = 0$ and $1/2$ (Fig. 2). The organic cations are anchored onto successive layers and connect them via N-H...Cl hydrogen bonds to form an infinite three-dimensional network. What is especially interesting about this structure is that it consists of one-dimensional tubes center to the axes located at the intersection of the planes ($x = 0$, $y = 1/2$) and ($x = 1/2$, $y = 0$), linked together so as to form the open framework structure. In this work, we report the synthesis and the characterizations of a novel hybrid complex $[\text{CuCl}_4](\text{C}_6\text{H}_{16}\text{N}_2)$. In addition, The nature and proportion of contacts in the crystal packing were studied by the Hirshfeld surfaces. Furthermore IR, the optical and photoluminescence properties of the compound were achieved at room temperature in the solid state. Finally the thermal analysis shows that this compound is stable until 400° .

A comparative Study on the Physical, Thermal and Electrochemical Properties of Dicyanamide Based Ionic Liquid in Molecular Solvents

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In this work we present a comparative study of binary mixture of 1-allyl-3-methylimidazolium dicyanamide AMIM-DCA ionic liquid (IL) with acetonitrile (ACN), gamma-butyrolactone (γ -BL) and propylene carbonate (PC) as function of temperature and composition of IL. The influence of solvent addition on volumetric and transport properties have been studied for all composition range from 293 to 323K. The excess volume was calculated for each IL/solvent mixture and different behavior were recorded for each solvent. Variation of ionic conductivity with IL composition were well described by Casteel-Amis equation. The highest ionic conductivity value was recorded for ACN mixture ($62 \text{ mS} \cdot \text{cm}^{-1}$ for $x_{\text{IL}}=0.2$) while γ -BL and PC mixtures showed similar conductivities. The temperature dependence of dynamic viscosity and ionic conductivity of binary system were graphically described by Arrhenius equation for all IL/solvent mixtures. Through the Walden rule which shows that viscosity is highly correlated to conductivity, the ionicity of binary system at each fraction was evaluated and all mixtures show a behavior of "true electrolytes". Thermal and electrochemical properties of IL mixtures have been studied only for the optimum fraction. Differential Scanning Calorimetry DSC results showed that all mixtures are stable up to very low temperatures so those electrolytes could be interesting for low temperatures device application. According to three-electrode method, the electrochemical potential windows (EPWs) of optimum system and pure IL were measured to investigate the electrochemical stability and the addition of solvent seems to affect their EPW. In a supercapacitor cell, the optimum IL mixtures were applied as electrolytes and the performances of the supercapacitor were determined by cyclic voltammetry and galvanostatic charge discharge measurements.

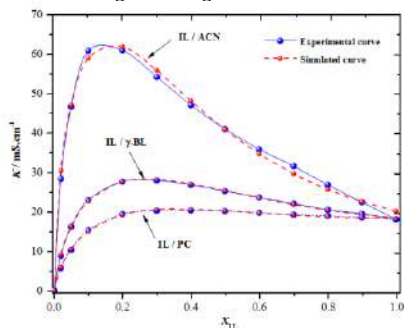


Figure 1: Evolution of experimental and simulated value of ionic conductivity with composition of IL+solvent mixtures at 298K

Theoretical investigation of the structural, electronic, optical, elastic and thermodynamic properties of the quaternary diamond-like semiconductors $\text{Cu}_2\text{MgSiS}_4$ and $\text{Cu}_2\text{MgGeS}_4$

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Structural, electronic, chemical bonding, optical, elastic and thermodynamic properties of quaternary diamond-like semiconductors $\text{Cu}_2\text{MgSiS}_4$ and $\text{Cu}_2\text{MgGeS}_4$ were investigated through density functional theory and quasi-harmonic Debye model (QHDM). The optimized structural parameters of the two studied compounds agree well with those obtained experimentally. Electronic band structure calculation showed that these materials are direct band gap ($I-I$) semiconductors. The calculated energy band gap using LDA-CAPZ (GGA-WC) is equal to 2.007 (1.820 eV) and 1.262 (0.964 eV) for $\text{Cu}_2\text{MgSiS}_4$ and $\text{Cu}_2\text{MgGeS}_4$, respectively. By analyzing the total and partial densities spectra and also based on the results of the Mulliken population analysis, we have demonstrated that the bonding of $\text{Cu}_2\text{MgSiS}_4$ and $\text{Cu}_2\text{MgGeS}_4$ are characterized by a mixture of covalent-ionic character. Dielectric function, refractive index, extinction coefficient, optical reflectivity and electron energy loss are calculated for different light polarizations. Single-crystal and polycrystalline elastic constants and some related properties namely isotropic sound velocities, Debye temperature acoustic Grüneisen parameter, Vickers hardness and minimum thermal conductivity at high temperature have been computed. The studied material is characterized by a relatively high hardness. It is found that the studied compounds exhibit a striking elastic anisotropy. The analysis of B/G ratio indicated that the examined materials might classify as ductile. The computed Debye temperature is about 369 and 342 K for $\text{Cu}_2\text{MgSiS}_4$ and $\text{Cu}_2\text{MgGeS}_4$, respectively.

Keywords: ab-initio, diamond-like semiconductors, electronic properties, optical properties

Crystal structure, Vibrational spectroscopy, Optical properties and Hirshfeld surface analysis of Quinolinium Dichromate

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The crystals of Quinolinium Dichromate ($C_9H_8N)_2 [Cr_2O_7]$ were grown by slow evaporation technique and characterized by X-ray diffraction. The compound crystallize in the monoclinic system, space group $P2_1/c$ with $Z=4$ and $a= 12.1699(3)\text{\AA}$, $b= 9.9344(2)\text{\AA}$, $c=15.2133(3)\text{\AA}$, $\beta=98.364(2)^\circ$.

The title compound has been characterized by IR spectroscopy, RAMAN, UV spectroscopy, Luminescence and Hirshfeld surface.

The X-ray study of quinolinium dichromate (QDC) (I), was undertaken in order to study the hydrogen-bond patterns and crystal packing. QDC is reported to be a selective oxidant for a wide range of substrates in view of its ease of preparation and high stability (1).

The quinolinium cations and a dichromate anion are connected through N-H...O and N-H...O intermolecular hydrogen bonds and by aromatic stacking interactions.

Keywords : X-ray diffraction, IR spectroscopy, RAMAN, UV spectroscopy, Luminescence, Hirshfeld surface.

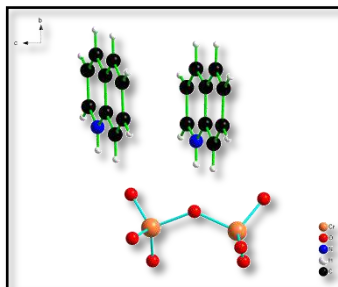


Fig. Projection of the asymmetric unit along the a axis

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^{13}C NMR Chemical Shifts and Atomic Charges in $\text{C}_3\text{H}_4^{++}$, $\text{C}_3\text{H}_6^{++}$ and $\text{C}_4\text{H}_6^{++}$ Dication Structures: A DFT Study

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Structures of $\text{C}_3\text{H}_4^{++}$, $\text{C}_3\text{H}_6^{++}$ and two isomers of $\text{C}_4\text{H}_6^{++}$ dication were investigated by using DFT calculations at B3LYP/6-31G(d) level. Geometry optimization shows that the two structures 1a and 2b were identified as minima on the potential energy surface, whereas 2a and 1b were found to be maxima. ^{13}C NMR chemical shifts were calculated by using GIAO-DFT/B3LYP/6-31G(d) method, and were applied to explore the nature of the carbocationic centers in carbocationic species. Correlations between various atomic charge (Mulliken, NBO, ChelpG, MK and AIM) of carbon atoms and their ^{13}C NMR chemical shifts show a linearity only with AIM charges. In addition, NBO analysis provided more informations about charge distribution and chemical bonding in carbocationic species.

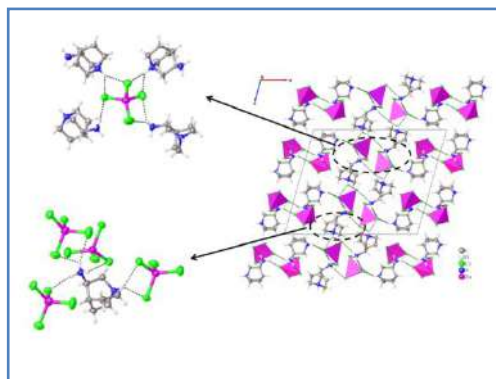
Keywords: Dications, $\text{C}_3\text{H}_4^{++}$, $\text{C}_3\text{H}_6^{++}$, $\text{C}_4\text{H}_6^{++}$, DFT/B3LYP/6-31G(d), Optimization Geometry, ^{13}C NMR Chemical Shifts, Carbocationic Centers, Atomic Charge, NBO Analysis.

Structural, optical, electrical and ferroelectric properties of metal-halide compound $[C_7H_{16}N_2][ZnCl_4]$

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A new organic–inorganic hybrid compound $[C_7H_{16}N_2][ZnCl_4]$ was synthesized by the hydrothermal method and characterized by X-ray diffraction, IR and Raman spectroscopy, optical absorption, differential scanning calorimetry and dielectric measurements. Single crystal diffraction results showed that $[C_7H_{16}N_2][ZnCl_4]$ crystallizes in the monoclinic system, space group $P2_1/c$ at room temperature. In the molecular arrangement, the tetrachlorozincate anions are connected to organic cations through $N-H\cdots Cl$ hydrogen bonds. The Raman and IR analyses confirm the presence of the organic groups and the anionic entities. UV–Visible absorption spectrum revealed the energy of the optical band gap. DSC measurements indicated that $[C_7H_{16}N_2][ZnCl_4]$ undergoes three sequential phase transitions at 287, 338 and 356 K. The dielectric study proved the ferroelectric properties below the 338K and indicates their classical character for this compound. The analysis of Nyquist plots was revealed the contribution of the bulk mechanism and the grain boundaries. The electrical properties as a function of temperature are characterized the transitions phase detected in the DSC study.



Keywords: Hybrid material, Crystal structure, Optical absorption, Phase transitions, Ferroelectric properties, Conduction mechanism.

Co(II)/Co(III) Mixed–valence complex: Synthesis, crystal structure, spectroscopic and magnetic characterizations.

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The bidentate ligand 2-picolyamine (2-aminomethylpyridine) and the concentrated hydrobromic acid have been employed to synthesize a dinuclear Co(II)Co(III) mixed-valence complex. Single crystals of the novel compound were grown by slow evaporation solution process at room temperature. This new product was subjected to the following characterization techniques: single crystal X-ray diffraction, FT-IR and FT-Raman spectroscopies and temperature dependent magnetic susceptibility measurements. The title compound crystallizes in the monoclinic system, space group $P2_1/n$, with $a=14.624(5)$ Å, $b=10.302(5)$ Å, $c=23.743(5)$ Å, $\beta=95.280(5)^\circ$ and $Z=4$. The crystal structure consists of three crystallographically independent bromide ions, one deprotonated amine (2-picolyamine), one water molecule and two crystallographically independent Co(II) and Co(III) ions: one has an octahedral geometry while the other is tetrahedrally coordinated. The crystal packing diagram reveals interesting non-covalent interactions involving N-H...Br, N-H...O, O-H...O and O-H...N hydrogen bonds, leading to the generation of 3D supramolecular architecture. The structural data, the magnetic and the spectroscopic measurements are in agreement with a six-coordinate Co^{III} and four-coordinate Co^{II} mixed-valence complex.

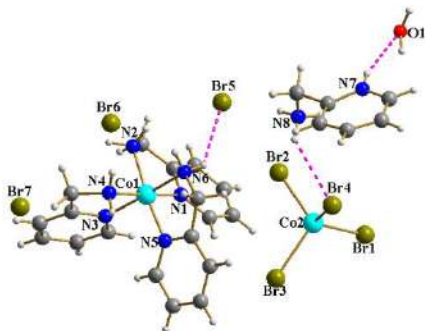


Fig.1. The asymmetric unit of $(C_6H_{10}N_2)[Co(C_6H_8N_2)_3][CoBr_4]Br_3 \cdot H_2O$ showing the atom-numbering scheme.

Keywords: Crystal structure, mixed–valence complex, spectroscopic and magnetic susceptibility measurements, 3D supramolecular architecture.

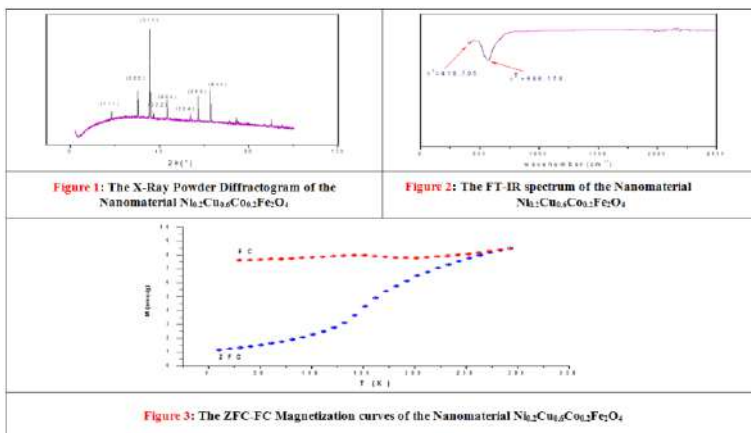
Synthesis by the Sol-Gel Autocombustion Method and Physicochemical Characterizations of Nanoferrimagnetic ferrite $\text{Ni}_{0.2}\text{Cu}_{0.6}\text{Co}_{0.2}\text{Fe}_2\text{O}_4$

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The nanoferrite $\text{Ni}_{0.2}\text{Cu}_{0.6}\text{Co}_{0.2}\text{Fe}_2\text{O}_4$ was synthesized via a self-combustion process using stoichiometric amounts of raw materials: aqueous Nickel-Copper-Cobalt-Iron nitrates and citric acid. The pH of the latest mixture was then adjusted to 7 by adding the concentrated ammonia solution. However, the black powder, obtained after heating at 900 °C during 2 h, was analyzed by different techniques as: XRPD, FT-IR and magnetic measurements ZFC-FC. The XRPD analysis (**Figure 1**) proves well the obtaining of only the spinel cubic structure with space group Fd-3m, whereas the Fourier transform infrared spectrum (**Figure 2**) puts in evidence the presence of the two characteristic peaks, corresponding to the vibration modes of octahedral (410.705 cm^{-1}) and tetrahedral (566.178 cm^{-1}) sites of spinel structure. Moreover, the magnetic measurements in the ZFC-FC modes (**Figure 3**), at 10 and 300 K respectively, have confirmed the ferrimagnetic behavior below the blocking temperature which is around 292.70 K, and the superparamagnetic behavior above it.



Kinetics of oxidative degradation of the antibiotic Sulfachloropyridazine by the novel Heterogeneous electro-Fenton process with solid catalyst Chalcopyrite

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The electrochemical advanced process, Electro-Fenton has been applied to oxidative degradation of sulfachloropyridazine in aqueous solution using chalcopyrite as source of Fe^{2+} and Cu^{2+} ions instead of a soluble catalyst salt used in conventional EF electrolyses were conducted in an open cylindrical cell equipped with a boron-doped diamond (BDD) or PbO_2 anode and carbon felt cathode. The powerful hydroxyl radical formed from water oxidation and in the bulk from Fenton's reaction Fe^{2+} and H_2O_2 react with the antibiotic leading to its overall degradation. The effects of operating parameters such as chalcopyrite concentration, applied current and anode material were investigated.

Keywords: Heterogeneous catalysis, chalcopyrite, Electro-Fenton, Sulfachloropyridazine, wastewater treatment, mineralization.

NEW TYPES OF NANOCOMPOSITES USED AS ELECTRODES IN SUPERCAPACITORS

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This work is interested in the formulation and characterization of new types of electrodes for super-capacitors. In the case of NPC based MMT/ PPy(Cl), relatively high capacities were obtained in aqueous medium, rivaling the results of the literature (410 F.g⁻¹). These capacities were "optimized" by controlling the temperature, the montmorillonite/pyrrole ratio, the pH of the solution during the elaboration of the nanocomposite material. These results are partly explained by the impact of these parameters on the conductivity of the nanocomposite.

The same phenomena are observed in the case of NPCs based PPy(Cl) with ZHY and Z4A, where values of 310 F.g⁻¹ / 1.7 S.cm⁻¹ and 380 F.g⁻¹ / 6.6 S.cm⁻¹ are respectively observed.

The preliminary study we conducted on these NPCs provided qualitative information, and understanding a mixture of two constituents requires further study.

Keywords: Conductive Polymer, Nanocomposite, Supercapacitor

Acknowledgments: I would like to thank MESRS for accepting me in the scholarship program for residential education abroad for teachers and researchers for the academic year 2016-2017 (PNE)

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Accelerated aging of biobased/kenaf fibres composite: Visual appearance, color and structural changes

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In this presentation, a comparison between the degradation behaviour of starch-grafted-polypropylene reinforced with 30 %wt of kenaf fibres (S-g-PP/KF) and the virgin matrix (S-g-PP) were carried out, when materials were subjected to UVA and UVB radiations, for various periods. Changes induced by radiations on the structure, visual and morphological appearance, were evaluated.

Results of visual appearance have shown colour changes with the progression of exposure, from brown to chalky white colour in case of UVB exposed composite. Matrix samples have shown also chalky white colour after exposure to UVB, while a complete discoloration followed by yellowing was observed for UVA exposed matrix. Colour measurements demonstrated an increase in lightening and total colour changes after UV exposure, in parallel to a decrease in yellowness and redness parameters. Changes were more accentuated in UVB exposed composite.

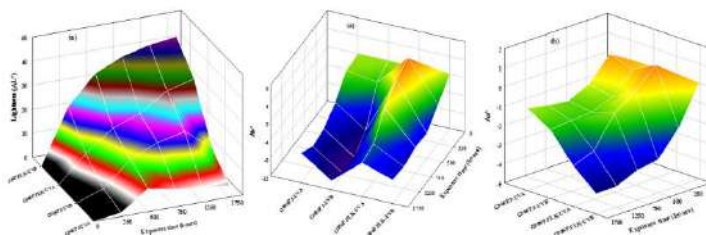


Fig. 2 Lightness, Yellowness and Redness parameters change of UV exposed samples.

FTIR-ATR analysis confirmed the deterioration of the chemical structure of exposed samples. A complex mechanisms occurs which evidenced the co-existence of crosslinking and chains scission reactions. Fibres has found to not affect the mechanism of oxidation while it is, visibly, affected by the irradiation intensity.

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Electrogenerated base-promoted synthesis and antimicrobial activity of 2-imino-1,3-thiazolidin-4-one derivatives

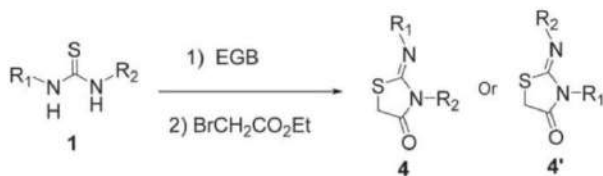
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We report in a simple method for the synthesis of 2-imino-1,3-thiazolidin-4-one dervatives in good yields under mild conditions. The electrogenerated cyanomethyl base, obtained from electroreduction of acetonitrile assists the reaction between thiourea dervatives **1** and ethyl bromoacetate. The reaction pathway was discussed based on the kinetic and thermodynamic data obtained by computational methods. In addition, the biological activity of these new compounds was also investigated.



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A novel and convenient synthesis of new 2-imino-1,3-thiazolines and thiazolidin-4-ones involving the electrogenerated cyanomethyl-anion

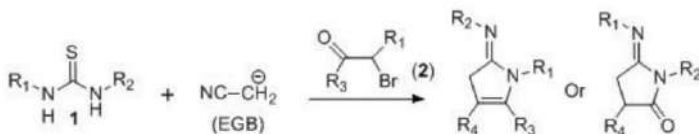
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A novel and convenient strategy is described for the regioselective conversion of N,N'-disubstituted thioureas with 1,2-dielectrophiles into the highly biologically valuable 2-imino-1,3-thiazolines and 2-iminothiazolidin-4-one derivatives. The synthesis proceeds through a process with good yield promoted by an electrogenerated base (EGB) obtained with high current efficiency and a magnesium rod as a sacrificial anode.



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Assembly and weak interactions in the crystal structure of 2-amino-4-(3-bromophenyl)-1,3,5-triazinobenzimidazolium chloride studied by X-ray diffraction, vibrational spectroscopy, Hirshfeld surface analysis and DFT calculations

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Experimental and theoretical investigations on the molecular structure, electronic and vibrational properties of the title compound (**1**) are presented in this study. The asymmetric unit of (**1**) consists of a discrete protonated cation assembled with the chloride anion (**Fig.**). Individual inversion dimers are connected through N5-H5A...Cl1 ($-x+3/2, -y+3/2, -z+1$), N5-H5B...N ($-x+3/2, -y+3/2, -z+1$) hydrogen bonds into 1D undulating chains running along the [110] direction. The chains are further extended into 2D layers packed along the [111] direction, mediated by N4-H44...Cl1 ($x+1/2, y-1/2, z$) and weaker C12-H12...Cl1 ($-x+3/2, y-1/2, -z+3/2$) hydrogen bonds. Moreover, the protonated aromatic system shows a π - π interaction adding an extra stability to the 2D architecture. Hirshfeld surface analysis has been used to analyze intermolecular interactions present in the solid state. The ground state geometry of (**1**) was optimized using density functional theory (DFT) at the 6-311+G(2d,2p) level of theory. Molecular parameters calculated using CPCM model of solvation has resulted in better agreement with measured vibrational spectra.

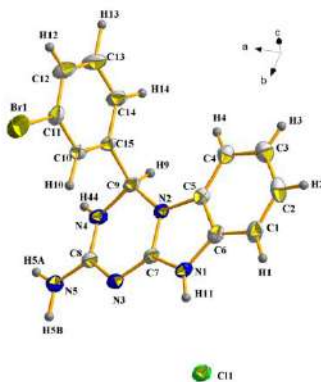


Fig. The asymmetric unit of the crystal structure of (**1**)

Key words: Molecular structure, electronic and vibrational properties, Hirshfeld surface analysis, DFT calculations.

Mechanical behavior of ion-substituted bioceramics

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Bone loss can have many origins such as trauma or severe bone disease. Its repair may require the establishment of an implant. Various materials can be used, such as metallic or inert materials, but those based on calcium phosphates, being the closest by their both composition and structure to the mineral part of bone, are of particular interest [1-6]. Several trace elements such as Mg^{2+} , Na^+ , K^+ , F^- , Cl^- are contained in biological apatite of natural bones. The presence of these elements in bones is indispensable in mechanisms of their calcification and mineralization. This was the starting idea to investigate calcium hydroxyapatite biomaterials doped with the aforementioned ions. Three formulations of ion-substituted hydroxyapatite powders were prepared via a wet-chemical precipitation method. After calcination at 500°C, the powders were uniaxially isostatically cold compacted into pellets, followed by pressureless sintering in the temperature range of 900-1250°C. Analysis and characterization by several techniques confirmed that well crystallized powders of apatitic nature were obtained. The samples sintered at temperature 1150°C during 1 hour were found to have the maximum densification value of 95%. A secondary phase of $\beta-Ca_3(PO_4)_2$ was found to form at 730°C due to a partial decomposition of the apatitic phase. The sintered materials were mechanically characterized by measurements of compressive and flexural strengths, fracture toughness, Young's modulus and microhardness and the maximum values were found to be 154MPa, 60MPa, $1.55MPa \cdot m^{1/2}$, 151GPa and 600Hv, respectively.

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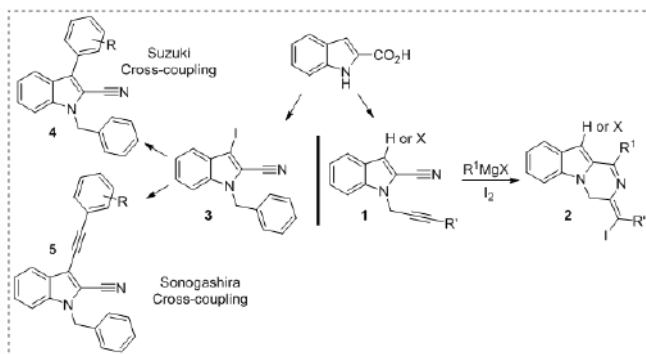
Synthesis of Novel 1H-Indole-2-Carbonitrile Via Sonogashira and Suzuki Coupling Reactions

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Dihydropyrazino[1,2-*a*]indole derivatives **2** can be readily synthesized from various 1-(propargyl)-1H-indole-2-carbonitriles **1** via an efficient Grignard reagent-promoted cyclization of nitrile to alkynes. Products **1** are obtained from 2-carboxylic acids. The reaction of heterocyclization with the magnesiumians is during the laboratory, some results will be presented in this work. Similarly, the products **3** are obtained in 4 steps from the acid indoles. A study of the reactivity of iodine in position 3 was studied by the use of cross-coupling reaction in particular. Sonogashira's reaction^[1,2] on **3** allowed us to synthesize 5 examples of molecule **4** as well as the reaction of Suzuki^[3] on **3** allowed us to synthesize 6 examples of molecule **5**.



Keywords: 1H-indole-2-carbonitriles, heterocyclization, Sonogashira, Suzuki

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NEUTRAL 1,3-DIMETHYL-2,4-DIMETHYLAMINO-2,4-DITHIO CYCLODIPHOSPHAZANE LIGAND [EtNP (S) NMe₂]₂: COMPARATIVE STUDIES OF X-RAY DIFFRACTION AND DFT CALCULATION RESULTS

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The material [EtNP(S)NMe₂]₂ (**I**) is a member of a family of ligands that may be used in the extraction of several metals. In order to better understand the complexing properties of (**I**) as well as other homologous ligands (mono- or bidentate ligand, active sites, ...), theoretical studies by the semi-empirical PM6 and DFT methods using the functional B3LYP and the base 6-31G (d) are realized. The results from these methods are compared firstly with the structural data of (**I**) (**Fig. 1**). It shows a good agreement between the theoretical and experimental geometric parameters. Secondly, these results, in particular the atomic charges calculated at the B3LYP level, show that (**I**) is a ligand potentially complexing by the sulfur atoms [**1**] with calculated loads of -0.37e (e: elementary charge). These obtained values are comparable to those obtained for the ligand bis (N, N, N', N' tetramethylthiophosphoramidoyl) methylamine P₂S₂N₅C₉H₂₇ [**2**].

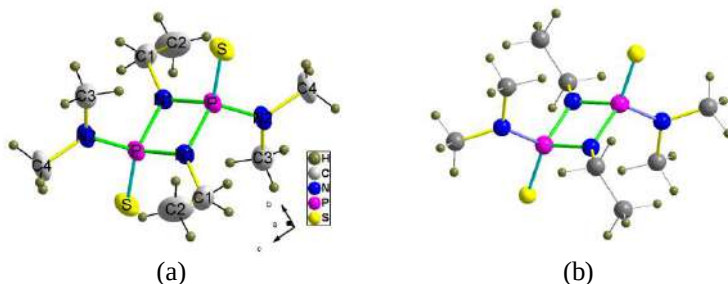


Figure 1: Perspective representation of the [EtNP(S) NMe₂]₂ molecule from: (a) the DRX and (b) DFT calculation data.

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Hydrothermal synthesis of Ni complex: Single-crystal structure, and catalytic evaluation

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A new mononuclear nickel (II) material with bi-atomic bridging ligands has been reported in this paper. This new Ni-based hybrid compound, $[\text{Ni}(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_4]\text{SeO}_4$, has been synthesized by hydrothermal method. The blue crystals are characterized by X-ray single crystal diffraction. They crystallize in the monoclinic system, space group $\text{P2}_1/\text{c}$, with the following unit-cell parameters: $a = 9.6916(2) \text{ \AA}$, $b = 9.7534(2) \text{ \AA}$, $c = 17.8240(4) \text{ \AA}$, $\beta = 93.20^\circ$, $V = 1682.20(6) \text{ \AA}^3$, and $Z = 4$. Their crystal structure consists of metallic cations octahedrally, coordinated by four water molecules and two nitrogen atoms of organic molecule $[\text{NiN}_2\text{O}_4]$, and selenate anion $(\text{SeO}_4)^{2-}$. Their crystal packing is ensured by a three-dimensional network of $\text{O-H}\cdots\text{O}$ hydrogen bonds between the cation and anion moieties, and $\pi\cdots\pi$ interactions between the pyridine rings of the organic moieties of the same layer.

The catalytic study of $[\text{Ni}(\text{dmbpy})(\text{H}_2\text{O})_4]\text{SeO}_4$ on Heck and Sonogashira coupling reactions activated by ultrasonic irradiation results in encouraging yields for a very short duration of time with a very remarkable preference of the form (E) with respect to (Z) during the arylation of styrene. These results allow us to consider this complex as a good catalyst for both types of reactions.

Keywords: hybrid compound, RXD, Catalytic properties.

Graphical Abstract:



Ultrasonic activation of Heck and Sonogashira reaction in the presence of
 $[\text{Ni}(\text{C}_{12}\text{H}_{12}\text{N}_2)(\text{H}_2\text{O})_4]\text{SeO}_4$

Nonlinear optical properties of a new centrosymmetric compound (4-Dimethylaminopyridinium nitrate gallic acid monohydrate).

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A new centrosymmetric material has been successfully synthesized using the slow evaporation method. Despite the fact that of having a centrosymmetric structure, the nonlinear optical properties of our single crystal, which was tested by Kurtz-Perry technique, proved that its second harmonic generation efficiency was 1.22 times more than that of KDP (potassium dihydrogen phosphate) single crystal. This nonlinear optical behavior of the studied compound was also determined through the calculations of polarizability and first hyperpolarizability values. So, we can say that the experimental and theoretical results have shown that this material provides a high value of quadratic susceptibility and certainly having high quality single crystal with equitable thermal stability, valuable transparency and a high nonlinear optical efficiency is the best choice for the technologists. Therefore, the title compound is a suitable choice for doubling frequency.

A green pathway for Friedel-Crafts acylation under solvent free conditions

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Since the pioneering study by Charles Friedel and James M. Crafts [1], the Friedel-Crafts reaction has been drawn in great interest the past several years [2] in the academic and industrial levels. We report here the development of a new green method for the Friedel-Crafts acylation of aromatic compounds with various acid anhydrides using iron (III) under solvent free-conditions. We are especially interested in terms of synthetic step, atom-economy, the efficiently catalytic activity of $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$ and the increased reactions yields. Thus, all the structures were confirmed by spectroscopic data.

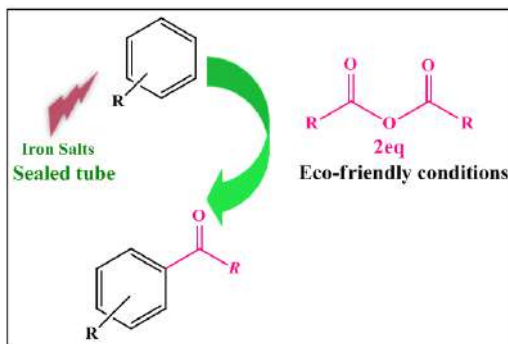


Fig. 1

Key words: Friedel-Craft, acylation, acid anhydrides, iron salts, solvent free conditions, atom-economy, high purity.

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Synthesis, Crystal structure, Electrical conductivity and Dielectric properties of a Decavanadate Cluster

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A new decavanadate cluster $(C_2H_5N_4)_6 [V_{10}O_{28}].7(H_2O)$ (I) has been isolated by slow evaporation at room temperature and characterized by single –crystal diffraction, IR, UV –visible and fluorescence spectroscopy measurement. Compound (I) crystallizes in triclinic system with $a= 11.051$ (4) Å, $b=11.172$ (3) Å, $c= 12.009$ (3) Å, $\alpha= 112.840$ (19)°, $\beta =101.22$ (2)° and $\gamma= 108.11$ (4)°. The structure analysis shows that compound possesses a 3-D supramolecular networks, which is built up of decavanadate anions $[V_{10}O_{28}]^{6-}$, organic cations and water molecules related by multiple H-bonds. Besides, the luminescent emission indicates a blue photoluminescence. Furthermore, the electrical conductivity, the dielectric properties and the relaxation behavior of this material were studied in detail using the impedance spectroscopy technique, in a frequency ranging from 200 Hz to 5 MHz at several temperatures.

Key-Words: Decavanadate. Synthesis. Fluorescence. Electric Conductivity

Biosorption of mercury (II) from aqueous solutions by moringa oleifera bark: equilibrium and kinetic studies.

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A biosorbent prepared from moringa oleifera bark was used to remove mercury (II) from aqueous solutions. The initial pH, biosorbent dose, contact time, and initial mercury concentrations, were evaluated. The ability of moringa oleifera bark to remove mercury at various pH (1 - 8) was studied. The maximum capacity (q_{max}) of biomass Calculated from Langmuir isotherm was found to be 33.22 mg Hg²⁺/g (pH 7). Biosorption equilibrium was established in approximately 120 min. The equilibrium data were described well by Langmuir and Freundlich models. Adsorption kinetics data were analyzed using the pseudo-first-, pseudo-second-order equations. Infrared (IR) spectral and X-ray diffraction (XRD) analysis of pure and mercury loaded biomass were performed. The adsorbed mercury on biomass was desorbed using 10 ml of 4.0 M HCl solution, which it could be reused for other biosorption assays. This study consider the possibility of using bark of moringa oleifera tree as an inexpensive biosorbent for the removal of Hg (II) from contaminated chemical and mining industry wastewaters. It is also suggested that the dried biomass might be simply kept and used in a very low cost metal ion removal system.

Keywords: Biosorption, Moringa Oleifera, Mercury, Isotherm, Kinetic.

Synthesis, structural study and characterization of a new iron complex $[\text{FeCl}(\text{phen})_2\text{H}_2\text{O}]\text{Cl}\cdot 3\text{H}_2\text{O}$

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The title compound, was prepared by slow evaporation at room temperature and characterized through single-crystal X-ray diffraction, photoluminescence, IR and UV-Vis diffuse reflectance spectroscopy (UV/DRS) from which the optical properties were determined (**Fig. 1**).

A new iron complex $[\text{FeCl}(\text{phen})_2\text{H}_2\text{O}]\text{Cl}\cdot 3\text{H}_2\text{O}$ (**1**) crystallizes in the centrosymmetric space group P-1 of triclinic system with the cell parameters: $a=9.718(3)\text{\AA}$, $b=11.512(2)\text{\AA}$, $c=13.066(3)\text{\AA}$, $\alpha=64.13(2)^\circ$, $\beta=86.35(3)^\circ$, $\gamma=78.45(3)^\circ$, $Z=2$, and volume $V=1293.8(1)\text{\AA}^3$.

The asymmetric unit of (**1**) consists of a cationic unit $[\text{FeCl}(\text{phen})_2\text{H}_2\text{O}]^+$, one anionic chloride (Cl^-) and three water molecules of crystallization (**Fig. 2**).

The crystal structure of (**1**) is stabilized by O-H...Cl and O-H...O hydrogen bonds. Moreover, the cations show a π - π interaction [1] adding extra stability to the three-dimensional architecture.

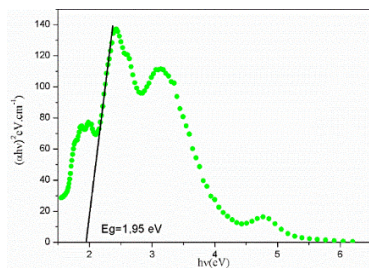


Fig. 1 Tauc Plots of $(\alpha h\nu)^2$ versus $h\nu$.

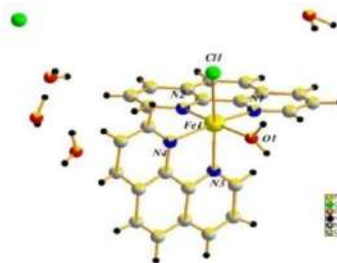


Fig. 2 The asymmetric unit of the crystal

Key words: phenanthroline (phen), crystal structure, photoluminescence, IR, UV-Vis diffuse reflectance spectroscopy.

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HYDROTHERMAL SYNTHESIS OF A TiO₂ MIXED PHASE WITH A HIGH PHOTOCATALYTIC ACTIVITY

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Water pollution resulting from the organic dyes in residential use is becoming a very big problem all over the world. To solve this problem, different works have shown that photocatalysis is an effective solution [1, 2]. Several photocatalysts were used but Titanium oxide offers the most successful application in photocatalysis because of their low cost, high photosensitivity, non-toxicity and environmentally friendly nature [3, 4]. TiO₂ exists in several crystallographic forms, among which there are three of the best known anatase, rutile and brookite. Several research studies have shown that the crystalline form has a great effect on the photocatalytic activity but the size and shape of the crystallites can also play an important role for the degradation of the polluting molecules[5]. In this work the titanium oxide was prepared by hydrothermal root. The synthesized product was characterized by various techniques such as scanning electron microscopy, X-ray diffraction, Raman spectroscopy. The X-ray diffractogram shows that the synthesized material is a mixture of phase: 62% rutile and 38% anatase. Scanning electron microscopy shows that the material is not formally homogeneous. There are elongated shapes that look like needles and agglomerations of fine particles. The SEM photo can explain the result found by the XRD.

The photocatalytic activities of the photocatalysts are evaluated by the photodegradation of methylene blue under UV light irradiation.

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STUDY ON CADMIUM REMOVAL BY PRECIPITATION OF CALCIUM PHOSPHATES POWDERS

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Cadmium is a heavy metal that finds applications in many fields. The human activities related to its exploitation contribute to the contamination of the soil and the groundwater leading to a serious heart to environment and health. Therefore, the technical and economic methods of Cd treatments are of great interest. Among a variety of remediation techniques, in situ phosphate formation has the potential to be relatively one of the most environmentally attractive methods due to approach in which toxic metals are immobilized into a stable edifice of phosphoapatites. This study was conducted to evaluate the efficiency of cadmium removal by a reprecipitation of calcium phosphates.

Thus, hydroxyapatite and tricalcium phosphate having the chemical formula $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ and $\text{Ca}_3(\text{PO}_4)_2$, respectively, were prepared according to the “double decomposition method” by adding a solution of diammonium hydrogen phosphate into a boiling solution of calcium nitrate with a molar ratio of reactants Ca/P equal to 1.67 and 1.55 for hydroxyapatite and tricalcium phosphate, respectively. These minerals were subjected to a characterization by IR spectroscopy and X-ray diffraction technique.

The extraction of Cd from aqueous medium consists in adding various amounts of the dissolved phosphates into the contaminated water at room temperature. The incorporation of cadmium in the apatite structure occurred by pH adjustment. The mixture was stirred for one hour then sampled through filtration. The remaining metal was determined by absorption atomic spectroscopy (SAAF).

Based on the ion exchange mechanism, the obtained phases are solid solutions having the general formula $\text{Ca}_{10-x}\text{Cd}_x(\text{PO}_4)_6(\text{OH})_2$ and $\text{Ca}_{3-x}\text{Cd}_x(\text{PO}_4)_2$. The IR analysis of the solid phases resulting from the depollution experiments revealed a displacement of the vibrational frequencies of the functional groups in both phosphates. That phenomenon indicates the distortion of the PO_4^{3-} tetrahedron induced by the decrease of the lattice volume which is related to the ion exchange occurred in the cationic sites.

According to this study, Cd was immobilized at high levels reaching 8.837 and 2.465 moles per mole of hydroxyapatite and tri-calcium phosphate, respectively. Moreover, the equilibrium extraction was quickly reached mainly for high concentrations. Hence, the proposed technique could be a promising alternative for the neutralization of this element from industrial wastewaters.

Keywords: Calcium phosphates; Cadmium extraction; Wastewaters.

HEAVY METALS RECOVERY FROM AQUEOUS SOLUTIONS BY POLYACRYLIC ACID ASSISTED ULTRAFILTRATION

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Heavy metals that are going out to the environment caused by human activity are or will be in aqueous solution, which must be removed before water recycling or discharging directly into surface (or sometimes subsurface) water. Unlike organic contaminants, heavy metals are not biodegradable and tend to accumulate in living organisms and many heavy metal ions are known to be toxic or carcinogenic. Toxic heavy metals of particular concern in treatment of industrial wastewaters include zinc, copper, and cadmium. Cadmium exposes human health to severe risks. Chronic exposure of cadmium results in kidney dysfunction and high levels of exposure will result in death. Zinc is a trace element that is essential for human health. It is important for the physiological functions of living tissue and regulates many biochemical processes. However, too much zinc can cause eminent health problems, such as stomach cramps, skin irritations, vomiting, nausea and anemia [1].

Copper does essential work in animal metabolism. But the excessive ingestion of copper brings about serious toxicological concerns, such as vomiting, cramps, convulsions, or even death [2].

Nowadays, heavy metals are the most environmental pollutants and becoming one of the serious environmental problems. So these toxic heavy metals should be removed from the wastewater to protect the people and the environment.

Many industries do not treat wastewater contaminated by heavy metals; these latter are rejected in water reserves such as sanitation networks, rivers and sea.

Thus, people need effective water cleaning methods. Among the membrane methods, there are two widely used separation techniques for the removal of heavy metal ions from aqueous solutions: Micellar-enhanced Ultrafiltration (MEUF) [3] and Polyelectrolyte- Enhanced Ultrafiltration PEUF [4].

Membrane filtration technologies with different types of membranes show great promise for heavy metal removal for their high efficiency, easy operation and space saving. The membrane processes used to remove metals from the wastewater are ultrafiltration, reverse osmosis, nanofiltration and electrodialysis. One of the recent developed water treatment processes is the Polyelectrolyte Enhanced Ultrafiltration. This technique combine a membrane filtration process (Ultrafiltration) and a cation–polyelectrolyte complexation technique.

This complexation–membrane technique of filtration proved to be a promising alternative to technologies based on precipitation and ion exchange.

In this proposal, the removal of three heavy metals (cadmium, copper and zinc) from aqueous solutions by polyelectrolyte enhanced ultrafiltration (PEUF) process was investigated. The poly(acrylic acid) (PAA) with an average molecular weight 100 kDa was used as complexing agent. The ultrafiltration experiments were performed using a tangential cell system equipped with a polyethersulfone membrane having a 10.000 (MWCO). To improve the retention of the heavy metal ions, the effect of some operating parameters and solution characteristics were studied.

For different PAA concentrations, all permeate fluxes increased linearly by increasing transmembrane pressure.

For three studied metals, the best retentions were observed at $2 \cdot 10^{-3}$ mol L⁻¹ PAA concentration, 3 bar transmembrane pressure and pH above 5. The removal of cadmium, copper and zinc exceeded respectively 80%, 93% and 70%.

Selectivity was studied using a solution containing three metal ions that demonstrate the copper retention is higher than cadmium and zinc for all PAA concentrations.

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Synthesis, Structural and Spectroscopic Characterization of Hybrid Materials based on polyoxoborates

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A novel Co(II)-hexaborate containing $[\text{Co}\{\text{B}_6\text{O}_7(\text{OH})_6\}_2]^{2-}$ decorated with piperazinium organic cation; $\text{C}_4\text{N}_2\text{H}_{12}[\text{Co}\{\text{B}_6\text{O}_7(\text{OH})_6\}_2]\cdot 6\text{H}_2\text{O}$ was synthesized from aqueous solution and the crystals were grown by the slow evaporation technique and characterized by means X-ray diffraction, IR UV–Vis and fluorescence spectroscopy measurements, elemental analysis and TDA-TG thermal analysis. The powder and single crystal XRD analysis show that the isolated pure crystals crystallizes in the triclinic system. The structure exhibits interesting porous 3D hydrogen-bonded network built by $[\text{Co}\{\text{B}_6\text{O}_7(\text{OH})_6\}_2]^{2-}$ monomers. The piperazinium dications are filled in the free void channels of the inorganic framework and interact by means extensive hydrogen bonds. This hydrated mixed hexaborate thermally decomposed in multiple steps involving dehydration and release of organic cation leading to a novel unknown phase which undergoes crystallization. Moreover, the fluorescent properties of $\text{C}_4\text{N}_2\text{H}_{12}[\text{Co}\{\text{B}_6\text{O}_7(\text{OH})_6\}_2]\cdot 6\text{H}_2\text{O}$ have also been carried out, showing a red photoluminescence.

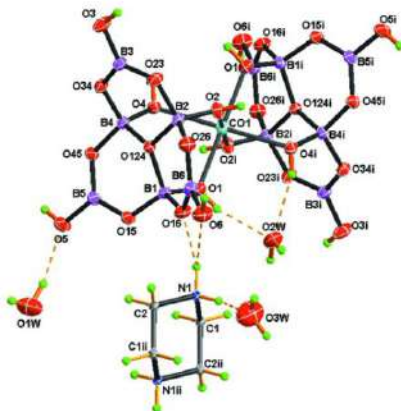


Fig. An ORTEP view of $\text{C}_4\text{N}_2\text{H}_{12}[\text{Co}\{\text{B}_6\text{O}_7(\text{OH})_6\}_2]\cdot 6\text{H}_2\text{O}$ with displacement ellipsoids drawn at the 30% probability level.

Key words: Hydrated Co(II)-hexaborate. X-ray diffraction. Thermal analysis. Photoluminescence.

Synthesis, crystal structure and ionic conduction pathways simulation of $\text{Ag}_{2-2x}\text{Na}_{2x}\text{Mn}_2(\text{MoO}_4)_3$ ($x=0.925$)

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A new mixed molybdate $\text{Ag}_{0.15}\text{Na}_{1.85}\text{Mn}_2(\text{MoO}_4)_3$ has been synthesized by a solid-state reaction and its crystal structure determined from single crystal X-ray diffraction data. It crystallizes in the triclinic system, space group $P-1$, with $a=7.0668$ (7) Å, $b=8.7951$ (8) Å, $c=10.7556$ (9) Å, $\alpha=113.214$ (6)°, $\beta=102.295$ (5)°, $\gamma=103.084$ (3)° and isostructural to $\text{Ag}_2\text{Mn}_2(\text{MoO}_4)_3$. Its structure can be described as being composed of $\text{Mn}_2\text{Mo}_2\text{O}_{14}$ double-chains that are interconnected by corner-sharing with MoO_4 tetrahedra, leading to a three-dimensional framework with channels propagating in [100], [010] and [001] in which the monovalent cations are located. The structural model was validated by the bond valence sum (BVS) and charge distribution (CHARDI) methods. The BVS-P and BVS-E analysis were extended to simulate the ionic conduction properties of monovalent cations in the anionic framework, correlate the crystallographic and electric properties and discuss the effect of partial substitution of silver in $\text{Ag}_2\text{Mn}_2(\text{MoO}_4)_3$ by sodium on ionic conduction.

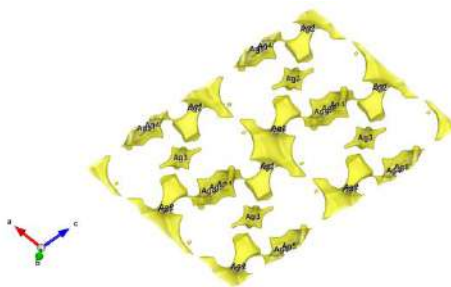


Fig. 1 BVSE maps for sodium paths in $\text{Ag}_{0.15}\text{Na}_{1.85}\text{Mn}_2(\text{MoO}_4)_3$

Key words: Single-crystal structure, Charge-distribution, X-ray diffraction, Bond-Valence-Sum-Pathways (BVS-P), the bond-valence-site-energy (BVS-E).

Synthesis, crystal structure and characterization of a new manganese molybdate $\text{Li}_2\text{Mn}_2(\text{MoO}_4)_3$

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In this paper, $\text{Li}_2\text{Mn}_2(\text{MoO}_4)_3$ compound was prepared by solid-state reaction at high temperature. The Structural, morphological, vibrational and optical properties have been investigated by X-ray diffraction (XRD), atomic force microscopy (AFM), Scanning Electron Microscopy (SEM) and spectrophotometry. X-ray powder diffraction analysis revealed that the titled compound crystallizes in the orthorhombic system with $Pnma$ space group. Microstructural parameters such as crystallite size suggest the good crystallinity of the tittle compound. Vibrational study by means of Raman and FTIR spectroscopies confirms the existence of the MnO_4^{2-} functional group. Optical analysis by means of reflectance (R) measurement allowed us to determine the optical constants for $\text{Li}_2\text{Mn}_2(\text{MoO}_4)_3$ compound. The refractive index dispersion was adequately described by the Wemple-Di-Domenico model. The values of oscillator energy E_0 , dispersion energy E_d , high-frequency dielectric constant ϵ_∞ as well as the ratio of the carrier concentration to the effective mass N/m^* were estimated according to both Wemple-Di-Domenico and Spitzer–Fan models.

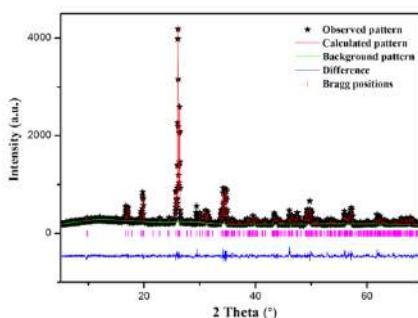


Fig. 1 Rietveld plot of the powder X-ray diffraction pattern of $\text{Li}_2\text{Mn}_2(\text{MoO}_4)_3$

Key words: X-ray diffraction, Rietveld, Optical properties, Optical gap, Refractive index.

THIA MICHAEL ADDITION OF SIMPLE AND FUNCTIONALIZED THIOLS TO DIALKYL (ALLYLOXYMETHYL)PHOSPHONATES USING MILD CONDITIONS

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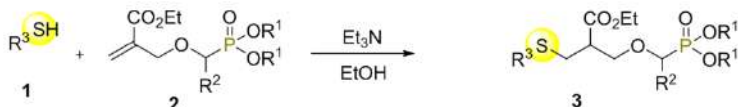
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The Michael addition of nucleophiles to electron deficient alkenes is one of the most efficient reactions in organic chemistry for the formation of carbon–carbon and carbon–heteroatom bonds¹. Among various nucleophilic additions, the reaction of thiols to form a carbon-sulfur bond constitutes a key step in the synthesis of biologically active compounds². Our contribution in this area is to extend the thia Michael reaction on the addition of functionalized thiols **1** to Dialkyl (allyloxymethyl)phosphonates **2** in order to obtain highly functionalized thia Michael adducts **3** under smooth reaction conditions involving Et₃N as the base and ethanol as the solvent. All the synthesized products are characterized by NMR ¹H, ¹³C, ³¹P, and HRMS spectra.



Scheme: Thia Michael addition of various thiols to Dialkyl (allyloxymethyl)phosphonates

Key words: Thia-Michael addition, allyloxymethylphosphonates, thioether.

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Sol-gel synthesis and characterization of rare earth doped TiO₂.

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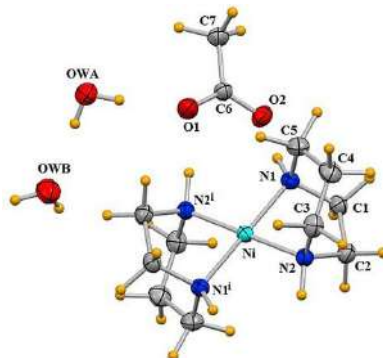
Pure and rare-earth ion (La³⁺, Pr³⁺ and Er³⁺) doped TiO₂ monoliths were prepared through a modified Sol-Gel method. The chemical composition, microstructure and optical properties were characterized using X-ray diffraction (XRD), Raman microscopy, scanning electron microscope, (SEM), liquid fluorescence and the analysis of porosity and surface area (BET method). The XRD and Raman analyses confirm that rare earth doped TiO₂ crystallized in the pure anatase phase. Also, it is found that rare earth ions having practically a total solubility up to 2% mol/mol ratio. Overall, doping very low concentrations of rare earth greatly alters the structural morphology.

A HIRSHFELD SURFACE ANALYSIS, SYNTHESIS, STRUCTURE AND CHARACTERIZATION OF A NEW Ni(II) DIAMAGNETIC COMPLEX WITH THE BIDENTATE LIGAND HOMOPIPERAZINE

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A new Ni(II) complex with the bidentate ligand homopiperazine, $[\text{Ni}(\text{C}_5\text{H}_{12}\text{N}_2)_2](\text{CH}_3\text{COO})_2 \cdot 4\text{H}_2\text{O}$, has been prepared and characterized by single crystal X-ray diffraction, elemental analysis and IR spectroscopy. The basic coordination patterns of the homopiperazine coordinated metal cations are slightly distorted square planar. In the atomic arrangement, the cationic complexes $[\text{Ni}(\text{C}_5\text{H}_{12}\text{N}_2)_2]^{2+}$ are interconnected by the CH_3COO^- anions via $\text{N} \cdots \text{O}$ and $\text{C} \cdots \text{O}$ hydrogen bonds to form layers parallel to the (a, b) plane. These layers are connected by hydrogen bonds generated with water molecules to build a three dimensional network. The charge density of the compound could be refined from X-ray diffraction data measured at cryogenic temperature. Intermolecular interactions were investigated by Hirshfeld surfaces. The title compound is diamagnetic as confirmed by theoretical calculations, allowing its ^{13}C and ^{15}N solid-state NMR spectra to be recorded. Absorption bands were identified by infrared spectroscopy. Electronic properties such as HOMO and LUMO energies were also obtained.



Structure of the title compound showing the atom-numbering scheme and displacement ellipsoids drawn at the 40% probability level. (i: $-x, -y+1, -z+1$).

Keywords: Ni(II) diamagnetic complex X-ray diffraction Coordination compound Hirshfeld surface DFT calculations Solid-state NMR

**(C₄H₁₂N₂) [MnCl₄(H₂O)₂]:
CHEMICAL PREPARATION, CRYSTAL STRUCTURE,
SPECTROSCOPIC ANALYSES AND THERMAL DECOMPOSITION**

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The chemical preparation and the structural characterization of the new complex (C₄H₁₂N₂)[MnCl₄(H₂O)₂] are described. The crystal structure determination shows that the title compound crystallizes in the P-1 space group with the following unit-cell parameters: $a = 6.5983 \text{ \AA}$; $b = 8.2155 \text{ \AA}$; $c = 11.751 \text{ \AA}$ and $Z = 2$. The crystal structure of this salt was solved by Patterson methods and refined by full-matrix least squares on F^2 giving rise to final values of $R = 0.04$ and $wR = 0.13$. The structure of the supramolecular compound consists of manganese(II) cation octahedrally coordinated by two water molecules and four chloride anions $[\text{MnCl}_4(\text{H}_2\text{O})_2]^{2-}$ and piperazinedium cation linked together via two types of hydrogen bonds; O–H...O and N–H...O. The zero-dimensional structure is described as an alternation between cationic and anionic layers along the crystallographic c-axis. The title compound was characterized by several techniques such as single-crystal X-ray diffraction, spectroscopic analyses, IR and Raman, and thermogravimetry. The thermal decomposition of the precursor proceeds through three stages leading to the formation of the manganese oxide as a final product.

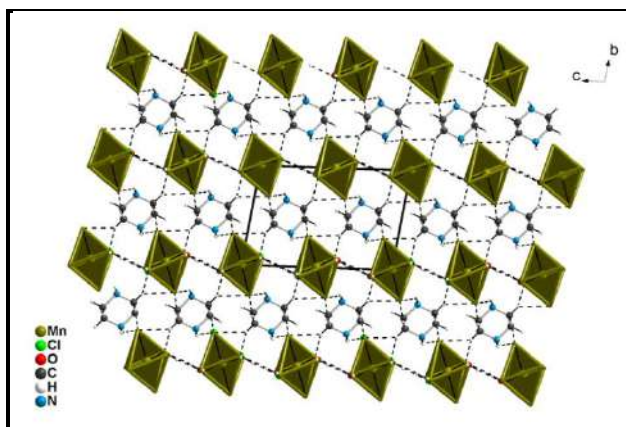


Figure. Projection of the structure of the title compound along the a axis.

Key words: Crystal structure, thermal decomposition, IR and Raman spectroscopy.

Cyclodialcoxyphosphites: Synthesis and stereochemistry of cis/trans 5-methyl-5-propyl-2H-2-oxo-1,3,2-dioxaphosphorinane

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The increasing importance of phosphorus compounds in organic synthesis and biological applications has stimulated advances in dioxaphosphorinane synthesis^[1].

Hydrolysis of diastereomeric 2-chloro-5-methyl-5-propyl-1,3,2-dioxaphosphorinane leads to the formation of corresponding cis/trans 5-methyl-5-propyl-2H-2-oxo-1,3,2-dioxaphosphorinane which are identified by NMR (³¹P, ¹H, ¹³C, MR-SM)^[2].

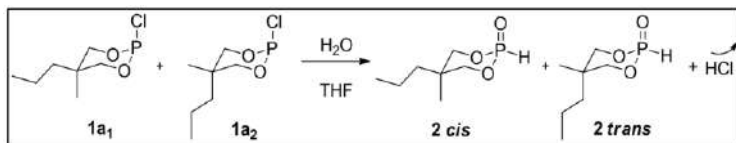


Fig 1. Synthesis of cis/trans 5-methyl-5-propyl-2H-2-oxo-1,3,2-dioxaphosphorinane

There is four possible conformations for 5-methyl-5-propyl-2H-2-oxo-1,3,2-dioxaphosphorinane. In order to determine preferred conformations, density functional theory calculation (DFT) is used.

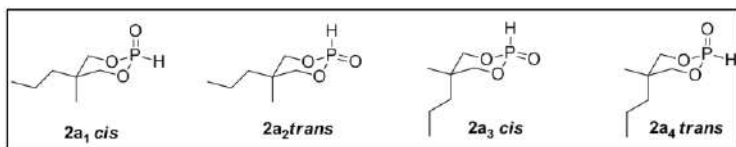


Fig 2. Possible conformations for 5-methyl-5-propyl-2H-2-oxo-1,3,2-dioxaphosphorinane

Key words: dioxaphosphorinane, Hydrolysis, diastereomeric products, density functional theory calculation (DFT)

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Synthesis and characterizations of a copper complex, from a symetric tetradentate schiff base ligand.

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This resume reports the synthesis, spectroscopic characterizations and electrochemical behavior of the obtained tetradentate copper (II)-Schiff base complex with its two wings as ferrocenylaniline moieties. This new ferrocenic derivative with two ferrocenylaniline entities surrounding the copper (II)-Salen complex (FcEDCu) was synthesized by reacting N-ferrocenmethyl-N-phenyl-5-aminomethyl-2-hydroxyacetophenone (FcClm) with one half equivalent of 1,2-diaminoethane in absolute ethanol. As for the intermediates involved in this synthetic sequence, the compound (FcClm) was prepared in tetrahydrofuran (THF) by reacting N-ferrocenmethylaniline (FcAN) with 5-chloromethyl-2-hydroxyacetophenone (Clm).

The compound (FcClm) condensed on the diamine yields the Schiff base ligand (FcED). Under a nitrogen atmosphere and stirring at 50 °C, the ligand dissolved in absolute ethanol with stoichiometric amount of copper acetate monohydrate ($\text{Cu}(\text{COOCH}_3)_2 \cdot \text{H}_2\text{O}$) formed the expected tetradentate Cu(II)-Schiff base complex (FcEDCu) after 6 h of reaction.

All these synthesized compounds gave yields varying from 50 to 90%. Their purities were estimated from elemental analysis while the molecular structures were elucidated with FT-IR, UVeVis, ¹H- and ¹³C- NMR. For the obtained copper complex, it is tetracoordinated in a distorted square planar environment with two nitrogen and two oxygen atoms as donor sites.

Key words : schiff base, ferrocen, metal transition, copper.

Structural, conductivity and dielectric properties of activated clay-based SiP₂O₇ material

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The manufacturing of SiP₂O₇ powder, using low-cost material, namely, phosphoric acid and activated clay (AK) as a natural source of silica, was the purpose of this study. This powder has been obtained at low temperature 350°C. The mineralogical characterization by XRD and NMR analysis showed that the SiP₂O₇ has a well-crystalline structure. The conductivity and dielectric behavior have been studied over a frequency range of 40–5×10⁶ Hz at several temperatures in the range of 20–300°C. The results showed that the SiP₂O₇ have a high ionic electrical conductivity value passes from 2.96 10⁻⁶ Scm⁻¹ at room temperature to 8.8 10⁻³ Scm⁻¹ at 300°C. Furthermore, the powder exhibited high values of dielectric constant (120×10⁵) and loss factor (350×10⁵) at 300°C, these values decreased with the increase of frequency. The imaginary electric modulus (M'') showed that the dielectric relaxation time (τ) almost varies linearly with temperature.

Keywords: Activated clay; Silico-phosphate; Electrical properties; Dielectrics.

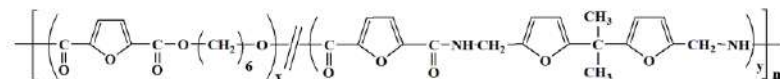
Fully bio based Furanic-Polyesteramides From Renewable Monomers: Synthesis, Characterization and Degradation Study

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Polymers from renewable resources have attracted an increasing amount of attention over the last two decades, predominantly due to two major reasons: Firstly environmental concerns, and secondly the realization that our petroleum resources are finite. Furanic polymers have been considered as alternative environmentally friendly polymers^[1]. In our earlier work, modifying furanic polyesters by incorporation of amide functions along their backbone, lead to a particular class of polymer (polyesteramides), was investigated to combine the excellent mechanical properties of polyamides and the biodegradability of polyesters^[2]. As a continuation of our studies a new series of furanic polyesteramides (PEAFs) was synthesized from mixture of the monomer system (FDCA/DAF/HD) by the melt polycondensation made in two phases. The formation of the expected polyesteramides has been confirmed with NMR1H and FTIR. The hydrolytic degradation in different aqueous conditions (pH= 4.35,7 and 11.9) at 37°C over the period of four weeks show that polyesteramides was stable. The oxidative degradation was also performed in solution composed of 30 vol% H₂O₂ and in solution composed of 20 vol% H₂O₂ in combination with 0.1 M CoCl₂ for 15 days at 37°C. Sample weighting was used to follow the rate of the oxidative degradation and this study highlight the stability of all PEAFs. These polyesteramides behave as amorphous copolymers. Studies are now in progress to explore the mechanical properties of such copolymers.



Keywords: Furanic Monomers, Polyesteramides, Bulk Polycondensation.

References

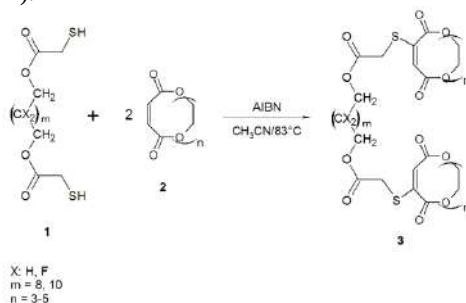
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Synthesis and Physical Chemical Properties of Highly Fluorinated Bolophile Surfactants Derivatives of Crown Ethers Succinate

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Bolophiles are molecules comprising two polar heads joined by one or more hydrophobic chains. Crown ethers and derived surfactants find applications as ion carriers through lipid bilayers¹ and in a lot of membrane mimetic chemistry effects². Due to their peculiar molecular properties, it is expected that alkyl crown ethers may work in ion transport across membranes by a flip-flop mechanism.³ Bolophiles would be able to keep their elongated configuration in bilayers, and thus, may operate as permanent holes in the membrane. In this work we describe the synthesis of nonionic bolophiles from the reaction of fluoroalkylene (dimercaptoacetates) with maleate crown ethers in presence of AIBN⁴ (Scheme 1).



Scheme 1 : Synthesis of bolophiles **3**

Surface activity of the new surfactants was evaluated on the basis of surface tension measurements. The dependence of the surface activity on the structure of surfactants **3** has been studied taking into consideration the length and type of the alkyl chain and the size of the crown ether (polar head). As foreseen, surface tension values of fluorinated bolaamphiphiles **3** are lower than those of nonfluorinated analogues. On the other hand, the increase in alkyl chain length leads to a decrease of surface tension whatever the cyclic size.

Keywords: Bolaamphiphile, Crown ether, Fluorine

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Modelling of Polyphenol Recovery from *Thymus algeriensis* by Response Surface Methodology.

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Thymus algeriensis Boiss. and Reut. (Lamiaceae), popularly known as “mougecha” or “mazoukcha” is prolific in Mediterranean regions, mostly in North Africa, and is used in folk medicine to treat of stomach diseases.

Factorial design and Response Surface Methodology (RSM) were used to model the recovery of polyphenols from **Thymus algeriensis** (TA) by solvent extraction. Experiments carried out according to a Central Composite Design (CCD) allowed evaluation of the effects of temperature, extraction time, solvent composition and liquid-to-solid ratio on the yield of polyphenol extraction. Statistical analysis of the results showed that temperature was the most influential factor. A reduced polynomial model was developed by the stepwise regression method. The model was checked by performing validation experiments both inside and outside the factorial region. A very good agreement was observed between experimental and calculated extraction yields, thus supporting the use of the model to quantitatively describe the recovery of polyphenols from TA.



Fig. *Thymus algeriensis*

Key words: *Thymus algeriensis* and polyphenols.

Texture Evolution of 6060 Aluminum Alloy Processed by ECAP

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Samples of a commercial AA 6060 alloy were subjected to severe plastic deformation at room temperature using equal channel angular pressing (ECAP) up to 12 passes via route Bc. The texture of the processed samples was analyzed through electron backscatter diffraction (EBSD). The texture after ECAP was mainly of ECAP shear type whose components shifted slightly from their ideal positions. It should be noted that the existence of the reinforced A* component after 8 passes may be explained by the excess of the low-angle grain boundaries produced in the sample because of the continuous introduction of dislocations when processing through severe plastic deformation.

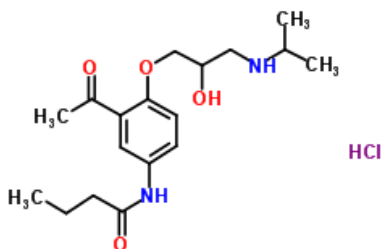
Keywords: ECAP, AA6060, EBSD, texture

STUDY OF THE ACEBUTOLOL DEGRADATION'S KINETIC BY HIGH PERFORMANCE LIQUID CHROMATOGRAPHY (HPLC)

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This work aims to study the acebutolol hydrochloride's intrinsic stability in conditions of forced degradation. The selected pharmaceutical is one of the commonly used β -blockers for the treatment of cardiovascular diseases, which structure is as follows:



Chemical structure of acebutolol hydrochloride.

Successful chromatographic separation of the drug degradation products formed under stress conditions was achieved on Thermo Hypersil (150*4.6mm, 5 μ), using an isocratic method with mobile phase composed of acetonitril: water in the ratio 60:40 v/v adjusted to pH 3.5 with acetic acid. The flow rate was 1.0 mL/min, temperature of the column was maintained at ambient and detection was made at 240 nm.

In addition to chromatographic separation, the identification of degradation products was carried out by using ¹H NMR, ¹³C RMN, IR spectroscopy and UV.

Several stress conditions were tested in order to stimulate the degradation behavior of the target compound.

Forced degradation study of acebutolol under hydrolysis's conditions in acidic forms was accomplished, acebutolol showed significant degradation at concentrations of 0.1 M for 6 hr at 60°C, 70°C, 80°C and 90°C. Moreover the selected compound's Hydrolytic degradation proceeds as a pseudo-first order reaction.

Keywords: Acebutolol, HPLC, degradation.

Aluminum slag effect on the physical properties of natural hydroxyapatite

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Calcium phosphate ceramics represent a family of bone substitute biomaterials due to their specific physico-chemical and biological characteristics. Hydroxyapatite and **tricalcium phosphate** (α -TCP, β -TCP) are usually used as artificial implants in osseous substitution. These materials were imperatively used in biomedical since their composition is closer to that of the bone, as well as to properties of biocompatibility which make them particularly attractive. In this work, we prepared by reaction sintering different composites based of hydroxyapatite by using two different sources of hydroxyapatite such as: the natural phosphate from Djebel el-Onk (Tébessa, East of Algeria) and the bone bovine. Different experimental techniques, including density, porosity, DTA/TG, XRD and SEM techniques were used to analyze the formation and transformation of phases at different temperatures.

Keywords: Hydroxyapatite, biomaterials, experimental techniques.

Magnetism and structure proprieties of nanostructured Fe-Co-Ni-Si alloys prepared by mechanical alloying

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The nanostructured Fe₅₅Co₂₅Ni₁₅Si alloy was prepared by high energy mechanical alloying. The magnetic characterization was studied by SQUID magnetometry in different times. After 100 hours of milling, the hysteresis loops have a low coercive force (H_c), which implies a moderate ferromagnetic behavior. Similarly, by increasing the milling time, values of the saturation magnetization (M_s) and the ratios (M_r/M_s) were changed when machining times are longer. The dissolution of the Si, Co and Ni atoms in the iron lattice favors the formation of solid solutions and the homogeneity of crystalline system induces a behavior of a soft magnetic alloy.

Keywords: Magnetic properties, X-Ray diffraction, solid solutions.

Microwave assisted facile and green route for synthesis of Zn(II) (NO₃)₂ - Amide and Their Antibacterial Activities.

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This work concerned the study of the reactivity of the metal complexes of Zn(II) with two ligands therapeutic in particular the isonicotinohydrazide and the 2-(Phenylcarbamoyl)benzohydrazide. This complexes were isolated by by novel, green routes using sonication, stirring, and microwave irradiation.

They were characterized by methods of analysis such as gravimetric, the IR spectroscopy and spectroscopy UV-VISIBLE. The two ligands were revealed to act like agents bidentate chelating [1].

The antibacterial activity of the ligands and their complexes was evaluated *in-vitro* against two bacteria pathogenic (Escherichia Coli and staphylococcus aureus) by the method of diffusion on agar. The able antibacterial of the compounds is relatively weak for the bacterial stock with gram negative (E.coli) [2]. On the other hand an inhibition is notable for the bacterial stock with gram positive (S.aureus) with the various concentrations (50mg/ml, 100 mg/ml).

Key words: Isonicotinohydrazide, 2-(Phenylcarbamoyl)benzohydrazide, metal complexes, Antibacterienn Activity.

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Synthesis, Characterization, Evaluation of the catalytic activity of Nickel Complexes.

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In this study, we report the synthesis of oximato-nickel complexes by adopting the hydrothermal method. This process is rarely used for the preparation of coordination compounds. New complexes of nickel were isolated and were thoroughly characterized by elemental analyses and the commonly used spectral techniques. EPR investigation confirms the oxidation state of the nickel in all complexes. Infrared spectroscopy (IR) and nuclear magnetic resonances (¹H and ¹³C) indicate the formation and the presence of new reduced forms of oximes within the complexes. The metal complexes have been tested for catalase-like activity in order to assess their catalytic properties.

Keywords: Nickel complexes, hydrothermal method, catalytic properties.

Applicability of electrochemical methods to paper mill wastewater for reuse. Anodic oxidation with BDD and TiRuSnO₂ anodes

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The electrochemical oxidation of paper mill wastewater belonging from Halfa industries (Tunisia) was performed by galvanostatic electrolysis using boron-doped diamond (BDD) anodes and Ti-Ru-Sn ternary oxide (TiRuSnO₂). The effect of several operating parameters, such as applied current density, flow rate, temperature, initial pH value and addition of NaCl was evaluated. Chemical oxygen demand (COD) and ammonium measurements were carried out to study the treatment of the actual wastewater. The energy consumption analysis has been also discussed. The experimental results exhibited that galvanostatic electrolyses with BDD always allowed efficient COD removal in any conditions thanks to the reaction with hydroxyl radicals electrogenerated on BDD surface during electrolysis. On the contrary, using the TiRuSnO₂ anode, the complete COD removal was only obtained in the presence of chloride ions. Comparison of the results of the two electrodes showed that BDD provided a faster removal with higher efficiency and lower energy consumption, while TiRuSnO₂ was more efficient for ammonium removal.

Stability of Hassi-Messaoud Asphaltenes in Media of Different Polarities

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Asphaltenes represent the heaviest and most polar crude oil fractions¹ and are made responsible for many problems in oil industry since they aggregate to form flakes of bigger sizes. This flocculation leads to the formation of deposits which induce the reduction in the production and generate overcosts. The intensities of these drawbacks are intimate related to the physical status (molecular or aggregate) in which the asphaltenic particles are. These problems can be definitively solved only by the thorough comprehension of the factors and mechanisms involved during the process of flocculation.

In this context, we explored the flocculation behavior of asphaltenes, extracted from a deposit recovered from a Hassi-Messaoud oil well field, in solution in toluene according to the polarity of the flocculating medium. The flocculation thresholds related to the addition of two flocculating agents of different polarities (n-heptane and acetone) for three asphaltenic concentrations are obtained by means of the near infra-red absorption spectrophotometry². The Hildebrand solubility parameters³ of the flocculated asphaltenic fractions are deduced using the Donagio method based on the Flory-Huggins theory⁴.

The results obtained indicate that the interactions between the flocculated asphaltenic molecules within the toluene/acetone mixture (the least polar fraction) are weaker than those in the toluene/n-heptane mixture (the most polar fraction).

Key words: Asphaltenes, Hassi-Messaoud, flocculation, close IR spectroscopy, solubility parameter.

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Revised Jiang model's « New formula of Prediction of lattice constant in cubic perovskites »

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ABX₃Perovskite materials are of great interest in the new technology because of the possibility of modifying their physical properties by numerous ionic substitutions.

The mesh parameter prediction model used is useful for providing the predicted structural information for estimating the physical properties of materials for which accurate structural data are not available.

It is also useful as a guide for synthetic exploratory efforts as a starting point for structural characterization improvements of new materials.

Our reformulation of Jiang's model allowed us to obtain a new equation of parameter prediction of cubic perovskite structures taking into account 158 materials.

The results obtained are in good agreement with the experimental with a relative error of the order of 2.64%.

This prediction equation allowed us to predict the mail parameter of 20 new perovskite oxides.

Key words: mail parameter prediction, cubic perovskite, tolerance factor.

Structure and Hirshfeld surface analysis of [C₇N₃H₂₀]₂V₁₀O₂₈·4.21H₂O.

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Crystals of [C₇N₃H₂₀]₂V₁₀O₂₈·4.21H₂O (I) were prepared and characterized through single-crystal X-ray diffraction and IR spectroscopy. The crystal structure of the title salt is stabilized by hydrogen bonds and Van Der Waals interactions. The overall intermolecular interactions involved in the structure were quantified and fully described by Hirshfeld surface analysis. The three-dimensional Hirshfeld surface (3D-HS) [1] and their relative two-dimensional fingerprint plots (2D-FP) [2] reveal that the structure is dominated by H...O/O...H (70.8%) and H...H (18.5%) contacts.

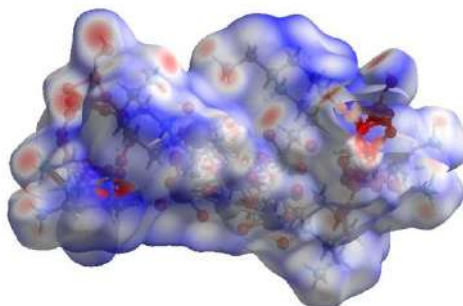


Fig. View of the three-dimensional Hirshfeld surfaces (3D-HS) of (I) mapped over d_{norm} .

Key words: Crystal structure, Hirshfeld surface analysis, Fingerprint plots

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Comparative study of the characteristics and reactivity of catalysts based on acidified mesoporous zirconia and alumina with telluric acid: Acetic acid esterification with ethanol

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Xerogel catalysts are based on zirconia and alumina each one of them is acidified with telluric acid in the same ratio of $n\text{Te}/n\text{M}$ ($\text{M} = \text{Zr}, \text{Al}$), were synthesized by the sol-gel method using a simple drying solvent in an oven.

The characterization of these catalysts was made by N_2 -physisorption, X-ray diffraction, FTIR spectroscopy and adsorption of Hammett's indicators. The reactivity of prepared catalysts was tested in the esterification reaction of acetic acid with ethanol.

N_2 adsorption-desorption shows that the adsorption-desorption isotherm is of type IV for the two kinds of acidified oxides. Whereas acidified alumina have a more developed specific area. The calcination of solids at 500°C causes a considerable decreasing of the specific surfaces but does not change the behavior of the isotherms adsorption-desorption.

XRD analysis shows that the zirconium oxide doped with telluric acid is amorphous. Calcination at 500°C develops the tetragonal ZrO_2 phase. However acidified aluminum oxide presents bohemite (AlOOH) phase which is more developed by calcination.

Analysis by IR spectroscopy shows that doped zirconia with telluric acid is characterized by bands of Te-OH , Te-O , and Zr-O which that of Te-OH disappear completely after calcinations at 500°C . Acidified aluminum oxide is characterized by the same bands of Te-OH , Te-O which that of Te-OH disappear by calcination. However, the bands of Al-O in the bohemite phase increase in intensity by calcination.

Acidity study by Hammett indicators shows that acidified zirconia is more acidic than acidified alumina. This property provides reactivity of catalyst in the acetic acid esterification by ethanol despite a lower specific area.

Keywords: Xerogel; zirconia; alumina; acidified; acetic acid esterification

Chemometrically assisted optimization and validation of reversed phase liquid chromatography method for the quantification of direct acting antivirals in pharmaceutical dosage forms.

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Hepatitis C virus (HCV) infection is one of most deadly diseases in the world. Several direct acting antivirals (DAAs), recently approved, has revolutionized treatment paradigms of HCV. A combination of DAAs has high efficacy and safety in genotype 1, 2, 3 and 4 and is widely used for CHC management. Also, their effects were accompanied with attenuation of liver fibrosis. Furthermore, this combination can be used for treating HCV patients co-infected with HIV. Thus, there is great analytical significance for simultaneous determination of the novel hepatitis C antivirals.

A new procedure for the simultaneous separation of four DAAs by reversed phase high performance liquid chromatography (RP-HPLC) was optimized, developed and validated. It is based on changing gradually the experimental conditions all along the chromatographic procedure as a function of the physical properties of the eluted compounds.

Fractional factorial design was used for screening the most influential factors on separation and time analysis. These significant factors were optimized using central composite design.

The optimum resolution was carried out by using Waters X-Bridge C18 column (150×4.6 mm I.D., 5µm) at temperature of 35°C and acetonitrile/sodium perchlorate buffer (10mM, pH=2.5) (43:57% v/v) as mobile phase at a flow rate of 1.5 mL min⁻¹. UV detection was set at 210 nm. A short chromatographic separation time less than 4 min was achieved. The developed method was validated according to the accuracy profile approach and the method was found specific, precise and accurate. The detection Limits were between 0.07 and 0.13 µg mL⁻¹. Hence, this optimized method can be employed for the routine analysis in quality control laboratories and in dissolution profile studies.

Keywords: Direct acting antivirals, chemometric, fractional factorial designs, response surface, HPLC-UV, accuracy profile.

First principles calculations of the structural and thermal properties of ZnO

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First-principles calculations are performed to investigate the structural and thermal properties of ZnO in Zinc blende and rock-salt structures using the full-potential linearized augmented plane wave method. In this approach, the generalized gradient approximation (GGA-08) and the new form of GGA (WC) which are an improved form of the most popular Perdew-Burke-Ernzerhof (PBE) were used for exchange correlation potentials. Ground state properties such as the lattice parameters a , bulk modulus B and pressure derivative B' have been directly calculated and compared to previous experimental and theoretical results when available. In addition, pressure and temperature effects on the volume cell, the bulk modulus, the heat capacity, and the thermal expansion coefficient are investigated in the 0-25 GPa pressure range and in the 0-800 K temperature range.

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Theoretical investigation of first hyperpolarizabilities of disubstituted benzene: Experimental and theoretical comparison

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Nonlinear optical (NLO) materials can be useful for a variety of applications Computational investigation in electronic and optoelectronic properties of π - conjugated molecules could keep financial capitals and time, but it is important to choose the best method that reproduces experimental results.

To verify the prediction of first hyperpolarizabilities (β) in push–pull (D- π -NO₂) molecules by theoretical semi-empirical (RM1, AM1, PM3, PM6 and PM7), calculations were performed and analyzed through linear fitting analysis to investigate the accuracy of such theoretical predictions in comparison to the experimental ones. Solvent polarity effects on geometry, hyperpolarizabilities, frequencies dispersion and the strength of donor /acceptor pairs are taken into account.

From our results, it is found that solvent polarity, frequency and the strength of substituted groups strongly affect the second-order NLO property of p-NA and its derivatives. Furthermore, RM1 methodology better agrees with (β) experimental results.

Key-words: NLO, push–pull, semi-empirical, solvent, BLA

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Synthesis, Crystal structure, Spectral, Thermal characteristics and Antimicrobial studies of a new hybrid material
 $(C_{11}H_{18}N_2O)_4(Sb_4Cl_{20})_4 \cdot 60$

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A new organic-inorganic hybrid material of formula $(C_{11}H_{18}N_2O)_4(Sb_4Cl_{20})_4 \cdot 60$ was synthesized and characterized by X-Ray diffraction analysis. It crystallizes in the orthorhombic system with the space group $Pca2_1$ and the following unit cell parameters $a=32.6159(5)$ Å, $b=9.0135(1)$ Å, $c=26.3296(3)$ Å, $Z=4$ and $V=7740.47(17)$ Å³. The examination of the structure shows that the two dimensional frameworks are produced by N-H...O and N-H...Cl hydrogen bonding. In addition, the infrared spectrum of this compound reported from 400 to 4000 cm⁻¹ confirmed the presence of the principal bands assigned to the internal modes of cations of the title complex. The optical band gap is calculated and found to be 3.29 eV. The fluorescent properties of this compound have been investigated in the solid state at room temperature. Differential scanning calorimetry (DSC) has revealed a series of endothermic peaks. The synthesized compound exhibited significant antimicrobial activities. The antimicrobial activity of this complex was reported.

Keywords: Chloroantimonates(III), Crystal structure, Spectroscopies, Photoluminescence, antimicrobial activity.

Comparative Study of the γ -Alumina to α -Alumina phase transformation spectra by XDR and FTIR

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In this work, we studied the aptitude to sintering of green bodies using γ -Al₂O₃ transition alumina as raw powder. We focused on the influence of the heating rate on densification and microstructural evolution. Phase transformations from transition alumina $\gamma \rightarrow \delta \rightarrow \theta \rightarrow \alpha$ -Al₂O₃ were studied by in situ X-rays diffraction from the ambient to 1200°C and Fourier transform infrared (FTIR) spectroscopy. XRD patterns revealed coexistence various phase transformations during the heating cycle. FTIR patterns showed that in the range 4000–3000 cm⁻¹ the spectra are characterized by two bands located at 3701 cm⁻¹ and 3630 cm⁻¹, and a wide band centred at 3449 cm⁻¹ for MDD1, and for MDD3 bands are respectively located at 3698 cm⁻¹, 3618 cm⁻¹ and 3453 cm⁻¹, these bands are due to stretching vibration hydroxyls.. DTA and dilatometry results showed that low heating rate leads to a significant reduction of the temperature of formation of the α -Al₂O₃ alumina. It was found around 1190, 1217 and 1240°C when using 5, 10 and 20°C.min⁻¹ of heating rate, respectively. The activation energy for θ -Al₂O₃ $\rightarrow$ α -Al₂O₃ transformation was calculated by Kissinger and JMA equations using dilatometry method were 464.29 and 488.79 kJ/mol, respectively and by DTA method were 450.72 and 475.49 kJ/mol, respectively. In addition, the sintering of the green bodies with low heating rate promotes the rearrangement of the grains during θ -Al₂O₃ $\rightarrow$ α -Al₂O₃ transformation, enhancing the relative density to 95% and preventing the development of a vermicular structure.

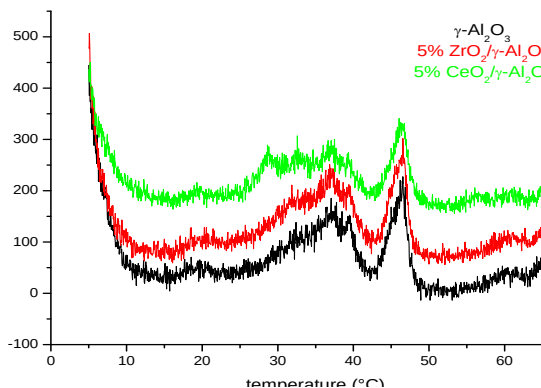
Keywords: Transition alumina, phase transformation, densification, microstructure.

Enhancement of catalytic wet air oxidation of para-hydroxybenzoic acid by $\text{ZrO}_2/\gamma\text{-Al}_2\text{O}_3$ and $\text{CeO}_2/\gamma\text{-Al}_2\text{O}_3$ catalysts

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Catalytic wet air oxidation (CWAO) is considered as one of the most promising techniques of (AOP), it's frequently used for the treatment of wastewater [1]; this work concerns the degradation of p-HBZ acid in aqueous media. The modified aluminum oxide catalysts $\text{ZrO}_2/\gamma\text{-Al}_2\text{O}_3$ and $\text{CeO}_2/\gamma\text{-Al}_2\text{O}_3$, synthesized with simple impregnation, are characterized by X-ray diffraction (X-ray diffraction), N_2 adsorption-desorption and programmed reduction temperature of hydrogen (H_2 -TPR) [2,3]. The treatment of p-HBZ acid was studied under air pressure of 50 bars and at 140  C. The catalytic performances of the developed catalysts were examined and compared with the CWAO tests of para-hydroxybenzoic acid. The results showed a significant increase in the catalytic activity of $\text{ZrO}_2/\gamma\text{-Al}_2\text{O}_3$ compared to Al_2O_3 and $\text{CeO}_2/\gamma\text{-Al}_2\text{O}_3$ matrix.



Keywords: Aluminum oxide $\gamma\text{-Al}_2\text{O}_3$; ZrO_2 ; CeO_2 , CWAO ; parahydroxybenzoic acid (p-HBZ).

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DFT, X-Ray and FTIR studies of the hybrid compound : Cyclohexylammonium Nitrate

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In the last decade, hybrid materials have been intensively studied, they have created large impact in materials research society with their efficiency and supremacy in having multiple desirable properties in one phase [1,2]. In this work, the prepared compound consists of nitrate as inorganic anion and cyclohexylammonium as organic cation. This mix between organic-inorganic matrices, allowed us to obtain an organic nitrate formula ($C_6H_{11}NH_3$)NO₃. The elaborate compound is then characterized by different physico-chemical analytical techniques, a theoretical study is also provided for better interpretation. We report in this work the molecular structure, vibrational frequency, and HOMO-LUMO calculations of the organic cation nitrate ($C_6H_{11}NH_3$)⁺(NO₃)⁻ in the electronic ground state. All calculations were carried out using the density functional method (B3LYP) and the 6-31G* basis set implemented in Gaussian 09 [3]. The optimization of the geometry using the DFT method led to very similar results of the structural data obtained by the technique of X-ray diffraction which validates the calculation method used. A set of H-bonds (N-H...O) in addition to electrostatic and van der Waals interactions, generating a two-dimensional supramolecular network (figure1).

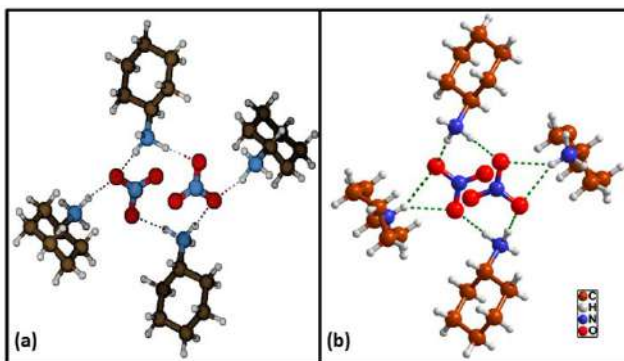


Fig 1: Geometry optimized at DFT / B3LYP / 6-31G * of ($C_6H_{11}NH_3$)NO₃ (a)
Perspective view of the structure obtained by XRD (b)

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DFT, X-Ray, FTIR and biochemical studies of a new compound: trans-2,5-Dimethylpiperazine-1,4-dium tetrachloridocobaltate

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A new two-dimensional (2D) organic-inorganic hybrid compound, trans-2,5-Dimethylpiperazine-1,4-dium tetrachloridocobaltate grown by slow evaporation method at ambient temperature and its structure was characterized by FT-IR, UV and single-crystal X-ray diffraction (XRD) techniques' means. X-Ray diffraction shows that the newly prepared compound crystallizes in the monoclinic system with space group C2/c and cell parameters:

$a = 7.6431(3) \text{ \AA}$, $b = 11.9347(6) \text{ \AA}$, $c = 14.0058(7) \text{ \AA}$ and $\beta = 95.519(4)^\circ$. The structural unit of $[\text{C}_6\text{H}_{16}\text{N}_2]\text{CoCl}_4$ consists of one half cation and one half anion completed by inversion symmetry. The crystal packing is stabilized by **N-H...Cl** and **C-H...Cl** hydrogen bonds. This interaction were investigated by Hirshfeld surfaces.

We have carried out a structural and vibrational theoretical study. The geometry were fully optimized at the DFT/B3LYP/LanL2DZ level of theory to study its structure and vibrational properties. These calculations gave us a precise knowledge of the normal modes of vibration of this compound and were compared to the experimental crystal structure and FT-IR spectra. The antioxidant properties was determined, in vitro, using 1,1-diphenyl-2-picrylhydrazyl (DPPH), hydroxyl radical and reducing power and with ascorbic acid as a control. The results show that the synthesized compound possesses high antioxidant activities.

Keywords:

Crystal structure, X-ray diffraction, DFT calculations, Optimized geometry, Hirshfeld surface analysis, Hydrogen-bonding, Antioxidant activities.

Phytochemical study and evaluation of the antioxidant activity of the most used five plants in traditional medicine to treat diabetes in Oran

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Introduction/Objectives:

Diabetes is one of the non-communicable diseases that constitutes a major public health burden despite the existence of a variety of chemically synthesized medicines for treating this pathology. Currently more and more patients are using herbal medicine. For this, we set the following objectives:

- To determine the rate of type 2 diabetic patients who are using medicinal plants;
- To identify the composition of some ready-to-use herbal teas;
- To perform a phytochemical study about five plants reputed as anti-diabetic.

Material/patients and methods:

An ethnobotanical survey was carried out among 314 type 2 diabetic patients. Data collection was completed via a survey card. The EpiData 3.1 software was used to analyze all investigated parameters.

Composition identification of some herbal teas, sold in our region, intended for diabetics, was performed using a stereoscope, magnifying glasses and a camera.

The first five plants, quoted during our investigation, were considered as antidiabetic and were used for the phytochemical analysis (determination of total polyphenols, flavonoids and condensed tannins) and for evaluating the antioxidant activity. In this part, we were based on spectrophotometry.

Results and discussion:

Our investigation showed that 35.40% of the study population used medicinal plants, of which 56 species were listed belonging to 28 families. The composition identification of the herbal teas revealed several falsifications, which enlightens a bad regulation of these products.

The phytochemical analysis and the evaluation of the antioxidant activity, which were carried out on the five plants: fenugreek, olive tree, white sagebrush, berberis, oregano, showed high contents in total polyphenols, which concord with appreciable antioxidant activities.

Conclusion:

Herbal medicine is still a practice used by diabetics in addition to conventional treatment. The ethnobotanical survey carried out amongst diabetics allowed us to list the main plants used by this population. These plants can offer a broad response to the complex problems of diabetes mellitus and therapeutic perspectives for better management.

Key words: diabetes, herbal medicine, ethnobotany investigation, total polyphenols, antioxidant activity.

Synthesis and structural study of $(C_4N_2H_7)_4(C_6N_2H_{10})V_{10}O_{28} \cdot 2H_2O$

Myriam Louati^a, Roukaya Ksiksi^{a,b} & Mohamed Faouzi Zid^a

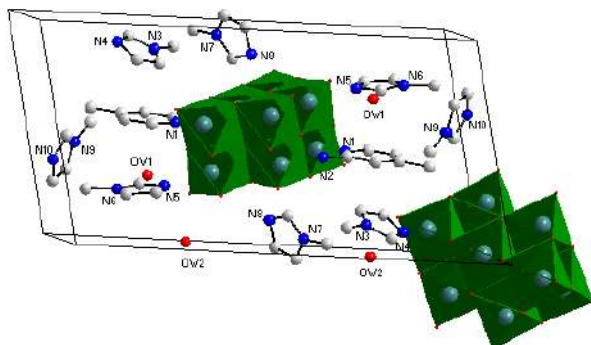
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The polyoxometalates have been extensively studied due to their potential applications in various fields such as catalysis and materials science [1].

A new decavanadate, $(C_4N_2H_7)_4(C_6N_2H_{10})V_{10}O_{28} \cdot 2H_2O$, was synthesized by slow evaporation at room temperature and characterized by single-crystal X-ray diffraction and UV-Vis spectroscopy.

The compound crystallizes in the triclinic system, P-1 space group with the cell parameters: $a=11.200(5)\text{\AA}$, $b=12.056(9)\text{\AA}$, $c=20.511(7)\text{\AA}$, $\alpha=73.40(4)^\circ$, $\beta=84.67(3)^\circ$, $\gamma=63.51(5)^\circ$, $Z=2$ and volume $V=2373.67(1)\text{\AA}^3$.

The formula unit is composed of two centrosymmetric decavanadates $[V_{10}O_{28}]^{6-}$ anions, eight 2-methylimidazolium $(C_4N_2H_7)^+$ cations, two 2-amino-4-picolinium $(C_6N_2H_{10})^{2+}$ cations and four water molecules (Fig 1).

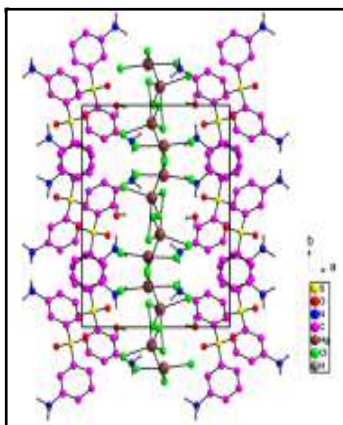


CRYSTAL STRUCTURE, VIBRATIONAL STUDY AND THERMAL DECOMPOSITION OF NEW COMPOUND CONTAINING MERCURY (II)

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A new organic inorganic crystal, $C_{12}H_{14}N_2O_2S(Hg_4Cl_{12})_{0.5} \cdot H_2O$ has been synthesized by slow evaporation. The prepared compound was studied by X-ray diffraction, infrared absorption, Raman spectroscopy scattering, thermogravimetric analysis and differential scanning calorimetric. This compound crystallizes in the monoclinic system and $P2_1/c$ space group. The cell parameters are: $a = 12.4741(5)$ Å, $b = 15.0020(6)$ Å, $c = 11.6397(4)$ Å and $\beta = 101.860(1)^\circ$. The atomic arrangement can be described as inorganic chains parallel to the (b, c) plane at $x=0$ and $x=1$ governed with the organic groups by means of N-H...O and N-H...Cl hydrogen bonds. The mercury environment presented distorted trigonal bipyramidal geometry on the one hand and a trigonal geometry on the other hand. The infrared absorption and Raman diffusion confirms the existence of the different modes of vibration of the groups observed in the structural study. The thermal analysis for the title compound shows two weight losses.



Projection of the structure of $C_{12}H_{14}N_2O_2S(Hg_4Cl_{12})_{0.5} \cdot H_2O$
in the (a, b) plane

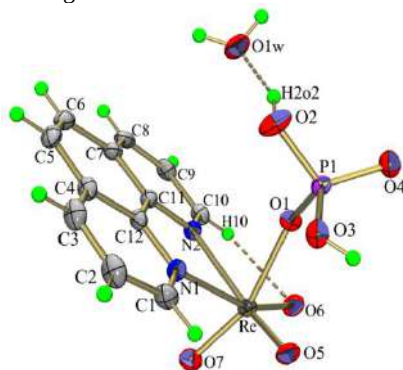
Keywords: X-ray diffraction, Mercury, Hybrid material, Spectroscopic study.

Synthesis, bio-physic-chemical properties and antibacterial Activity of the Re(VII) Complex:

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The coordination chemistry of Re is actually intensively explored owing to use of this element in several fields, more particularly in radiopharmaceuticals for therapy. Rhenium radiopharmaceuticals constitute a class of therapeutic agents in which the bio-distribution is determined by the size, charge and lipophilicity of the complex. Among these compounds, the chemistry of oxo rhenium complexes is of particular interest. The interesting chemistry results from the favorable nuclear properties of the ¹⁸⁶Re and ¹⁸⁸Re nuclides, which make the radioisotopes useful for diagnostic nuclear medicine and applications in radioimmunotherapy. In this contribution, single crystals of a Re(VII) complex, the dihydrogenophosphato phenanthroline tri-oxorhenium monohydrate of formula [ReO₃(phen)(H₂PO₄)]·H₂O [where phen = phenanthroline], were prepared in aqueous solution. X-Rays analysis shows that it crystallizes in the monoclinic space group *P*2₁/*c* with the unit cell parameters: *a* = 8.611(2), *b* = 13.881(2), *c* = 14.502(4) Å and β = 120.87(2)°, *V* = 1487.9(6) Å³ and *Z* = 4. Its crystal structure consists of [ReO₃(phen)(H₂PO₄)]·H₂O units held together by different interactions. The rhenium is in oxidation state (VII), coordinated by two nitrogen atoms of the bidentate phenanthroline, one oxygen of H₂PO₄⁻ and three terminal oxygen atoms in an octahedral environment N₂O₄. The thermal stability, IR, UV/Vis and fluorescence spectroscopic properties and antimicrobial activities against five microbes are given.



An ORTEP view of the title complex. Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented as small spheres of arbitrary radii.

Hydrogen bonds are shown as dashed lines.

DRX study of $\text{Pr}_{1-x}\text{Mg}_x\text{CuO}_3$ for $x = 0$, $x = 0.1$, $x = 0.2$ and $x = 0.3$

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$\text{Pr}_{1-x}\text{Mg}_x\text{CuO}_3$ ($x = 0.0, 0.1, 0.2$ and 0.3) was prepared by Sol-Gel method which is a process based on the hydrolysis and condensation of molecular precursors. In sol-gel method we have used citric acid, ethylene glycol and samples were calcined at 900°C for 10 hours. The sample was characterized by X-ray diffractometry. The prepared sample had single phase perovskite structure. The lattice constant, unit cell volume and average grain size were calculated using XRD data. According full proof soft, $\text{Pr}_{1-x}\text{Mg}_x\text{CuO}_3$ adopts the orthorhombic crystalline system and Pnma space group.

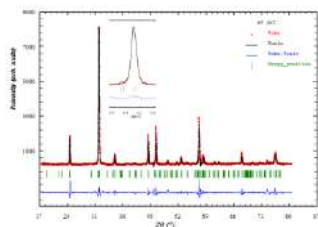


Fig.1 Rietveld fit of XRD patterns of PrCuO_3 at room temperature. The red dots represent the experimental data, the continuous black curve is the calculated pattern, the blue curve at the bottom represent the difference between the experimental and calculated profiles. The green bars show the position of Bragg reflections. Insets show the fitting of the main peaks at around $2\theta = 32.5^\circ$.

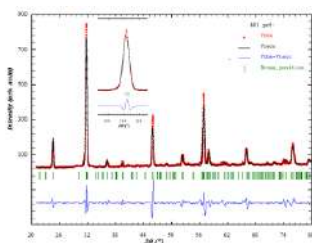


Fig.2 Rietveld fit of XRD patterns of $\text{Pr}_{0.9}\text{Mg}_{0.1}\text{CuO}_3$ at room temperature. The red dots represent the experimental data, the continuous black curve is the calculated pattern, the blue curve at the bottom represent the difference between the experimental and calculated profiles. The green bars show the position of Bragg reflections. Insets show the fitting of the main peaks at around $2\theta = 32.5^\circ$.

Keywords: Perovskite, XRD, full proof, praseodymium, sol-gel, $\text{Pr}_{1-x}\text{Mg}_x\text{CuO}_3$

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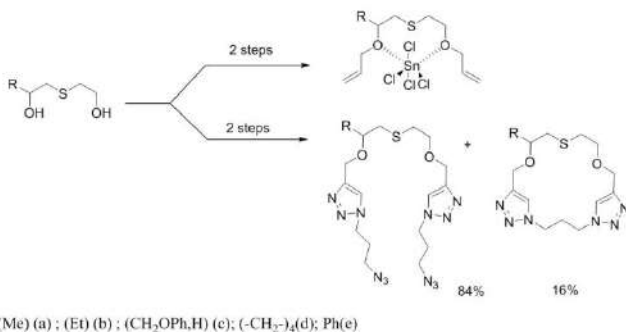
Synthesis and reactivity of 1,5 bis-allyloxy and 1,5 bis-propargyloxy-sulfides

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Sulfur-containing organic compounds have various applications in the area of medicinal chemistry for their antibiotic, antioxidant, calcium channel antagonist, antimicrobial, anti-inflammatory, antitumor, and antiHIV activities¹. β -Hydroxysulfides act as precursors in the synthesis of compounds having biological importance such as pharmacophores². Herein, we report on the synthesis of novel substituted 1,5-bis(allyloxy) and 1,5 bis-propargyloxy sulfides obtained from the products of opening of epoxides by mercaptoethanol³. The study of coordination chemistry of these 1,5-bis(allyloxy) sulfides as new ligands towards tin tetrachloride was carried out. The ¹H and ¹³C NMR data show that both oxygen atoms of these molecules are coordinated to the tin center in a bidentate fashion. The 'click' 1,3-dipolar cycloaddition reaction of 1,5 bis-propargyloxy sulfides and the diazide in the presence of catalytic amounts of copper (I) gives a mixture of the corresponding crown thioether (16%) and the bis azide (84%).



Keywords: Thioethers diol, 1,5-bis(allyloxy) sulfides, 1,5 bis-propargyloxy-sulfide, tin complex,, click chemistry.

¹ Fringuelli F, Pizzo F, Tortoioli S, Vaccaro L. *J Org Chem.* **2004**;69:8780

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Synthesis, Crystal structure, vibrational spectra and optical properties of the novel hybrid bis (4-fluorobenzylammonium) tetrachloridozincate (II)

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A novel organic- inorganic hybrid material $[\text{C}_7\text{H}_9\text{NF}]_2\text{ZnCl}_4$ 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 $\text{P2}_1/\text{n}$ with the following cell parameters: $a = 15.1956(10) \text{ \AA}$, $b = 7.2108(3)$, $c = 36.103(2) \text{ \AA}$, $\beta = 93.100(6)^\circ$, $V = 3950.1 \text{ \AA}^3$ 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 $[\text{ZnCl}_4]^{2-}$ anions and 4-fluorobenzylammonium $[\text{C}_7\text{H}_9\text{NF}]^+$ cations which are interconnected by hydrogen bonding contact $\text{N-H}\cdots\text{Cl}$ 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.

Analysis of organic micropollutants in sediments from the Bizerte Lagoon and Rivers using gas chromatography-tandem mass spectrometry

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16 Polycyclic aromatic hydrocarbons (PAHs), 7 Polychlorinated biphenyls (PCBs), 3 organochlorine pesticides (OCPs) and its isomers, 2 alkylphenols, 8 plasticisers (APS), 9 organophosphorus flame retardants (OPFRs), 3 organophosphorus and Nicotine were studied in sediments from the Bizerte Lagoon (northern Tunisia) and from rivers around the lagoon in April 2017. The samples were extracted by ultrasonic extraction [1] and analyzed using GC-EI-MS/MS [2].

The sum of PAHs concentrations in Bizerte lagoon ($\sum \text{PAH}_{16}$) ranged from 68.03 to 624.50 ng g⁻¹, $\sum \text{APS}_8$ from nd to 6.60 ng g⁻¹, $\sum \text{PCB}_7$ from 4.23 to 14.65 ng g⁻¹, $\sum \text{alkylphenols}_2$ from 1.69 to 70.55 ng g⁻¹, $\sum \text{OPFRs}_9$ from nd to 36.59 ng g⁻¹, $\sum \text{organophosphorus}_3$ from nd to 2.97 ng g⁻¹ and $\sum \text{plasticisers}$ ranged from 1.69 to 70.55 ng g⁻¹.

Concerning the rivers, the sum of PAHs ranged from ($\sum \text{PAH}_{16}$) ranged from 63.35 to 99.46 ng g⁻¹, $\sum \text{PCB}_7$ from 1.06 to 5.65 ng g⁻¹, $\sum \text{plasticisers}_8$ ranged from 0.64 to 7.07 ng g⁻¹. And for the organophosphorus, Alkylphenols (APS) and OPFRs are not detected in these samples.

Nicotine is not detected in all samples.

Keywords: HAP, PCB, POC, OPFRs, APS, organophosphorus, plasticisers, Ultrasonic extraction, GC-EI-MS/MS.

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Development of SPE Method for the Analysis of POPs in treated waste water

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This study is interested to the developpement of SPE method to analyze the residue of 9 congeners of polychlorinated biphenyles (PCB) and 6 organochlorine pesticides (POC) in treated waste water by gaz chromatography (CPG-ECD) [1]. This study has allowed us to became familiar with several technics and methodologies of analysis of organic compound.

The protocol used for the treatment of water is solid phase extraction (SPE). It's easy to applied and gived a good recoveries between 70 and 94%.

Levels of PCB and POC measured in samples shown a general contamination with a variable concentration. The highest concentration for highly chlorinated congeners was in relation to their high bioaccumulation [2].

Key words: PCB, POC, SPE, GC-ECD.

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Adsorption of Lead and Cadmium Pb(II), Cd(II) by a derivative of phenolic resins

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In this work, we are interested in the capacity of a synthesized derivative of phenolic resins to adsorb cadmium Cd^{2+} and lead Pb^{2+} , and to determine the factors conditioning the fixing process : kinetics and equilibrium in batch conditions.

This resin has been characterized by spectroscopy IR, NMR^1H , NMR^{13}C and viscosity.

We also showed, through a thermodynamic study, that the two isotherms of adsorption for lead and cadmium on the resin are in conformity with the Langmuir model in the range of the studied concentration, with a maximum adsorption's capacity about 27,54 mg/g for lead and 8,06mg/g for cadmium.

Key-words : p-hydroxybenzoic acid, synthesis, phenolic resins, lead, cadmium, adsorption.

Morphological design, hierarchical structure and fiber swelling properties of fibrous networks from *Opuntia* (Cactaceae)

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The present study focuses on the morphological, hierarchical and swelling fibre characterizations of natural cellulosic fabric from *Opuntia* (Cactaceae). This plant was constituted by numerous separated fibrous layers with intricate structures. The detailed arrangement, layer distribution, fibre thickness, bulk density and fibre swelling (water uptake test) of the fibrous networks were determined. The studied fibrous networks exhibit good layer distribution, different values of bulk density and important rate of water uptake. The morphological design (topology and geometric parameters), hierarchical structure (internal and anatomical structures) of fibrous networks were studied using both bright-field microscopy and scanning electron microscopy. The fibrous layers present high diversity of fibres (macro and microstructures) having a complex hierarchical structure.

Keywords: *Opuntia* (Cactaceae), fibrous networks, design, hierarchical structure, fiber swelling.

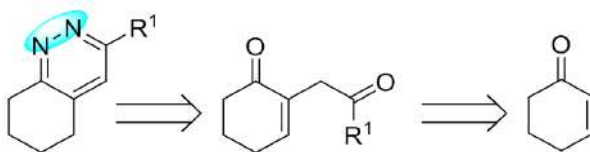
EFFICIENT ACCESS TO CINNOLINIC DERIVATIVES FROM 1,4-DIKETONES: EVALUATION AS ANTIBACTERIAL AGENTS

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Over the last decades, several synthetic strategies have been developed allowing the preparation of many heterocyclic compounds such as : furan, pyrrole, thiophene and cinnolinic derivatives.¹ Indeed, Cinnolinic derivatives have been shown to act as anticancer, fungicidal, bactericidal and anti-inflammatory.^{2,3} Several methods have been developed for the synthesis of many derivatives of cinnolines these last years. In this context we have focused our attention into the preparation of new cinnolines using 1,4-diketones. Herein we propose a new and simple strategy based firstly on the synthesis of 1,4-diketones from 2-cyclohexen-1-one then the preparation of cinnolinic derivatives in simple conditions. Our previous work demonstrated that the synthesized compounds showed good antibacterial activities.



Scheme : Access to 3-alkyl-5,6,7,8-tetrahydrocinnolines.

Key words : 1,4-diketones, cinnolines, antibacterial activities.

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Chemical composition determination of different date palm organs using HPLC-DAD-ESI-MS/MS method and related biological activities

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Date palm is a particularly vital plant in arid and semi-arid regions of the world. Chemical composition of different date palm organs and related biological activities were studied here. Ethanolic extracts of pollen, male and female flowers and fruits were investigated. Twenty compounds were tentatively identified using HPLC-DAD-ESI-MS/MS analysis, on the basis of their mass spectra in full scan mode (MS). Besides two fatty acids, one lipid and five phenolic acids, twelve flavonoids were identified which are derivatives of quercetin, luteolin and isorhamnetin. Total phenolic (TPC), flavonoid (TFC) and tannin (TC) contents were determined for all organs. The highest TPC and TFC values were noted in pollen extract. TC recorded values varied in the following order: fruit □ pollen □ male flower □ female flower. The role of the studied organs in diabete and obesity was investigated.

SYNTHESIS, CRYSTAL STRUCTURE, PHYSICOCHEMICAL PROPERTIES OF AN HYBRID COBALT (II) HALIDE MATERIAL WITH HIRSHFELD SURFACE ANALYSIS AND MAGNETIC PROPERTIES

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A new complex of cobalt (II), (C₁₁H₁₈N₂O)CoCl₄, has been synthesized and structurally characterized. Crystal structure determination shows that the compound crystallizes in Pbc_a of the orthorhombic system. The Co (II) centre has distorted tetrahedral geometry. Furthermore, the organic cation develop in parallel chain. The structure is stabilized by different hydrogen bonds ensuring the interaction between the organic and inorganic entities to give 3D frameworks. The interactions variability of the independent units in this material is analyzed via Hirshfeld surface analysis. The IR spectrum prove the existence and independence of the organic and inorganic groups as well as a water molecule. The suitability of the crystal for optical application was studied by UV-Vis spectroscopy. The fluorescence spectral analysis of the compound shows double emission between 300 and 335 nm. The thermal stability of the compound was investigated by differential scanning calorimetric. Magnetic susceptibility measurements indicate that the crystal exhibits a weak antiferromagnetic coupling interaction. The bioassay results showed that the structure exhibits significant antibacterial and antifungal activities.

Keywords: Metal transition, Crystal structure, Hirshfeld surface, Spectroscopies, DSC thermogram, Antiferromagnetism.

Influence of concentrations Zn^{2+} on Raman and photoluminescence spectra of TiO_2 -ZnO film modify by anodic anodizing.

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Titanium dioxide (TiO_2) thin films were modified by anodic anodizing using different concentration of Zinc. The crystalline of the film has improved with the increase Zn^{2+} concentrations. The X-ray diffraction and Raman scattering results showed that the incorporation of Zn^{2+} into TiO_2 impedes the rutile-phase growth, facilitates the anatase phase growth and promotes the formation of the junction TiO_2 -ZnO. The effect of Zn^{2+} concentration on optical, photoluminescence and Raman spectra of TiO_2 films were investigated.

The peaks in Raman spectra depicts that they TiO_2 films were anatase phase and heterojunction is formed by increasing the ZnO level during synthesis by the electrochemical method. The films show high refractive index, good optical quality and photoluminescence characteristics suggest that possible usage in opto-electronic and optical coating applications.

Keys words: TiO_2 , ZnO, Photoluminescence, Raman, anodic anodizing

Electromechanical actuator based on poly(vinylidene fluoride) with ([C₂mim][Cl]) and its electrodeposition on a platinum surface

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Low voltage actuator based on poly(vinylidene fluoride) (PVDF) with 40% 1-ethyl-3-methylimidazolium chloride ([C₂mim][Cl]) is prepared by solvent casting in order to evaluate the effect of anion size in the bending properties. The addition of IL leads to the crystallization of PVDF in the β -phase and decrease significantly the degree of crystallinity and the elastic modulus. The bending movement of the IL/ PVDF composite is correlated to their degree of crystallinity, mechanical properties and ionic conductivity value [1]. By means of cyclic voltammetry study in acetonitrile solution, we show that our blend undergoes an irreversible oxidation step and a consecutive electrodeposition step at a platinum disk.

Keywords: PVDF, Ionic liquid, Actuators, Bending, Cyclic Voltammetry

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Occurrence of halogenated and organophosphate flame retardant in eel (*Anguilla Anguilla*) from Bizerte Lagoon.

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Classic (polybromodiphenyl ethers, PBDEs) and emerging halogenated flame retardants (HFRs) such as hexabromobenzene (HBB), pentabromoethylbenzene (PBEB), decabromodiphenyl ethane (DBDPE) and halogenated norbornenes (HNs), as well as organophosphorus flame retardants were analyzed in 24 eel (*Anguilla Anguilla*) samples collected from Bizerte Lagoon, northern Tunisia. Agilent 7890 gas chromatograph connected to an Agilent was carried to the analysis of PBDEs, emerging PBDEs and HNs. As regards OPFRs were analyzed by LC-MS was performed with Thermo Scientific TurboFlowTM system. The levels of PBDEs, HNs and OPFRs ranged between 3.9 to 58, <loq to 103, and from 32.5 to 2161 ng/g lipid weight (lw) respectively. Thus, the levels of OPFRs are higher than both PBDEs and HNs.

PBDEs and HNs concentrations in (*Anguilla Anguilla*) samples are similar or slightly lower than other reports for other species. The health risks bounded to the consumption of sea urchin in Bizerte city no threat to public health concerning PBDE intakes.

Keywords: Bizerte lagoon, Halogenated norbornenes, PBDEs, OPFRs, *Anguilla Anguilla*.

Analysis of metabolites of organophosphorus flame-retardants in biological matrices using on-line turbulent flow chromatography-liquid, chromatography tandem mass spectrometry.

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A fast on-line analytical method based on combination with tandem mass spectrometry (MS-MS) has been applied for the analysis of eight metabolites of organophosphorus flame retardant (OPFRs) in human urine. The extraction was performed by centrifugation, followed by solid phase extraction (SPE), and then the extracts were directly injected to the chromatographic system. The analytes were purified into the cleanup-loading column. Thus, the analytes were passed into the analytical column for subsequent detection MS-MS. Analytical parameters display adequate, recoveries between (52 and 102%), with very low relative standards deviation (RSD) between (1.06 and 7.08). Moreover, mLODs ranged between (3.6×10^{-4} and 1.07 ng), mLOQs ranged between (1.2×10^{-3} and 3.57 ng). This new methodology for the analysis of metabolites of organophosphorus was demonstrated by the analysis of real samples corresponding to human urine with levels ranged between <loq and 186.53 ng.

Keywords: metabolites of organophosphorus, pressurized liquid extraction TFC-MS-MS, urine sample.

Temperature effect on the hydroxyapatite synthesis by the sol-gel route

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Loss of materials or bone reconstruction requires the research and development of biomaterials with specific characteristics for use in the human body. Research is more concerned with biocompatible materials that form a direct biochemical link when implanted in the human body, for example, hydroxyapatite. Hydroxyapatite (HA) is one of the most commonly used biochemical due to its similarity with the bone matrix. Its chemical formula (HA) $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ is a very important inorganic substance. The first bone mineral component is tooth enamel and ivory. It is very flexible in terms of composition and configuration. HA is known as a non-absorbable bioceramic and is mainly used for many medical applications due to its bio-compatibility with biological activity. The objective of this work is to study the effect of different temperatures (25 °C, 50 °C, 70 °C, 90 °C) on the formation of hydroxyapatite by sol-gel. It is possible to obtain well-crystallized hydroxyapatite at 700 °C. Formation of primary calcium nitrate and triphosphate. The synthesis was performed for 3 days. One day for stomach aging; one day to get a gel, one day to dry the gel. The results obtained at temperature 90 showed improvement in hydroxyapatite preparation in a liquid-gel method compared with different temperatures. The powder was prepared at 90 °C to dilute the solutions and obtain gel and dry the gel during 24h. X-ray analysis also showed hydroxyapatite after heat treatment.

Keywords: Hydroxyapatite, Sol-Gel route, Temperature

Efficient facilitated transport of lead and cadmium across a plasticized cellulose triacetate and polymer membranes mediated by crown-ethers.

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Polymer inclusion membranes (PIM) used for selective transport and separation of metal-lic ions has emerged in recent times. Their expansion depends on the method of preparation and their structure. This paper reports on the synthesis of a novel class of polymer inclusion membranes based on two polymers cellulose among which triacetate (CTA) plasticized by 2-Nitrophenyl pentyl-ether (NPPE) and doped with crown ethers incorporated into the poly- mer as a metal ion carrier. All the membranes were characterized by several techniques as well as Fourier Transform Infra - Red (FTIR), X-ray Diffraction (XRD), and Thermogravimetric Analysis (TGA). As application, transport of Pb(II) and Cd(II) ions in polymeric membranes (PIM) was studied. Overall, our results showed that the addition of plasticizer with two polymers resulted in homogeneous and hydrophobic membranes whose physical properties, such as density, thickness, and hydrophobicity, were modified. All membranes were thermally stable up to nearly 200 C. The study of the transport across a polymer in- clusion membrane has shown that the lead or cadmium transport efficiency was increased using NPPE as carrier.

Keywords: Key words: Polyvinyl alcohol, Cellulose triacetate, NEPP, polymers, membranes, heavy metals.

Transesterification reactions in 70PC30PET/MMT composites with and without catalyst

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The study presented deals with the reactive compatibilization of two thermoplastic polyesters, namely polycarbonate (PC) and poly (ethylene terephthalate) (PET), by transesterification reactions. For this, a catalyst, which is hydrated samarium acetylacetonate ($\text{Sm}(\text{acac})_3$), is incorporated with concentration of 0.01 phr into the 70PC/30PET mixture.

The organophilic nanoclay Nanomer 1.34TCN (MMT) was also added, at concentration of 3 %, to the mixtures with and without catalyst, to highlight the effect of the particles of the nanofiller, on the one hand on the dispersion of PET into the PC matrix in the absence of $\text{Sm}(\text{acac})_3$, and on the other hand on the intensity of the exchanges between the two polymers and this function of the concentration of the catalyst.

The characterization of the blends and composites by the different experimental techniques, in particular differential scanning calorimetry and thermogravimetry, revealed that, by increasing the catalyst concentration, significant variations are noticed on the structural and thermal properties. These modifications, due to the interfacial reactions between the two phases of the system, were also evidenced by variations in chemical and morphological properties observed after the study of solubility and atomic force microscopy (AFM). On the other hand, the characterization of the 70PC/30PET/MMT composite suggested that in the presence of the nanofiller, the inter-exchange reactions between the two polymers were relatively less intense.

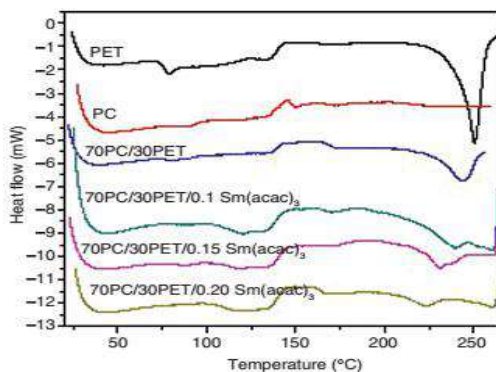


Figure : DSC thermograms of neat polymers and 70PC/30PET mixtures melt blended with and without $\text{Sm}(\text{acac})_3$.

Relationship between the diffraction peak intensity and composition in $(\text{Ti}_{1-x}\text{W}_x)\text{C}$ powders

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In this work, nanostructured $(\text{Ti}_{1-x}\text{W}_x)\text{C}$ ($x = 0$ and $x = 0.2$) powders were synthesized by mechanical alloying (MA) of Ti, W and C powder mixture. The mechanical alloying was performed in an argon atmosphere using a high-energy planetary ball mill. The powders were characterized by X-ray diffraction (XRD). The relationship between the changes in diffraction peaks intensity and the composition of obtained powders was determined by using the structure factor calculations. However, the obtained results were compared with the theoretical ones.

Keywords: Nanocrystalline; TiC; Mechanical alloying (MA); X-ray diffraction; Composition; Diffraction peak.

Mechanism of synthesizing nanocrystalline TiCrC powders in different milling atmospheres

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Nanocrystalline TiCrC powders were produced by mechanical alloying (MA) from the mixture of titanium, chromium and graphite in vacuum and argon atmospheres, respectively. MA was carried out in a high-energy planetary ball mill Fritsch Pulverisette 7, at room temperature. The morphology and the phase transformation of the powders were characterized by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The results showed that synthesizing mechanism and reaction velocity changed when Ti, Cr and C mixture were milled in different atmospheres. It was found that nanocrystalline (Ti,Cr)C were formed after 5 hours of milling in argon atmosphere and vacuum.

Keywords: Mechanical alloying (MA); Carbide; Microstructure; Powders; X-ray diffraction; Nanocrystalline.

Properties of P-doped $\text{La}_2\text{Mo}_2\text{O}_9$, oxygen ion conductors: Molecular structure, ^{139}La and ^{31}P NMR, and vibrational studies

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The effect of partial substitution of molybdenum by phosphorus on the global and local structural arrangement of the fast oxide-ion conductor $\text{La}_2\text{Mo}_2\text{O}_9$ (LAMOX) has been studied by X-ray powder diffraction as well as ^{139}La and ^{31}P solid state NMR. The diffraction patterns show that $\text{La}_2\text{Mo}_{2-y}\text{P}_y\text{O}_{9-y/2}$ forms a solid solution at low phosphorus concentrations, and that there is a structural phase transition upon increasing phosphorus concentration. This phase transition is also reflected in ^{139}La and ^{31}P NMR spectra. The possibility to excite ^{31}P multiple-quantum coherences of one of the ^{31}P NMR signals gives evidence of an accumulation of phosphorus atoms on neighbouring Mo-type sites already before formation of three-dimensional precipitates. On the basis of our X-ray and NMR results we propose a possible structural arrangement of the compound $\text{La}_2\text{Mo}_{2-y}\text{P}_y\text{O}_{9-y/2}$ that explains the experimental observations by crystal twinning. From infrared and Raman analysis it is confirmed that different vibration modes arise from the vibration of molybdenum–oxygen bands. Mo–O bond lengths are also found to be independent of P-doping.

Key words: $\text{La}_2\text{Mo}_2\text{O}_9$; X-ray powder diffraction; $\text{La}_2\text{Mo}_{2-y}\text{P}_y\text{O}_{9-y/2}$; ^{139}La and ^{31}P NMR; Infrared and Raman spectroscopy.

Study of Effect of aluminum addition on the sintering of hydroxyapatite

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In this paper, the effect of aluminum addition on the sintering of natural hydroxyapatite was investigated. Hydroxyapatite (HAp) bioceramic material have been widely applied as bone substitutes because of its excellent compatibility with the human body. Hydroxyapatite is one of those few ceramic materials which are bioactive. The addition of aluminum to the hydroxyapatite have been carried out to improve properties of sintered HAp. By mechanical treatment, hap properties were studied according to the different milling time. The reactions and phase transformations between hydroxyapatite and aluminum metal powder were studied using XRD, Raman spectroscopy and SEM. All samples were characterized by apparent density and open porosity measurements. The results of the mixture of hydroxyapatite and aluminum powder showed the formation of differents phases after high time of milling at high temperature. The addition of aluminum resulted the partial decomposition of hydroxyapatite at high temperature.

Keywords: Hydroxyapatite, aluminum, bioceramic, transformation, mechanical treatment.

Effect of aeration flow on the bioremediation of total hydrocarbons contaminated soil

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The impact of hydrocarbons on the environment remains a subject of great importance; this is due to their toxicity even at low concentrations. These harmful substances constitute a major part of soil and groundwater contamination, so their treatment is necessary. For several decades and until today, biological techniques have been particularly attractive in the treatment of soil, because they are cost-effective and eco-friendly.

In this framework, we were interested on variation of air flow in the bioremediation of soil polluted by total petroleum hydrocarbons (TPH) that was sampled from an old service station.

After physicochemical and biological characterization of the soil and the state of its pollution (initial concentration of the TPH = 90 g/kg of dry soil), three reactors gas-solid covered with aluminum foil were prepared, each containing 700g of sieved soil (<0.08mm) to follow different treatment by biostimulation at different air flow (Q), treatment A (Q1=0.6mL/min), treatment B (Q2=0.8mL/min) and treatment C (Q3=1mL/min). To study the performance of treatments recommended we conducted a control treatment without aeration (D). The various systems were incubated during 70 days in closed systems shielded from the light to avoid photo-oxidation and in a constant temperature equal to 28°C. Soil samples were collected periodically in different systems and were analyzed for TPH, biomass, humidity and pH.

It appears from the various tests that aeration flow hasn't a significant influence on biodegradation activity. Removal efficiency varied between 50 and 57 %, and the best rate was shown at low flow. This degradation were accompanied with increase of total microorganisms from $4.9 \cdot 10^4$ to meet the most favorable terms of an order of 10^7 CFU/g of soil.

We conclude from this study that the presence of nutrients in bioremediation process is more important than the presence of aeration.

Microstructure and thermal analysis of Fe-Mo nanostructured alloys

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Nanostructured materials are new functional materials with interesting properties, which play an important role in the materials science and engineering. The microstructural refinement is usually accompanied by enhanced mechanical and physical properties of the nanostructured materials. For this, their formation mechanism, structure and physical properties investigations have attracted increasing attention. In the present work, nanocrystalline iron based $\text{Fe}_{1-x}\text{Mo}_x$ solid solutions with x in the range ($0 \leq x \leq 1.6$ at. %) were prepared by mechanical alloying from elemental Fe and Mo pure powders. The effects of milling time and Mo concentration on the morphology, microstructure and thermal stability of the obtained powders were investigated by scanning electron microscopy (SEM) and differential scanning calorimetry (DSC) techniques. The SEM micrographs analysis indicates that the powders morphology is milling time and Mo concentration dependent. The DSC thermograms investigation show the presence of broad exothermic peaks, generally related to the structural relaxation and grain growth.

Keywords: Fe-Mo alloys, DSC, morphology, thermal stability.

Effect of the substrate and deposition time on the electrodeposited nanostructured Cobalt thin films

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During the last decades, nanostructured materials have attracted considerable attention owing to the wide range of their potential applications. The decreasing of the crystallite size to the nanometer scale is an effective way to enhance the mechanical and physical properties of nanostructured materials. In this paper, nanostructured Co thin films were electrodeposited on Cu and Sn substrates in sulphate solutions containing boric acid. The experiments were carried out in a conventional two-electrodes electrochemical cell at room temperature in an acidic environment with pH=6. Different deposition times (10, 15, 20 and 30 min) were performed during the process in order to study the formation mechanism of the particles. The effect of the deposition time, applied current density and substrate on the physical properties of Co nanoparticles has been investigated using XRD, DSC, SEM techniques.

The obtained results confirm the thermal transformation phenomenon of the cobalt coatings with different structures. The Co films thickness is sensitive to the substrate material, the applied current density and the deposition time. Thus, an increase in the thickness of the layers with the increase of the deposition time was observed for different experimental conditions.

Keywords: nanostructured alloys, Electrodeposition, DSC, thin films.

Synthesis, crystal structure, vibrational and optical properties of a new Pb(II) complex (2-hydroxyethyl)piperazine-1,4-diium tetrachloroplombate(II) $C_6H_{16}N_2OPbCl_4$

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A novel hybrid material, $C_6H_{16}N_2OPbCl_4$, has been successfully synthesized in nitrogen atmosphere by slow evaporation at room temperature. The compound structure was determined by single-crystal X-ray diffraction and crystallizes in the triclinic space group P-1 ($a = 5.9926(2)$ Å, $b = 10.3691(5)$ Å, $c = 11.3558(4)$ Å, $\alpha = 111.755(4)^\circ$, $\beta = 96.080(3)^\circ$, $\gamma = 105.948(4)^\circ$, $Z = 2$) at 293 K. The structure is built up from anionic 1-D polymeric chains of $PbCl_4O$ octahedral extended along the $(b + c)$ -axis. These chains are interconnected O-H...Cl hydrogen bonds to form inorganic layers parallel to $(a, b + c)$ plane. The organic layers are inserted between the inorganic ones and connect them through N-H...Cl and C-H...Cl hydrogen bonds to build a three dimensional network. To gain more information about intermolecular interaction we used Hirshfeld surfaces associated with 2D finger plots. The optical and PL properties of the compound were investigated in the solid state at room temperature and exhibited two bands at 250 and 290 nm and a photoluminescence emission at 529 nm. Raman and infrared spectra were used to gain more information for vibrational modes of the title compound. As for thermal analysis, DSC analysis shows that this compound is stable at temperature below melting point. Finally, XPS analysis is achieved for analyzing the surface chemistry of $C_6H_{16}N_2OPbCl_4$ crystals.

Keywords: Organic-inorganic hybrid; X-ray diffraction; Spectroscopy IR and Raman; Hirshfeld surface; Optic study; XPS and DSC.

Elaboration and characterization of Co-Fe-B-Ta alloy

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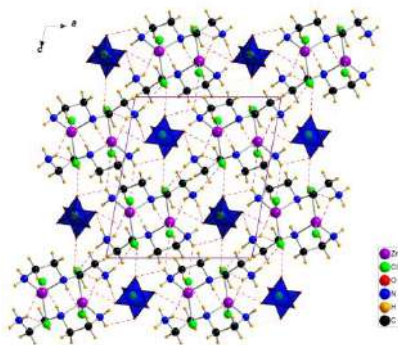
In this study, Co-Fe-B-Ta alloy was obtained by mechanical alloying (MA) of the elemental powder mixture under argon atmosphere. Scanning electron microscopy (SEM), X-ray diffraction (XRD) and differential scanning calorimetry (DSC) are used to study the structural, microstructural and thermal properties of the samples obtained. It has been found during the processes of mechanical alloying the development of new phases. We noticed the appearance of Co₂Ta and bcc-(Fe, Co) phases. A decrease of the crystal size of Co₂Ta phase after 105 h of milling, contrary to bcc-(Fe, Co) phase. The evolution of lattice parameter is also investigated. The DSC analysis of the initial powder and the milled samples for several times revealed only exothermic peaks which can be related to the recovery of defects, recrystallization and formation of new phases.

SYNTHESIS, STRUCTURE AND CHARACTERIZATION OF TWO NEW Zn(II) AND Cd(II) COMPLEXES WITH THE BIDENTATE LIGAND 2-[(2-AMINOETHYL)AMINO]ETHANAMINIUM (AEEA)

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Two new Zn(II) and Cd(II) complexes with the bidentate ligand 2-[(2- aminoethyl)amino]ethanaminium (AEEA), $[\text{ZnCl}_2(\text{C}_4\text{H}_{14}\text{N}_3)]\text{ClO}_4$ (1) and $[\text{CdCl}_2(\text{C}_4\text{H}_{14}\text{N}_3)]\text{ClO}_4$ (2), have been prepared and were characterized by single crystal X-ray diffraction, elemental analysis, CP-MAS-NMR and IR spectroscopies. The basic coordination patterns of the AEEA coordinated metal cations is highly distorted tetrahedral in (1) and distorted octahedral in (2). The crystal structure of (1) is characterized by ZnCl_2N_2 tetrahedra interconnected via $\text{N-H}\cdots\text{Cl}$ hydrogen bonds to form layers parallel to the (b, a + c) plane. In (2), the CdN_2Cl_4 entities form polymeric chains of edge-sharing octahedra extending along the a-axis direction. The crystal structures are stabilized by sets of hydrogen bonds, some of which are bi ortrifurcated. The ^{13}C and ^{15}N CP-MAS NMR spectra are discussed and the vibrational absorption bands were identified by infrared spectroscopy.



A projection of the structure of $[\text{ZnCl}_2(\text{C}_4\text{H}_{14}\text{N}_3)]\text{ClO}_4$ along the b-axis.
Dotted lines indicate hydrogen bonds.

Keywords: Coordination compound, X-ray diffraction, CP-MAS-NMR spectroscopy, Hydrogen bonds.

Detection of sulfa drugs in Chicken liver using Charm II system

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The screening methods have had an increasing success thanks to their ability of selecting the suspect samples at considerably reduced costs and times like Charm II test which is based on the irreversible binding reaction between the functional groups of antibacterial and receptor sites on or within the cells of the added microorganisms. The test employs ¹⁴C or ³H radiolabelled antibacterial (tracer reagent) to compete for the binding sites. This competition for the receptor sites prevents the radiolabelled antibacterial from binding. Thus, the more radiolabelled compound binds, the less analyte is in the sample. In this work thirty samples of chicken liver were studied from different industries for detection of sulfa drugs by Charm II and the effect of freezing time was studied. It was found that 20% of samples were contaminated and the freezing time was a very important parameter to distinct negative and positive samples.

Keywords: Charm II test, sulfa drugs, chicken liver

The recuperation of terephthalic acid from Poly(ethylene terephthalate) Waste Bottles by hydrolysis in the Presence of Phase Transfer Catalyst

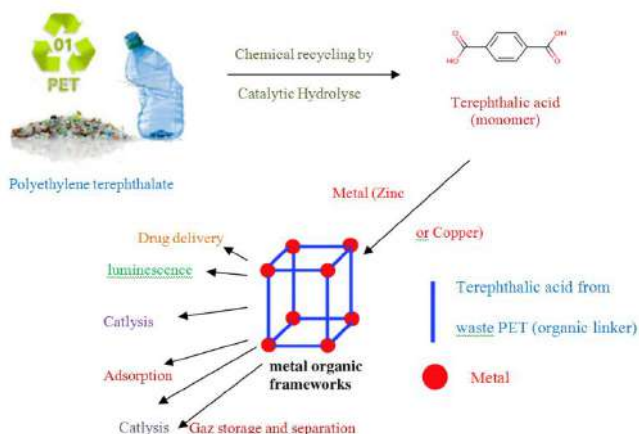
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Chemical recycling of waste poly(ethylene terephthalate) is the a promising alternative for the recuperation of raw materials (monomers) from waste. This work has been focused on the depolymerisation of PET by means of catalytic alkaline hydrolysis using Tributylhexadecylphosphonium bromide ($C_{28}H_{60}BrP$) as catalyst. The alkali used for the hydrolysis was NaOH at varying concentrations. Several parameters have been tested: concentration of NaOH, solid/liquid fraction of PET, quantity of catalyst and size of PET waste. All reactions were performed at atmospheric pressure and at 100 ° C. The time for complete hydrolysis (>95% conversion) of solid PET under alkaline conditions with Tributylhexadecylphosphonium bromide at 100°C varies from 1.5 hours to 4.5 hours. The recuperated products from PET hydrolysis are terephthalic acid (TA) and ethylene glycol.

The second phase of this work consists on the preparation of metal organic framework using recuperated terephthalic acid as organic linker and Zinc or Copper as metal cluster. This work presents a promising alternative for the conversion of waste to functional and value added material.



Elaboration of hybrid nanocomposites PMMA / montmorillonite in miniemulsion

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Hybrid nanocomposites are mixed organic particles with inorganic ones, with a nanometric dimensions [1,2], such as polymer/clay nanocomposite materials [3,4,5]. Recently these materials have attracted considerable interest both in industry and in academia, due to their potential for enhanced physical, chemical, and mechanical properties compared to conventionally filled composites [6]. In particular, and during the last decade, interest in hybrid polymer-clay (NPH) nanocomposites has rapidly been increasing. They have the potential of being a low-cost alternative to high-performance composites for commercial applications [7], in both the automotive and packaging industries [8]. Several methods have been reported in the literature for preparing these nanocomposites; in situ polymerization, intercalation of polymer from solution, and polymer melt intercalation. Miniemulsion polymerization is a nanodroplets dispersion within a particle size between 50 and 500 nm, obtained by mixing an aqueous phase (water, surfactant) and an organic phase (monomer and hydrophobic agent) using sonication [9]. This method involves the clay encapsulation within the monomer phase, then polymerization will take place in monomers nanodroplets, taking advantage of the one-to-one copy process [10].

In this work, we applied miniemulsion polymerization to obtain hybrid nanoparticles polymethylmethacrylate (PMMA) / montmorillonite. Several parameters, such as surfactant class, clay treatment, hydrophobic agent have been tested to obtain an optimum stability. These NPH particles size have been measured by dynamic light scattering. On the other hand, a structural analysis of these hybrid latex have been performed using X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy.

Key words: Hybrid nanoparticles, miniemulsion, clay, PMMA.

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Crystal structure, Hirshfeld surface analysis, DFT, thermal and optical properties of a new chlorobismuthate(III) hybrid material

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The research field of halobismuthate(III) hybrid organic-inorganic materials has developed over the past few decades to yield materials of interest for their non-linear dielectric and optical properties [1]. Single crystal of the new organic-inorganic hybrid material $(C_7H_{10}N)_3(BiCl_6) \cdot 2H_2O$ has been synthesized by slow evaporation method at room temperature and characterized by X-ray single crystal diffraction, Hirshfeld analysis, Infrared spectroscopy coupled with DFT calculation, optical absorption and thermal measurements. The single X-ray diffraction results have revealed that the compound crystallizes in the triclinic system with space group *P*-1 with the following parameters $a = 8.6856(10)$ Å, $b = 13.0671(16)$ Å, $c = 15.3445(18)$ Å, $\alpha = 93.648(4)^\circ$, $\beta = 109.832(4)^\circ$, $\gamma = 112.652(4)^\circ$, with $Z = 2$ and $V = 1473.52$ Å³. The structure is built up of $[BiCl_6]^{3-}$ octahedral anions, three P-Toluidinium cations and two uncoordinated water molecules. The cohesion between these entities is performed via N-H $\cdots$ Cl, N-H $\cdots$ O and C-H $\cdots$ Cl bonds. The optimized molecular structure and vibrational frequencies were calculated by the Density Functional Theory (DFT) method using the B3LYP function 6-311++G** for all atoms except for Bismuth, the LanL2DZ basis set was used. A satisfactory agreement has been found between the calculated and the experimental vibrational frequencies.

Keywords: Hybrid materials, crystal structure, chlorobismuthate(III), spectroscopy, DFT

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Synthesis, crystal structure, vibrational and optical properties of a new non-centrosymmetric hybrid material (1-phenylpiperazinium) dihydrogen diphosphate ($C_{10}H_{15}N_2)_2H_2P_2O_7$

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This present work undertakes the study of a novel organic–inorganic hybrid material, which has been obtained successfully by an acid-base reaction at room temperature and studied by the single crystal X-ray diffraction method. $(C_{10}H_{15}N_2)_2H_2P_2O_7$ crystallizes in the triclinic system with the non-centrosymmetric space group P1 with the following lattice parameters: $a = 5.9159(2) \text{ \AA}$ $b = 13.8451(6) \text{ \AA}$ $c = 14.5973(5) \text{ \AA}$ $\alpha = 74.507(2)^\circ$ $\beta = 89.980(2)^\circ$ $\gamma = 89.231(2)^\circ$ with $V = 1152.06(8) \text{ \AA}^3$ and $Z = 2$. The X-ray structural analysis supported by a detailed Hirshfeld surface analysis and fingerprint plots has been elucidated the different inter-contacts in the crystal structure mainly associated with $N-H\cdots O$, $O-H\cdots O$ and $C-H\cdots O$ between the different entities so stabilizing the 3D-supramolecular structure. An infrared spectrum was registered to reveal the vibrational modes of the title compound. The optical measurements have been carried out at room temperature. Theoretical calculations based in density functional theory (DFT) will be devoted to study the vibrational spectrum of the investigated molecule in its ground state.

Key words: Hybrid material; non-centrosymmetric organic–inorganic hybrid compound; nonlinear optical material; Hirshfeld surface; DFT calculations.

REMEDIATION OF PETROLEUM HYDROCARBONS-CONTAMINATED SOIL BY BIOSTIMULATION AND FENTON-LIKE AS POST TREATMENT

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Contaminated soils poor in nitrogen and phosphorous contents require the addition of nutrients to allow a sufficient increase in biomass and therefore significant degradation rates of petroleum hydrocarbons. These must be used at appropriate concentrations in a certain ratio of Carbon:Nitrogen:Phosphorous (C :N :P) which is the aim of our study. The objective of this work is to study the influence of coupling a chemical treatment by Fenton-like oxidation followed by a biological treatment on the effectiveness of remediation of soil contaminated by hydrocarbons at a rate of 3% under aerobic conditions in solid phase bioreactors by supplying appropriate nutrients and water contents. The effects of the C :N :P ratio (100:10:1) were investigated, using both abiotic and biotic systems. Humidity and temperature were held constant throughout treatment period.

The biodegradation efficiency of petroleum hydrocarbons reached 52%, while 73% of total petroleum hydrocarbons was eliminated by biological treatment and chemical one as a post-treatment. For higher N:P molar ratio greater than or equal to 10, the recorded depletion and consequently biodegradation ratios decreased significantly. The monitoring of temporal evolution of the biomass and C:N:P ratios highlighted that the N: P molar ratio may be a factor limiting which concurs with several studies. In addition to the ability of the indigenous microbial population to oxidize petroleum hydrocarbons to a large extent, the results highlighted the remediation feasibility in solid phase bioreactors.

Keywords: Petroleum hydrocarbons; Soil bioremediation; Biostimulation; Biomass evolution.

Extraction of the uranium from the phosphoric acid using new hydrophobic Ionic liquids

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The explosion in global demand for metals is depleting deposits, which has a direct impact on the production of strategic metals. Among these strategic metals, uranium is an indispensable element for military and especially energetic applications, since it is the only element possessing a fissile natural nucleus [1]. Similar to the case of rare earths, the recourse to the recycling of uranium would make it possible to avoid its shortage.

This work is part of the perspective of the renewal of nuclear energy and the development of processes that are more respectful of the environment. This includes the replacement of current volatile organic solvents (VOCs), such as long-chain carbon alkanes used in the PUREX process for uranium extraction, with so-called "green" solvents. This is why a growing interest is brought to the ionic liquids. In this work, these green compounds play both the role of the solvent and the extracting agent of the extraction process. A complete optimization of the process has been realized. The results show that the extraction of uranyl ions from an aqueous solution of phosphoric acid (0.4 mol / L) by the ionic liquid denoted Mor18-OP, is quantitative (% E > 98%). The extraction process follows the solvation neutral mechanism, suggesting the involvement of two molecules of ionic liquid. This green process represents an efficient and ecological alternative, the usual separation and recovery techniques for critical metals.

Keywords: uranium, ionic liquid, green chemistry, liquid-liquid extraction.

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Synthesis and antibacterial activity of a new sulfide chitosan

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A new sulfide chitosan was prepared in acid acetic solution from allyloxy- β -hydroxysulfide and chitosan. The chemical structure and physical properties of sulfide chitosan were characterized by FTIR, ¹H NMR and XRD techniques. The modified chitosan has been also tested as bactericides against *Staphylococcus aureus*, *Escherichia coli*, *Salmonella typhimurium* and *Pseudomonas aeruginosa*. By comparison with the native chitosan, the synthesized derivative shows an enhancement of the antibacterial activity and solubility.

Key words: Chitosan, Sulfide chitosan, Solubility, Antibacterial activity.

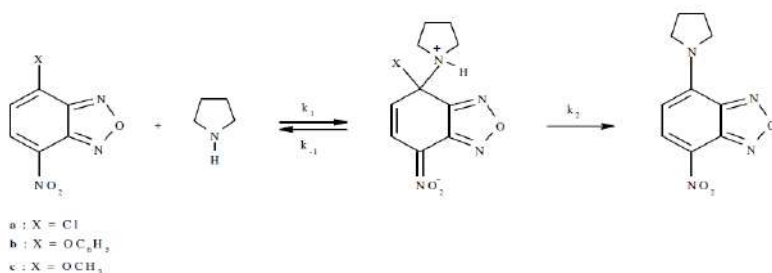
Reactivity of benzofurazan derivatives: Kinetic, Thermodynamic and Structure-Reactivity Relationships

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Second-order rate constants (k) have been measured spectrophotometrically for reactions of 7-X-4-nitrobenzofurazans ($X = \text{Cl}$, OC_6H_5 and OCH_3) with pyrrolidine in acetonitrile solution at various temperatures.

The data are consistent with the $\text{S}_\text{N}\text{Ar}$ mechanism and the substituent effects on the free energy ($\Delta G^\ddagger$), enthalpy ($\Delta H^\ddagger$) and entropy ($\Delta S^\ddagger$) of activation parameters have been determined on the basis of kinetic measurements.



Scheme 1

On the other hand, the effect of substituents on the electrophilic reactivity was examined quantitatively on the basis of activation parameters leading to linear correlation of $\Delta H^\ddagger$ (or $\Delta S^\ddagger$) with Hammett-Brown substituent constants $\sigma^\text{+}_{\text{para}}$.

Keywords: Activation Parameters, Substituent effects, Hammett's equation, Kinetic, Structure-Reactivity

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**Determination of Polychlorinated Biphenyls (pcbs) and
Organochlorine Pesticides (ocps) in a benthic fish (solea solea)
from the Ghar El Melh Lagoon, Tunisia**

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We propose in this work to develop a protocol interested in the analysis of the residue of 12 congeners of The aim of this study is to measure the concentrations of polychlorinated biphenyls (PCBs) and organochlorine pesticides (OCPs) in 21 benthic fish (*Solea solea*) samples collected from Ghar El Melh lagoon, North of Tunisia. The analytical procedure involved the application of microwave extraction, followed by purification by adsorption chromatography on a silica column. Finally, the gas chromatographic analyzes were carried out on a capillary column with an electron capture detector (GC-ECD-ECD). Compositional analyses of the POPs indicated that PCB 153, 138 and 180 were the predominant congeners accounting for 60 % of the total PCBs. In addition, p,p'-DDT was found to be the dominant DDTs, demonstrating recent inputs in the environment. Compared with some other regions of the world, the Bizerte lagoon exhibited low levels of PCBs and moderate levels of HCB and DDTs.

Keywords: PCB, OCP, fish (*Solea solea*), microwave extraction, GC-ECD-ECD.

Synthesis, characterization, and photophysical properties of a new pentacyclic helicene

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Helicenes are polycyclic aromatic hydrocarbons made of ortho-fused aromatic rings, forming an inherent regular helical shape, which arises from the steric hindrance between aromatic rings. For many years, they are regarded as little more than an academic curiosity. More recently, their extraordinary optical and electronic properties have rekindled an interest in these non-planar condensed aromatic in fields as diverse as liquid crystals¹, asymmetric synthesis and polymer synthesis,^{2,3}. In this work, a new helically chiral pentacyclic compound bearing suitable functional groups (Fig.1) has been prepared, in a good overall yield, through a four steps sequence involving coupling reaction and oxidative photocyclization.⁴ The target [5]helicene showed an interesting optoelectronic properties.

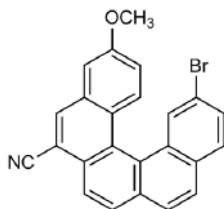


Fig 1. Synthesis of new [5]helicene

Key words: Phenanthrene, helicene, coupling reaction, Photocyclization.

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Control of geometric and intrinsic properties of Sr, Ni co-doped $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$: enhancement of dielectric properties

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$\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ (CCTO) ceramics have been widely demonstrated in the last few years, which are considered as potential material for capacitor applications. A novel strategy to improve the dielectric properties of $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ ceramics was proposed by codoping with Sr^{2+} and Ni^{2+} . In this work, effect of Sr^{2+} ions on the microstructure and electric properties of un-doped CCTO and Ni-doped CCTO was investigated. All the ceramics were synthesized by solid-state reaction method. SEM micrographs indicated that the grain growth of Ni-doped CCTO was strongly influenced by Sr doping ions at different ratios. EDX results revealed that the TiO_2 phase increased with Sr ratio at grain boundaries, which it is maximum for $\text{Ca}_{0.8}\text{Sr}_{0.2}\text{Cu}_{2.9}\text{Ni}_{0.1}\text{Ti}_4\text{O}_{12}$ accompanied after by a decrease in grain size. Additionally the Cu-rich phase decreased and migrated to grains and therefore influenced the dielectric and electric properties. The $\text{Ca}_{0.9}\text{Sr}_{0.1}\text{Cu}_{2.9}\text{Ni}_{0.1}\text{Ti}_4\text{O}_{12}$ exhibited not only the best dielectric properties at 10 KHz with good frequency stability ($\epsilon \approx 41320$ and $\tan\delta \approx 0.056$) but also the best resistivity values ($2 \times 10^8 \Omega \cdot \text{cm}$).

Key words: CCTO ceramics, TiO_2 phase, Raman, intrinsic and geometric properties.

Chemical analysis of essential oil from *Echinops spinosus* L. roots: Antimicrobial and antioxydant activities

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Echinops spinosus L. roots (ES) are traditional and popular medicinal plant in Tunisia. In this work, the essential oil obtained by hydrodistillation of roots of this species was analyzed by GC-FID and GC-MS. Twenty compounds were identified, representing 97.470% of the total oil. γ -cadinene (27.224%) was the main component followed by 5-(3-buten-1-ynyl)-2,2'-bithienyl (21.334%), 2,2',5',2''-terthiophene (18.024%), caryophyllene oxide (5.217%), agarospirol (1.627%), α caryophyllene (1.522%), thujone (0.328%) and 1,8-cineole (0.321%). The biological activities, including antioxidant and antimicrobial properties, of the *Echinops spinosus* roots essential oil were investigated by different methods. The antimicrobial activity was evaluated against gram-positive and gram-negative bacteria. Results showed that the ES essential oil exhibited strong antimicrobial activity against the tested species. The results suggested that the ES essential oil possesses antimicrobial and antioxidant activities, and therefore a potential source of active ingredients for food and pharmaceutical industry.

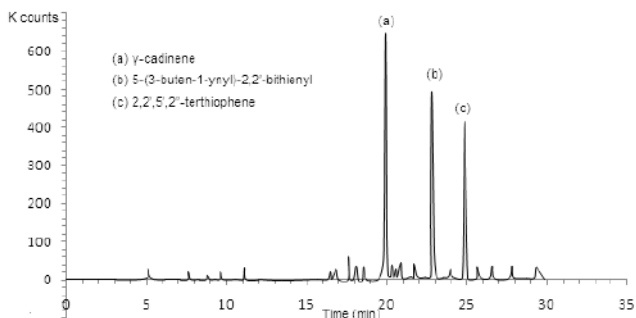


Fig. The main components in *Echinops spinosus* roots essential oil.

Key words: *Echinops spinosus*, antimicrobial activity, GC-MS and essential oil.

Oxidative stability of mayonnaise after enrichment with hydroxytyrosol extracted from olive by-product using a new selective method

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Many natural antioxidants show great potential for improving the oxidation stability of food products. These compounds also have a wide range of additional health. To the best of our knowledge, no study has been carried out the effect of polyphenols on the stability of the mayonnaise during the storage period. The effect of different hydroxytyrosol quantities ranged between 65 and 195 μL on oxidative stability of mayonnaise were studied after 4 weeks storage period. The free acidity, peroxide value as well as content of polyphenols and squalene were studied after 4 weeks storage period and the mayonnaise samples were stored protected from light at room temperature. The results obtained show that 195 μg of hydroxytyrosol may be of great benefit to improving the stability of the mayonnaise against oxidation.

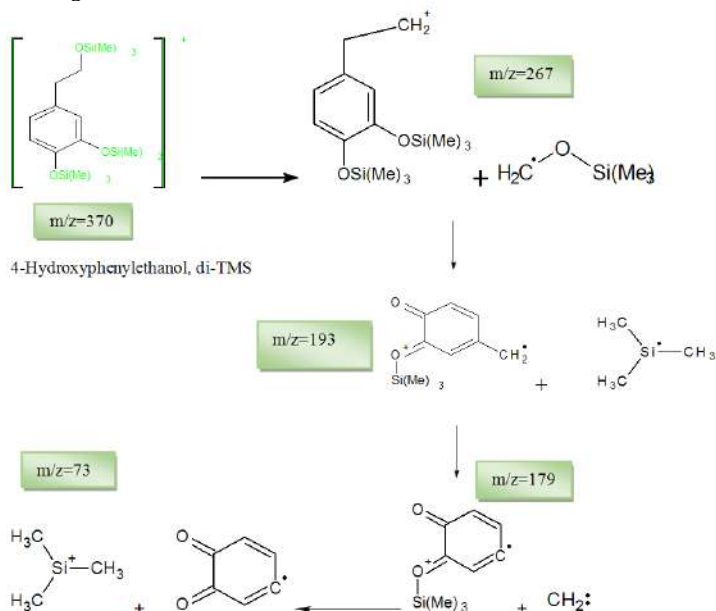


Fig : Proposal fragmentation of hydroxytyrosol.

Keywords: mayonnaise, hydroxytyrosol, phenolic compounds.

DESIGN AND SYNTHESIS OF NOVEL FUSED COUMARINYL PYRANOTRIAZOLOPYRIMIDINE DERIVATIVES

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Pyrimidine derivatives have been widely described as heterocyclic compounds known by their high chemical reactivity and their wide spectrum of biological properties [1].

On the other hand, the synthesis and biological activities of coumarin derivatives occupy an important position in heterocyclic chemistry as well as in medicinal chemistry. The compounds containing this heterocyclic moiety, which have been synthesized by Knoevenagel [2] reactions, are widely found their application as additives in food, in cosmetic products, and as pharmaceutical agents [3].

In view of these, it was considered of interest to synthesize some new class of heterocycle systems which incorporate the coumarin and the 1,2,4-triazolopyrimidine moieties **6(a-l)** via Knoevenagel condensation of salicylaldehydes with naphto [2,1-*b*]pyrano[3,2-*e*] [1,2,4]triazolo[1,5-*c*]pyrimidine-2-acetonitriles **4**, in the hope that they may be biologically active.

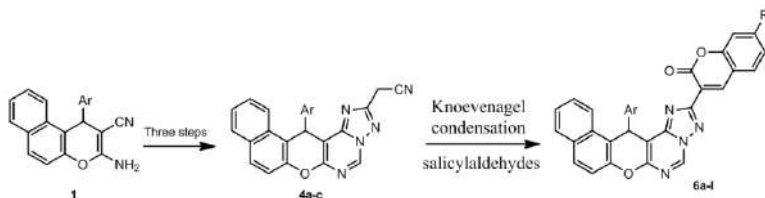


Figure 1. Synthesis of some novel fused coumarinyl naphtopyrantriazolopyrimidines **6a-l**

Keywords: triazolopyrimidines, Knoevenagel condensation, coumarinyl naphtopyrantriazolopyrimidines.

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DESIGN, SYNTHESIS AND BIOLOGICAL EVALUATION OF NOVEL HYBRID COMPOUNDS INCORPORATING TRIAZOLOPYRIMIDINE AND PHOSPHONATE MOIETIES AS ANTIDIABETIC AGENTS

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Heterocyclic compounds have drawn special attention in organic chemistry because of their abundance in natural products and their diverse biological properties [1]. Pyrimidine and its derivatives have been recognized as important heterocyclic compounds due to their variety of chemical and biological significance to medicinal chemistry [2]. On the other hand, phosphorus-containing compounds play a key role in living organisms as carriers of genetic information and important signaling, regulatory, energy transfer, and structural compounds [3]. Their diverse biological activity has, for a long time, attracted considerable synthetic and pharmacological interest [4]. Herein we report the synthesis of a series of novel naphthopyranotriazolopyrimidines dialkylphosphonates **4a-i** via the Arbusov reaction of naphthopyranotriazolopyrimidines chloride **3a-e** with trialkyl phosphite. The synthesized compounds were also screened for their antidiabetic activity.

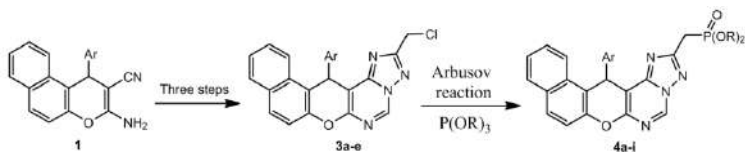


Figure 1. Synthesis of naphthopyranotriazolopyrimidines dialkylphosphonates **4a-i**

Keywords: trialkyl phosphite; Arbusov Reaction, phosphonate derivatives

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Design, synthesis and biological evaluation of Schiff bases of 4-amino-1, 2, 4-triazole derivatives as potent angiotensin converting enzyme (ACE) inhibitors and antioxidant activities

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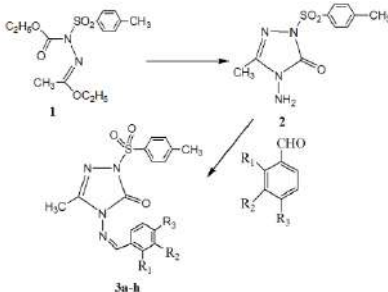
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This work reports a novel and highly efficient methodology for the synthesis of Schiff bases of 4-amino-1,2,4-triazole derivatives (**3a-h**) by the condensation of 4-amino-5-methyl-3-oxo-2-tosyl-1,2,4-triazol-3-one (**2**) derivative with various aromatic aldehydes under ultrasound irradiation. The major advantages of the reported method are its operational simplicity, extremely mild reaction conditions, short reaction times, and excellent yields. The structures of the synthesized compounds were elucidated by IR, ¹H NMR, ¹³C NMR, elemental analysis, and the X-ray crystallography (for compound **3f**).

The antioxidant activity of the synthesized compounds was determined by the 1,1-diphenyl-2-picrylhydrazyl (DPPH) method. The IC₅₀ value of synthesized Schiff bases were calculated and compared with standard BHA. All compounds showed excellent activity with inhibition values in the range of 71.22±0.98-96.54 ± 0.13% at 500 µg/mL.

The newly synthesized compounds were also evaluated for angiotensin I-converting enzyme (ACE) inhibition. The results were compared to captopril as a reference drug. All compounds showed ACE inhibition activity from 66% to 95%. Moreover, the synthetic compounds displayed virtually no cytotoxicity. The docking of chemical compounds in the ACE active site revealed possible inhibitory effect of all compounds on the catalytic activity of the enzyme, which would satisfactorily explain the anti-hypertensive effect of these compounds.



Keywords: Schiff bases, ultrasound, angiotensin I-converting enzyme (ACE) inhibitory activity, antioxidant activity

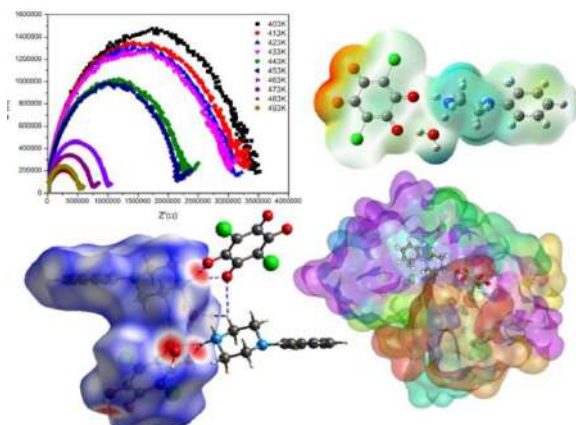
Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (C₆Cl₂O₄). 2(C₁₀H₁₄N₂F). 2H₂O

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A new chloranilate compound with 1-(2-fluorophenyl)piperazine has been synthesized and characterized using spectroscopic methods and X-ray diffraction. The atomic arrangement can be described by an H-bonded 3D network, formed by anionic entities, organic cations and H₂O molecules linked together via N-H...O, O-H...Cl, C-H...Cl and C-H...O hydrogen bonds. The vibrational absorption bands of the various characteristic groups of this compound have been identified by infrared spectroscopy. Moreover, the thermal and dielectric analyses have shown that the title compound has a phase transition at 393K. The surface mapped over the dnorm property, highlights the A...H (A=O, C, Cl and F) as the main intermolecular contacts. On the other hand, the geometry, intermolecular bonds and harmonic vibrational frequencies of the title molecule have been investigated using the B3LYP/ 6-31G (d, p) method. The stability of the structure obtained, as well as the charge transfer within the molecule, have been confirmed by determining the energies of the HOMO and LUMO levels and the theoretical gap energy. Molecular docking studies of the title compound have also been conducted as part of this study.

Keywords: Chloranilate, Vibrational spectra, Crystal structure, DFT, HOMO-LUMO.



Synthesis, Crystal structure, Spectroscopic, Optical and Thermal Properties of a New Hybrid Material (C₇H₁₁N₂)₂[CrCl₂(H₂O)₄]Cl₃·2H₂O

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A new chromium (III) hybrid compound with 4-dimethylaminopyridine was synthesized. The crystal was grown by slow evaporation method at room temperature. The single crystal X-ray diffraction proves that this compound crystallizes in the P2/c monoclinic space group. The structural unit is composed by an organic cation (C₇H₁₁N₂)⁺, an octahedral Cr(III) inorganic cluster [CrCl₂(H₂O)₄] surrounded by two chlorine and four water molecules, two other free chlorine anions and a water molecule as shown on Figure1. The structure exhibits an alternate organic-inorganic layered stacking along c-axis. The isolated octahedra are building a zero dimensional anionic network. The crystal structure is stabilized by N-H...Cl, O-H...Cl, O-H...O and offset π - π stacking interactions. Hirshfeld surface projections and fingerprint plots elucidate the relative contribution of the H...Cl, H...H, H...O intermolecular contacts in the crystal in a visual manner. Furthermore, the vibrational analysis of the structural groups in the compound was carried out by Fourier transform infrared (FT-IR). The thermal behavior of the material was studied by coupled thermogravimetric (TG) and differential scanning calorimetry (DSC). The optical properties were studied using absorption UV-visible and photoluminescence (PL) spectroscopy. Based on the structural investigation results, the electronic transition gaps such as HOMO and LUMO were calculated using PM3 algorithms.

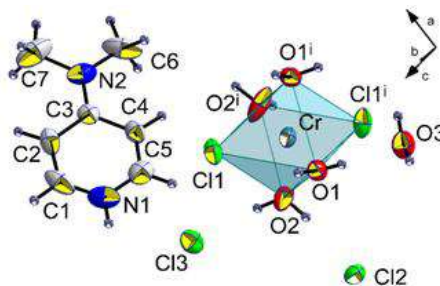


Figure 1. Structural unit of (C₇H₁₁N₂)₂[CrCl₂(H₂O)₄]Cl₃·2H₂O.
Thermal ellipsoids are shown at 50% probability.

Keywords: hybrid compound; synthesis; X-ray diffraction; FTIR; thermal analysis; optical studies; Hirshfeld surface analysis.

Structure, dielectric and impedance spectroscopic studies of $\text{CaCu}_{2.9}\text{Ni}_{0.1}\text{Ti}_{4-x}\text{Co}_x\text{O}_{12}$ ($x = 0.1, 0.2$ and 0.3) electro-ceramic

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In the present work, C and B-sites modified structured CCTO composition with the nominal formula $\text{CaCu}_{2.9}\text{Ni}_{0.1}\text{Ti}_{4-x}\text{Co}_x\text{O}_{12}$ ($x = 0.1, 0.2$ and 0.3) were prepared by solid state reaction. XRD analysis confirmed the formation of single-phase material in samples sintered at 1100°C for 12h and 24 h. The tailoring effects of nickel and cobalt were investigated thoroughly by Scanning Electron Microscopy, Raman spectroscopy and Impedance spectroscopy. SEM micrographs of co-doped samples noted (CCTO-Ni-Co) revealed amazing morphological change. Pure CCTO exhibits regular polyhedral grains while leaf grains occur in CCTO-Ni-Co particularly when the percentage of cobalt increases to 0.3. The complex dielectric and impedance properties of dielectric compound $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ co-doped by Nickel and cobalt as a function of frequency were interpreted to understand the grain and grain boundary contributions to its dielectric response. In this work we consider not only the electrical characterization, but also the microstructure in a discussion of the dielectric properties of the composition $\text{CaCu}_{2.9}\text{Ni}_{0.1}\text{Ti}_{4-x}\text{Co}_x\text{O}_{12}$ estimate.

An approach for correlating the structural and electrical properties of Ni²⁺ and Mg²⁺ modified CCTO ceramic

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CaCu_{3-x-y}Ni_xMg_yTi₄O₁₂ with (x=0/0.1/0.15/0.2) and (y= 0.1/0.2/0.3) noted CCNMTO ceramics were prepared by solid state method. The XRD pattern powder, calcined at 1000°C for 24h and 1100°C for 12h and 24h, shows that structure of the majority samples is basically single-phase. It is noted that compositions calcined at 1000°C and 1100°C for 24h whose magnesium percentage is of the order of 0.3 present CaTiO₃ as a minority phase. As the microstructures usually affect the dielectric characteristics of ceramics, we discussed the variation of microstructures for the present ceramics with composition and synthesis conditions. The SEM results indicate that the samples have porous structures. Microstructure shows spherical large grains size isolated by some fine grains regions independently of composition and synthesis conditions. Obviously, Ni²⁺ and Mg²⁺ dopants have distinct roles in grain growth as well as enhancement and inhibition mechanisms of CCTO ceramics, respectively. The experimental results of dielectric properties show that the dielectric constants are less than that of CCNTO ceramics. This can be related to mesoporous structures of CCNMTO ceramics.

Structural, magnetic and magnetocaloric properties of $\text{GdFe}_{10}\text{Cr}_2$ compound synthesized by arc melting

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We have synthesized the intermetallic $\text{GdFe}_{10}\text{Cr}_2$ compound by arc-melting with annealing at 800° C for one week. The Rietveld refinement shows that this compound crystallize in the tetragonal ThMn_{12} -type structure with the $I4/mmm$ space group (See Figure. 1). The temperature dependence of magnetization data reveals that $\text{GdFe}_{10}\text{Cr}_2$ exhibits a second-order ferromagnetic to paramagnetic phase transition at Curie temperature ($T_C = 580$ K). The magnetocaloric effect (MCE) of this compound was investigated by means of magnetic measurements in the vicinity of its Curie temperature. The maximum magnetic entropy change ΔS_M of $\text{GdFe}_{10}\text{Cr}_2$ in an applied field of 1.56 T, reaches a maximum values of 0.90 J/kg K(See Figure. 2). The relative cooling power around the magnetic transition and the Arrott plots are also reported.

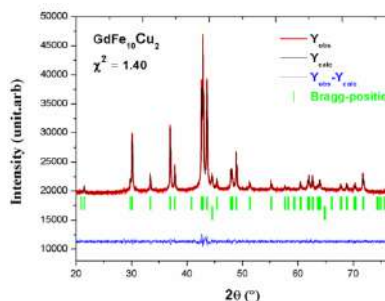


Figure. 1. Rietveld refinements for XRD pattern of $\text{GdFe}_{10}\text{Cr}_2$ compound.

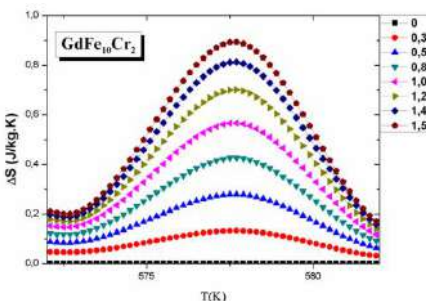


Figure. 2. Entropy change for $\text{GdFe}_{10}\text{Cr}_2$ compound.

Characterization and catalytic reactivity of catalysts based on acidified zirconia with carboxylic acids

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Xerogel catalysts based on zirconia acidified by tartaric and trifluoroacetic acids with different molar ratio ($n_{\text{acid}}/n_{\text{Zr}}$) were synthesized by the sol-gel route and tested in esterification reaction of acetic acid with methanol. Characteristics and reactivity of catalysts depend on several preparation parameters such as molar ratio ($n_{\text{acid}}/n_{\text{Zr}}$) and calcination temperature.

Characterization of these catalysts was carried out using N_2 physisorption at 77K, X-ray diffraction, FTIR spectroscopy, adsorption of Hammett's indicators and potentiometric acid titration.

The preparation of zirconia with tartaric or trifluoroacetic acids causes a slight lowering of the specific surface and generates more acidic sites on the surface with increasing acid content. This effect enhances the catalytic performance of catalysts. Furthermore, the calcination of each catalyst at 500°C develops the tetragonal ZrO_2 phase and causes the loss of acid, therefore acidity and reactivity of catalyst are reduced.

The comparative characteristics and the reactivity study of the two kinds of catalysts shows that zirconia prepared with trifluoroacetic acid has a more developed texture and more strong acid sites than zirconia catalyst prepared with tartaric acid. It seems that these properties provide a better reactivity in the esterification reaction of acetic acid with methanol.

Keywords: Xerogel; zirconia; acidified; tartaric acid; trifluoroacetic acid; acetic acid esterification.

Assessment of crude oils Compatibility by different methods

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Precipitation and flocculation of heavy organic compounds during the production of crude oils is a very serious problem, and is commonly encountered in the petroleum industry. Indeed, under certain hydrodynamic conditions of oil, the asphaltenes, which are the most polar compounds and the heaviest crude oils, can precipitate and form a deposit on the walls of the installations (valves, pumps, etc.), storage tanks and pipes.

In most cases, regardless of the quantities of deposits, the results are a reduction in the capacity of the lines of conduct and storage, which has the consequence the stopping of production.

Therefore, the mixing of the different crude oils during storage or when shipped by the same pipeline is likely to cause incompatibility problems due to the presence of asphaltenes. In order to avoid these problems, a characterization of the oils is necessary to better understand the behavior of their mixture.

The objective of our work is therefore the study of the mixture between two oils located in two different regions of Tunisia, by two methods in different volume proportions to determine their compatibility or incompatibility.

Key Word: crude oil, asphaltenes, deposit, compatibility.

Polyphenol composition and anti-corrosion properties of *Diplotaxis simplex* (DS) plant extract on 316L steel in H₂SO₄ (1M)

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Corrosion is a major problem for industrials for the use of metals. The bio inhibitor is a pre-treatment that can improve the corrosion resistance of metals. The aims of the present study are to investigate the effects of ethanolic extract (EE) of DS (Arial part) as a green inhibitor for corrosion of the metal (316L) to acid media (H₂SO₄ 1M) using electrochemical methods: polarisation curves and Electrochemical Impedance Spectroscopy (EIS). The polarisation results showed that DS acts as mixed inhibitor against the corrosion of 316L steel in H₂SO₄ (1M) and reduces the corrosion rate. In the same case, the EIS result suggests an increase in the corrosion resistance of steel in the presence of plant extract comparatively to the blank systems. This inhibition behaviour can be linked to the polyphenol richness of DS extract which are identified by the HPLC-UV.

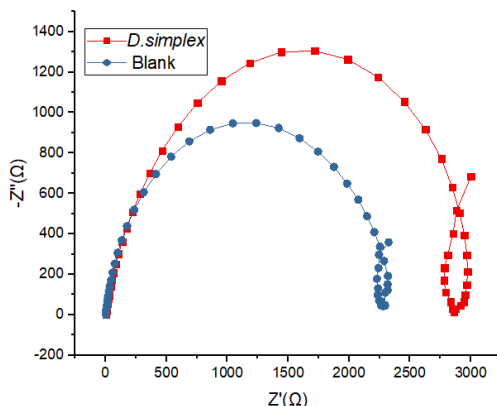


Figure: Nyquist plot of 316L steel in 1M H₂SO₄ solution in the absence and presence of (EE) of *Diplotaxis simplex*

VESICLES FORMATION IN BINARY CATIONIC DIBRANCHED SURFACTANT/WATER SYSTEM

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Molecular aggregates of surfactant molecules consisting of one or more bilayers arranged in a hollow, closed, with various geometry are termed as “vesicles”¹. This type of aggregate has intensively studied^{2,2} because of the many applications as emulsifier, corrosion inhibitors, membrane solubilization cell³, membrane manufacture², detergents and drug delivery⁴, etc... These vesicles are often observed through a transition after micelles formation in particular systems such dibranched surfactants systems where the vesicles forms spontaneously within a concentration range. The didodecylmethylammonium bromide (DDAB) surfactant studied here, has a double carbon chain and a quaternary ammonium terminal group.

In this work we investigated the micellar transition allowing the formation of vesicles in a binary system DDAB/ water. Micellar physico-chemical parameters have been obtained by tensiometry and conductimetry studies at 25°C in aqueous media. In the other hand, at higher concentrations the particular structure of DDAB vesicles was highlighted by the application of a small angle neutrons scattering method⁵ (SANS). Micelle structural parameters has been determinated by fitting the SANS data using analytical expression of the scattering intensity which is the product of the lamellar form factor $P(q)$ and the structure factor $S(q)$. The Nallet⁶ model used permit to measure the geometric quantities characterizing the lamellar phases, and the size measurements of these auto-associations.

Keywords: surfactants, SANS, DDAB, vesicles, bilayers, lamellar phase.

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Synthesis and photoluminescence of Eu^{3+} activated $\text{Li}_x\text{Na}_{1-x}\text{Y}(\text{PO}_3)_4$ under VUV-UV excitation

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Currently, alkali lanthanide phosphates were extensively investigated for their interesting optical applications [1–3]. The entire family of $\text{MRE}(\text{PO}_3)_4$ polyphosphate compounds form a nice study material for VUV-UV excited phosphors by selecting an appropriate combination of M and RE ions. The objective of the present work is to study the influence of substitution of alkaline ions on the spectroscopic properties of Eu^{3+} ions.

The $\text{Li}_x\text{Na}_{(1-x)}\text{Y}(\text{PO}_3)_4 \cdot \text{Eu}^{3+}$, where, $x = 0; 0.5; 1$ were synthesized by a solid-state reaction method. Structural behavior of the prepared matrix has been explored through XRD, FTIR and Raman spectral analysis. Optical characterization has been made using VUV excitation, luminescence and decay curves.

The X-ray diffraction pattern confirmed the monoclinic phase. The IR spectroscopy results show the presence of characteristic bands due to $(\text{PO}_3)_n$ polyphosphate chains. However, according to XRD and Raman data, the $\text{Li}_{0.5}\text{Na}_{0.5}(\text{PO}_3)_4 \cdot \text{Eu}^{3+}$ material seems to be a mixture of the Li and Na homologues.

The excitation spectrum of $\text{Li}_x\text{Na}_{(1-x)}\text{Y}(\text{PO}_3)_4 \cdot \text{Eu}^{3+}$ shows that both the CT bands of $\text{O}^{2-} \rightarrow \text{Y}^{3+}$ and $\text{O}^{2-} \rightarrow \text{Eu}^{3+}$ and efficiently absorb the excitation energy in the region of 130-250nm. Five emission bands have been observed from the $^5\text{D}_0$ excited state to the lower lying states $^7\text{F}_0$, $^7\text{F}_1$, $^7\text{F}_2$, $^7\text{F}_3$ and $^7\text{F}_4$ on exciting the sample with 394 nm wavelength. The luminescence intensity ratio of the $^5\text{D}_0 \rightarrow ^7\text{F}_2$ to $^5\text{D}_0 \rightarrow ^7\text{F}_1$ transition has been calculated to estimate the local site symmetry around the Eu^{3+} ions. Judd–Ofelt (J–O) intensity parameters Ω_2 ($\lambda = 2, 4$) were obtained from the emission spectra and the same is used to estimate the transition probability (A), and branching ratios (β_R) for the excited levels of the Eu^{3+} ions.

Key words: Solid-state reaction, FTIR, Raman spectroscopy, Excitation, Emission Judd–Ofelt (J–O), Branching ratios (β_R).

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Synthesis, thermal properties and electrical conductivity of lithium iron phosphate

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In this work, an amorphous compound Lithium Iron Phosphate was synthesized, the phase composition of the chemosynthetic powders was determined with X-ray diffraction, differential thermal analysis and electrical conductivity. The reaction of synthesis was carried out with mixtures of LiH_2PO_4 (2 g), and H_3PO_4 (1,3 ml g) with a molar ratio of 1 heated at 250°C for 48h, the mixture was filled into a 10 ml of water, a quantity of $\text{Fe}(\text{OH})_2$ was added in this solution until saturation.

The XRD traces of lithium Iron Phosphate material unheated and heated at varied temperatures clearly shows that unheated compound appeared amorphous. The onset temperature of crystallization was 550 °C, these crystalline phases were identified as $\text{Fe}_2\text{Fe}(\text{P}_2\text{O}_7)_2$ and $\text{LiFe}(\text{P}_2\text{O}_7)$ phases at 550°C, $\text{Fe}_2\text{Fe}(\text{P}_2\text{O}_7)_2$, $\text{LiFe}(\text{P}_2\text{O}_7)$ and $\text{Fe}(\text{PO}_4)$ phases at 650°C and at 750 °C, peaks correlated with the phase of $\text{Fe}_2\text{Fe}(\text{P}_2\text{O}_7)_2$ was transformed to $\text{Fe}_4(\text{P}_2\text{O}_7)_3$.

TG/DTA analyses of the title compound revealed the presence of a small exothermic peak observed at 530°C corresponding to reaction of crystallisation identified by X-Ray diffraction.

Two small exothermic peaks were observed at 620 °C and 780°C correlated with the crystalline phases transformations.

The conduction properties indicates first very low solid-state conductivity ($10^{-12} \text{ S.cm}^{-1}$ to $3.8 \cdot 10^{-11} \text{ S.cm}^{-1}$) under 275°C, the conductivity values is slightly higher around 325°C and begins to rise rapidly, reaching $3 \cdot 10^{-8} \text{ S.cm}^{-1}$ at 525°C.

Keywords: Amorphous compound, Thermal analysis, electrical conductivity.

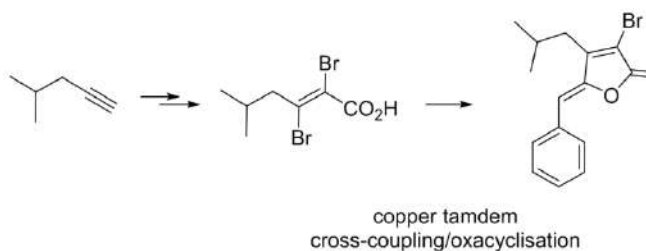
Total synthesis of Enhygrolide A

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“Enhygrolide A” is a metabolite isolated from a marine myxobacterium (*Enhygromyxa salina*) [1a,1b]. This alkylide-nebutenolide has antibacterial properties against *Arthrobacter crystallopoitit* (MIC = 4 µg/mL) which makes it an interesting structure for the development of new antibiotics [1c]. Since this compound has a structure that is structurally identical to the nostoclidides whose preparation has recently been completed in our laboratory [2], we have undertaken to carry out the total synthesis of “Enhygrolide A” in 5 steps from 4-methylpent-1-yne using a similar strategy. This sequence involves two metal catalyzed steps including a copper-palladium catalyzed Sonogashira/oxacyclization domino reaction.



Keywords: Enhygrolide, myxobacteria, Sonogashira, metal catalysts

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A new azo-phenylthiophene derivative for optical applications

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Azobenzene derivatives have received considerable experimental and theoretical attention. We describe herein the synthesis of a new azobenzene based phenylthiophene ligand obtained by a condensation reaction between 4-(4-nitrophenylazo)aniline and 5-phenylthiophene-2-carbaldehyde in ethanol with 83% yield. This ligand crystallizes in the monoclinic system, space group $P2_1/c$ with one independent molecule in the unit cell. The crystal structure of the ligand indicates that this ligand is not completely planar with the presence of a strong intramolecular C–H...S hydrogen bonding and S...N short contacts. Optical properties of this compound have been determined by UV-Vis spectroscopy.

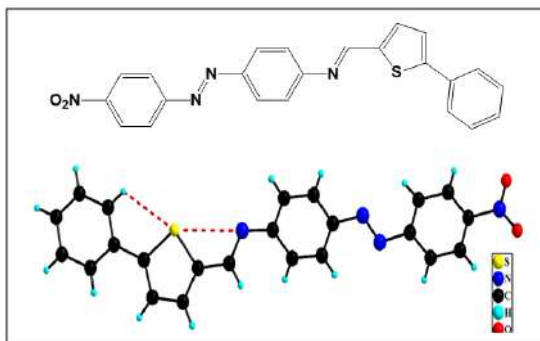


Fig. Structure of ligand

Key words: Azobenzene, phenylthiophene, UV-Vis spectroscopy,

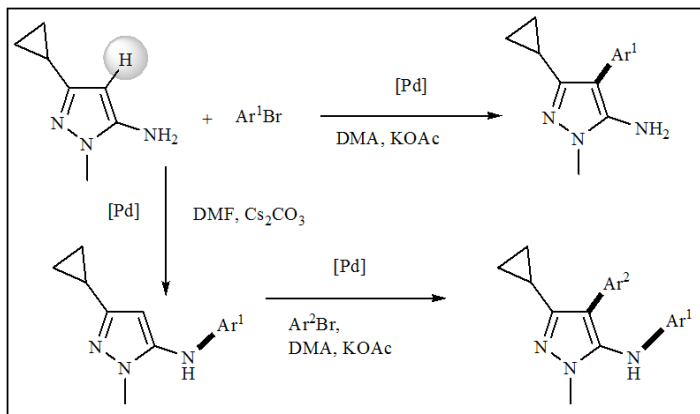
Palladium-catalysed controlled amination and arylation of 3-cyclopropyl-1-methylpyrazol-5-amine

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The reactivity of pyrazole derivatives bearing a cyclopropyl groupe at C3-position and an amino substituent at C5 in intermolecular palladium-catalysed direct arylations was investigated. These couplings were performed using air-stable $\text{PdCl}(\text{C}_3\text{H}_5)$ (dppb) catalyst associated to KOAc as inexpensive base. The target C4-arylated pyrazoles were obtained in moderate to high yields. A wide variety of functional groups on the aryl bromide including electron-withdrawing and electron-donating ones was tolerated. Conversely, the use of Cs_2CO_3 base afforded the amination products in good yields. No decomposition of the cyclopropyl group was observed for both procedures. [1]



Keywords: Palladium, Intermolecular arylation, Pyrazole, Aryl bromides.

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Fe₆₀Ni₃₀Cr₅B₅ powders obtained by mechanical alloying

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Fe₆₀Ni₃₀Cr₅B₅ alloy was prepared by mechanical alloying (MA) of elemental powders in a high-energy planetary ball mill type Fritsch (Pulvérisette P7). Scanning electron microscopy (SEM), X-ray diffractometry was used to study the mixing at nanometric scale. In addition lattice microstrain, average crystallite size, dislocation density, and the lattice parameter were determined. The patterns so obtained were analyzed using the Maud program. It is observed a gradual formation of mixture of phases as fcc and bcc with a nanoscale grain size. The final product of the mechanical alloying process after 50h of milling was nanocrystalline Ni(B) and Fe(Ni,Cr) phases with a mean crystallite size in the range of a few nanometers. The average grain size is decreased with a progressive enlargement of peaks of X-ray diffraction with increasing milling time.

Synthesis, X-ray single crystal structure, likelihood of occurrence of intermolecular contacts, spectroscopic investigation and DFT quantum chemical calculations of zwitterionic complex: 1-Ethylpiperaziniumtrichlorozincate (II)

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Polymeric and extended metal (II) halide complexes have recently received a great attention for their particular properties related to their ability to optimize both the inorganic and organic components. These materials have recently attracted further interest due to their potentially interesting catalytic, thermal, magnetic and electrical properties [1,2]. The synthesis and the X-ray structure of the Zn(II) zwitterionic complex are described. In the atomic arrangement, the ZnCl_3N entities, grouped in pairs, are deployed along the b-axis to form layers. The organic entities are inserted between these layers through $\text{N-H}\cdots\text{Cl}$ and $\text{C-H}\cdots\text{Cl}$ hydrogen bonds to form infinite three-dimensional network (Fig.1). The 3D Hirshfeld surfaces were investigated for intermolecular interactions. The optimized geometry, Mulliken charge distribution, molecular electrostatic potential (MEP) maps and thermodynamic properties have been calculated using the Lee-Yang-Parr correlation functional B3LYP with the LanL2DZ basis-set. The HOMO and LUMO energy gap and chemical reactivity parameters were made. The ^{13}C and ^{15}N -CP-MAS NMR spectra are in agreement with the X-ray crystal structure. The vibrational absorption bands were identified by infrared spectroscopy. DFT calculations allowed the attribution of the NMR peaks and of the IR bands.

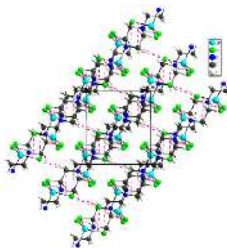


Fig.1. Projection along the *b*-axis of the crystal packing of the title compound. The dotted lines indicate hydrogen bonds.

Keywords: Crystal, Hirshfeld surface; enrichment ratio; Quantum; DFT; MEP

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A Hirshfeld surface analysis, crystal structure and physicochemical characterization of 1-ethylpiperazinium trichlorocadmate(II)

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In the past decades, coordination polymers have been subjected to a vast number of studies owing to their potential applications in catalysis, molecular adsorption, nonlinear optics and luminescence [1,2] as well as their intriguing structural motifs. As a part of our continued involvement in the investigation of coordination compounds, a novel organic–inorganic hybrid material, $\text{C}_6\text{H}_{15}\text{N}_2\text{CdCl}_3\cdot\text{H}_2\text{O}$, was synthesized, and its crystal structure is characterized by one-dimensional polymeric chains of an edge-sharing CdCl_5N distorted octahedral (**Fig.1**). These chains are linked to the water molecules via O–H...Cl hydrogen bonds to form layers parallel to the (b, a+c) plane. The crystal structure was stabilized by an extensive network of N–H...Cl, O–H...Cl and N–H...O hydrogen bonds which are analyzed by Hirshfeld surface calculations. The differential scanning calorimetry (DSC) reveals that the title compound is stable until 101.6 °C. The optimized geometry parameters, normal mode frequencies, and corresponding vibrational assignments of the present compound were theoretically examined by DFT/B3LYP method with the LanL2DZ basis set. The calculated results showed that the optimized geometry could well reproduce the crystal structure and that the theoretical vibrational frequency values were in good agreement with their experimental counterparts.

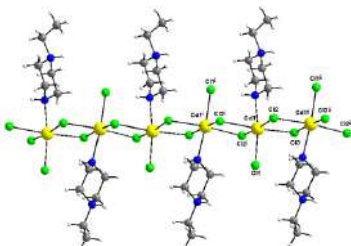


Fig. 1. $[\text{CdCl}_3\text{C}_6\text{H}_{15}\text{N}_2]_n$ polymeric chain in $\text{C}_6\text{H}_{15}\text{N}_2\text{CdCl}_3\cdot\text{H}_2\text{O}$.

Keywords: Crystal, Hirshfeld surface; enrichment ratio; Quantum; DFT; DSC

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EFFECT OF SOLVENT ON THE NUCLEOPHILIC REACTIVITY OF PYRROLIDINE: EXPERIMENTAL AND THEORETICAL APPROACH

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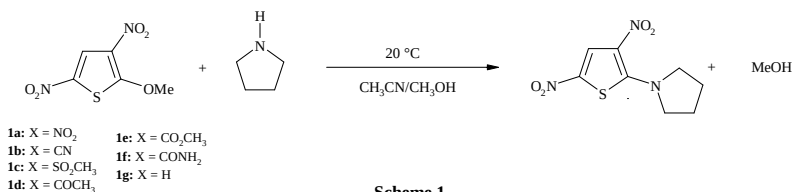
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The second-order rate constants for reaction of 2-methoxy-3-x-5-nitrothiophenes **1a-c** with pyrrolidine in various CH₃CN-CH₃OH mixtures at 20 °C have been employed to determine experimentally the nucleophile-specific parameters N and s of pyrrolidine according to the linear free energy relationship $\log k (20\text{ }^{\circ}\text{C}) = s_N (E + N)$.

A Density functional theory (DFT) protocol has been developed for the first time to predict the nucleophile parameters N of pyrrolidine in various acetonitrile-methanol mixtures using the package-program Gaussian 09 B3LYP /6-311++G (d,p).

As can be seen, a satisfactory correlation between the mole fraction of methanol values and the experimental and theoretical nucleophilic parameters N of pyrrolidine has been observed and discussed.



Key words: Pyrrolidine, Mary's Equation, Nucléophilicity, Density Functional Theory (DFT), Thiophene.

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**The lichens of Tunisia:
Use as indicators for the assessment of the level of pollution
Analysis by atomic absorption spectroscopy, plasma torch emission
spectrometry and high-performance liquid chromatography (HPLC)**

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The renewed interest for plants in both industrialized and developing countries has encouraged us to undertake a study on lichens in Tunisia. Nowadays, lichens are most known to the public for their role as pollution indicators.

Our study deals with air pollution, which is a major environmental concern nationally and internationally. The ability of lichens to capture and store both organic and inorganic air pollutants has been exploited to assess the air quality of the Bizerte region.. Our interest was in the behavior of lichens with respect to air pollutants such as heavy metals and polycyclic aromatic hydrocarbons.

Atomic absorption spectroscopy, plasma torch emission spectrometry and high-performance liquid chromatography (HPLC) techniques were used for the identification and characterization of contaminants accumulated by lichens collected from different harvesting sites in the Bizerte region.

Our results have identified about fifteen mineral pollutants, some of which are toxic such as: Pb, Hg, Co, As, ... The origins of these contaminants are diverse: industrial and road traffic (Zarzouna, Bizerte), agricultural (use of fertilizers at El Alia).

Five organic contaminants belonging to the family of polycyclic aromatic hydrocarbons (PAHs) (dibenzofuran, fluorene, phenanthrene, anthracene, and fluoranthene) were identified in lichens collected at Zarzouna. While no PAH pollutants are detected in those of El Alia and Sejnane, two rural areas far from emitting sources. The level of pollution in the Bizerte region is very low compared to those of European cities.

Short route to Abietanes Diterpenes

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Abietane diterpenes are widely distributed, naturally occurring products in the plant kingdom. Many of them exhibit significant biological activities, e.g. antibiotic¹, antitumor², anti-virus, antimalarial, anti-oxidant effects. Due to their wide distribution and interesting bioactivities, many synthetic studies have been reported. In this work we have investigated a simple route to abietanes.

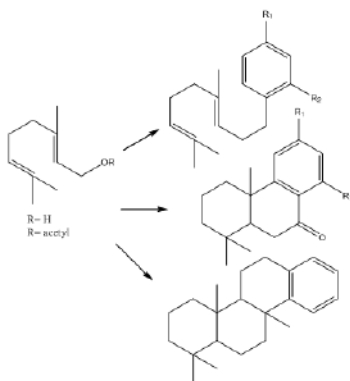


Fig. Synthesis of tricyclic and tetracyclic compounds

Key words: Abietane, Diterpenes, biological activities

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Characterization of amorphous solid dispersions of atorvastatin containing poly (vinyl pyrrolidone) PVP

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The aim of this study was to estimate the optimal amount of polymer required to generate stable amorphous formulation of a poorly soluble drug. Physical stability of amorphous molecular dispersions of atorvastatin prepared by mechanical process in the presence of poly (vinyl pyrrolidone) (PVP K40) was evaluated under humidity. Three different drug-polymer weight ratios (10, 25, and 50 wt. %polymer) were milled and characterized using differential scanning calorimetry DSC and X- ray diffraction.

The results obtained indicate that in contrast to the behavior of the pure amorphous drug recrystallization of atorvastatin was inhibited in the presence of PVP K40. Particularly solid dispersions of atorvastatin in 10% of PVP keep the amorphous form in the presence of moisture.

Keywords: Recrystallization, Solid dispersion, Atorvastatin, Poly (vinyl pyrrolidone) PVP K40..

Molecular structural and vibrational studies of a new non-centrosymmetric hybrid material (C₅H₉N₃)[ZnBr₄]H₂O

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The organic-inorganic hybrid materials have received a great attention in recent years due to their ability to combine the special structural features of inorganic compounds and the characteristics of organic molecules. In fact, they exhibit advantageous properties such as magnetic [1, 2] and optical properties [3]. The novel inorganic–organic hybrid (C₅H₉N₃)[ZnBr₄]H₂O were synthesized by evaporation lente conditions and was characterized by single crystal X-ray diffraction at room temperature, thermal analysis (DTA-TG) and vibrational studies. It crystallizes at room temperature in the non- centrosymmetric space group P1. The supramolecular crystal structure of these materials is built from the alternatively arranged inorganic and organic layers and stabilized by N—H···Br and N—H···O hydrogen bonds.

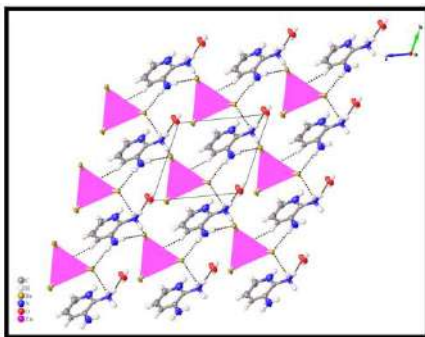


Figure. Projection of the crystal structure of (C₅H₉N₃)[ZnBr₄]H₂O along the a-axis.

Keywords: Crystal structure, slow evaporation, vibrational studies

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Study of Residue Analysis of Organochlorine Pesticides (POCs) in Honey by Gas Chromatography (GC-ECD)

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The present study concerns the preliminary evaluation of the contamination of some honey samples collected in different regions of Tunisia by organochlorine pesticides. The ten samples were taken in June and July. For each sample of honey collected, a data sheet was completed to specify, among other things, the identity of the site taken, the date of sampling and the honey storage methods. Once collected at the production sites, the honey samples were placed in glass containers, then stored at -20 ° C until chemical analysis. After the pretreatment step, the honey samples undergo a liquid-liquid extraction method, followed by purification by adsorption chromatography before being analyzed by gas chromatography. The chromatographic analyzes were carried out on two capillary columns of different polarity, a weakly polar SLB5-MS column (5% silphenylene / 95% dimethylpolysiloxane) and a moderately polar SPB-608 phase column used as a confirmation column to ensure reliability of analyzes. Finally Chromatographic analysis of organochlorine pesticides by high-resolution gas chromatography with electron capture detection achieves detection limits between 0.08 and 0.5 ng mL⁻¹ and accuracy less than 7% in terms of relative standard deviation DSR. The analysis of 10 honey samples from several Tunisian regions reveals that the majority of samples are contaminated by the desired pesticide residues. HCHs are the most common pesticides in honey samples analyzed with average recorded concentrations of 9,606 ng g⁻¹. This difference could be due to recent, unreported use of these insecticides.

Keywords: POC, GC-ECD, reliability of analysis.

EFFICIENT N-HETEROCYCLIC COPPER(I) COMPLEXES CATALYZED 1,3-CYCLOADDITION FOR THE SYNTHESIS OF TRIAZOLES AT AMBIENT CONDITIONS: SYNTHESIS AND BIOLOGICAL ACTIVITIES

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Click chemistry is one of the most powerful tools for the construction of various triazoles, which are often considered in pharmaceuticals, drug discovery, polymers and material science [1-3]. We herein report the synthesis of (Cu-NHC) complexes, bearing symmetrical and unsymmetrical ligands which is catalytically applicable to 1,3-dipolar cycloaddition reaction of in situ generated azides and phenyl acetylene to synthesize triazoles at low copper-NHC catalyst loading at ambient conditions. In addition, the biological activities of the new synthesized complexes (Cu-NHC) against food-borne pathogens and clinical micro-organisms, were studied. **Figure 1**

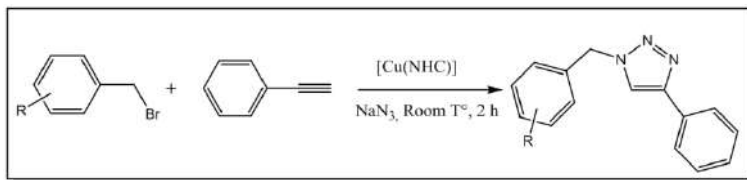


Figure 1: Cu-NHC complexes catalyzed formation of triazoles

Key words: click chemistry, 1,3-cycloaddition,, Cu-NHC complexes, triazoles, ambient conditions, biological activities.

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Synthesis, vibrational and optical proprieties of a new hybrid organic-inorganic material (C₇H₈N₃)₂[SnCl₆]

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Considerable attention has been focused on organic-inorganic hybrid materials due to their interesting architectures and topologies [1,2]. These compound represent an advanced field in material science [3-4]. A new organic-inorganic hybrid material, (C₇H₁₀N)₂SnCl₆, has been grown by the solvent evaporation method. A determination of the crystalline structure is performed from single X-ray diffraction data. This compound crystallizes at room temperature in the triclinic system with the Centro-symmetric P-1 space group. The atomic arrangement can be described by an alternation of organic and inorganic layers. The anionic layers are built up of [SnCl₆]²⁻ octahedron, while the cationic layers are arranged in sandwich between the inorganic ones. Crystal packing is governed by weak hydrogen bonds N-H...Cl to form zero-dimensional network. The detailed interpretation of the vibration modes has been carried out. Optical proprieties are investigated by photoluminescence (PL) spectroscopie.

Keywords

Organic-inorganic material, X-ray crystal structure, IR,, Photoluminescence.

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Transition metal halide salts of 1-methylpiperazine: Synthesis, Characterization and Magnetic properties

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During the past decades, construction of self-assembly of organic-inorganic hybrid compounds has attracted much attention in chemistry, physics and material science owing to their abilities to combine the desired properties of organic and inorganic compounds, so as to exhibit some interesting special properties, such as second order nonlinear optical (NLO) response, magnetism and even multifunctional properties. A new family of complexes of 1-methylpiperazine metal halides has been successfully synthesized by slow evaporation and characterized by single-crystal X-ray diffraction as well as with thermogravimetry, temperature-dependent X-ray powder diffraction and magnetic measurements. The compounds produced include $(C_5H_{14}N_2)[CuCl_4]$ (1), $(C_5H_{14}N_2)[CoCl_4] \cdot H_2O$ (2) and $(C_5H_{14}N_2)[MnCl_3(H_2O)_3]Cl^-$ (3). The magnetic measurements indicate that the compounds (1) and (2) exhibit antiferromagnetic interactions while Mn complex (3) is paramagnetic. The magnetic properties of this family are related to the interionic distances between the $[MX_n]^{2-}$ anions which are in turn strongly related to the properties of the organic cation.

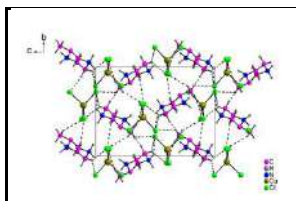


Figure. Projection of the crystal structure of $(C_5H_{14}N_2)[CuCl_4]$ along the a-axis.

Keywords: Crystal structures, Magnetic properties, Transition metal.

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Degradation of diclofop methyl used as an herbicide under gamma irradiation

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This study reports the efficiency of gamma irradiation to degrade diclofop methyl (DM) an herbicide deriving from aryloxy propionic acid. Aqueous solutions of DM were irradiated with ⁶⁰Co gamma-rays at doses of 0.5 -8 kGy. Measuring the reduction in Chemical Oxygen Demand (COD) and Total Organic Carbon (TOC) during the irradiation process showed that the mineralization efficiency increases with increasing radiation dose. During the mineralization, some aromatic intermediates were identified by GC/MS showing that degradation process starts with the fragmentation of the molecule followed by reaction involving the hydroxyl radical, which is generated by the radiolysis of water. As a result, a mechanistic pathway was proposed for DM degradation. Finally, based on spectrophotometric measurement experiments showed that the degradation process of DM is a pseudo-first order.

Keywords: gamma radiation, hydroxyl radicals, diclofop methyl

Kinetics of a reaction driven by evaporation: Thermal analysis of TEA decomposition.

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In many cases, the decomposition of solids or liquids occur in the gas phase [1–3]: therefore, the kinetics of the process is governed by the evaporation rate. Despite this fact, in the bibliography of thermal analysis there is a lack of evaporation kinetic studies. For this purpose, we analyse the kinetics of triethanolamine (TEA) decomposition.

A model that describes the evaporation kinetics is developed in films and crucibles that takes into account vapour diffusion and vapour carried away by the purge gas flow. This model takes into account gas diffusion and convective gas transport; it describes the evaporation kinetics under the general conditions of thermogravimetric measurements. The model is used to determine the equilibrium vapor pressure in a relatively wide temperature range. Also considers two different furnace setups: horizontal and vertical; i.e., the purge gas flow is either perpendicular or parallel to the liquid surface.

In this post it is shown that the thermal decomposition of TEA is governed by its evaporation. In this case the rate constant follows an Arrhenius temperature dependence where the activation energy is the standard evaporation enthalpy. We have shown that this model successfully describes TEA decomposition.

keywords: Triethanolamine, vaporization, thermal decomposition, Equilibrium vapor pressure, Thermogravimetric analysis.

Reference

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ISOLATION AND HEMISYNTHESIS OF CURCUMINOIDS OF *CURCUMA LONGA* L.

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In the present work, we report, purification and characterization of curcuminoids of turmeric longa L. These compounds are extracted from contact between turmeric rhizome powder and several organic solvents. The best yield (7.52%) is obtained using acetone as a solvent with pumice stones.

This study made it possible to isolate 4 natural products. Among these compounds, curcumin, which is the major compound obtained in (1.03%), is exploited in semisynthetic reactions of curcumin analogues. It was possible for us to react curcumin in esterification and nitration reactions and we obtained two original semisynthetic compounds.

The Structures of the synthesized compounds were determined using physical technics (fluorescence under UV light, IR), the ^1H NMR, ^{13}C NMR

Key words: Curcuminoids, turmeric longa L, semisynthesis, organic solvents, spectroscopic methods.

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Density functional theory mechanistic study of synthesis of 4-thiazolidinone derivatives

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In our work, we have studied by density functional theory the synthesis of the derivatives of 2-phenylimino-4-thiazolidinones according to the methods of ottana [1] and zhang [2]. Local and global reactivity indices and activation energy calculations were evaluated at B3LYP/6-31G+(d). The reaction path was followed by the calculation of the intrinsic reaction coordinates. We have obtained under kinetic control the derivatives 5-thiazolidinones while the derivatives 4-thiazolidinones are the thermodynamic products. The data from the energetic diagrams were in good agreement with the study of the local regioselectivity. The polar protic solvent (ethanol) has exhibited a remarkable effect on the values of the activation energy when studying the tautomeric equilibria of the obtained thermodynamic (2-phenylimino-4-thiazolidinone (P4)). We have obtained also that the dimeric forms of 2-phenylimino-4-thiazolidinones are stabilized by intermolecular hydrogen bonds of the N-H and O-H type.

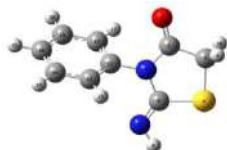


Figure 1: 2-imino-3-phenyl-4-thiazolidinone (P1)

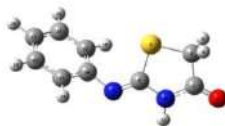


Figure 2: 2-imino-4-thiazolidinone (P2)

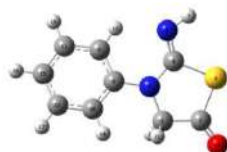


Figure 3: 2-imino-3-phenyl-5-thiazolidinone (P3)

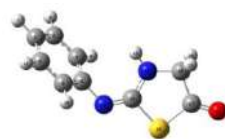
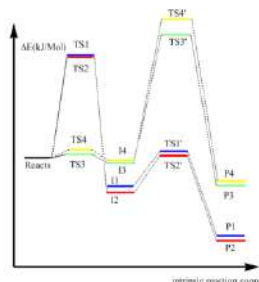


Figure 4: 2-imino-4-thiazolidinone (P4)



Scheme1: Energy diagram of the reaction between phenylthiourea and chloroacetyl chloride

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Synthesis, crystal structure and characterization of the new arsenate $\text{Na}_3\text{Al}_2(\text{AsO}_4)_3$

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A literature search revealed that studies on arsenates of alkalis and trivalent metals are much less numerous than phosphates. Indeed, for aluminum, only a few compounds have been the subject of a structural study [1,2].

In this context and in order to synthesize new materials with open framework, we undertook the investigation of the Na-Al-As-O system. A new phase $\text{Na}_3\text{Al}_2(\text{AsO}_4)_3$ (**1**) has been synthesized by solid state reaction. This compound is isostructural to $\text{Na}_3\text{M}_2(\text{AsO}_4)_3$ (M : Cr, Ga, Fe) ones [3]. The structure determined by single crystal X-ray diffraction is refined in the space group R-3c until the final agreement factors $R=0.026$ and $wR(F^2)=0.093$, with the cell parameters: $a = 13.334(1) \text{ \AA}$, $c = 18.480(1) \text{ \AA}$, $\gamma=120^\circ$, $Z = 12$ and volume $V= 2819.4 (16) \text{ \AA}^3$. The asymmetric unit of (**1**) consists of Al_4O_{18} clusters connected by AsO_4 tetrahedra. The structure can be described as a three-dimensional framework $[\text{Al}_2(\text{AsO}_4)_3]_\infty$ delimiting interstitial spaces in which are inserted Na^+ ions in a partially disordered distribution (**Fig. 1**). These cations are statistically distributed on several independent positions. The obtained structural result is confirmed by the Bond Valence Sum model (BVS) and the Charge Distribution method (CHARDI). Qualitative analysis of the diffraction powder diffractogram X-ray based on the Rietveld method revealed its purity. Spectroscopic analysis methods (IR and Raman) was conducted to identify the absorption bands characteristic of AsO_4 group.

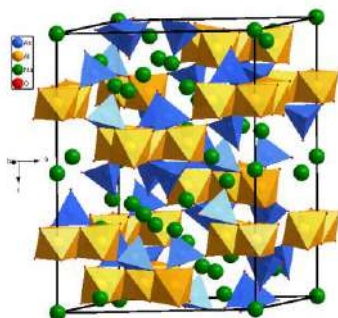


Fig. 1. The structure of $\text{Na}_3\text{Al}_2(\text{AsO}_4)_3$ prespective view

Key words: clusters, X-ray diffraction, purity.

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Chemical composition and antioxidant activity of essential oils from different Organs of Tunisian *Pituranthos chloranthus* (Apiaceae)

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The present study reports the variation of the chemical composition and the antioxidant properties of essential oils from an endemic species of North Africa "*Pituranthos chloranthus*", collected from two areas of the South-East of Tunisia (Boughrara and Naffatia) at the fruiting stage. The essentials oils extracted from the seeds and stems by hydrodistillation were analysed by Gas Chromatography/Flame Ionization Detector (GC-FID) and Gas Chromatography/Mass Spectrometry (GC-MS). Seventy compounds were identified accounting for 90.4 to 99.7 % of the whole essential oil showing the predominance of monoterpene hydrocarbons. The most abundant compounds of the seeds oils of Boughrara and Naffatia were α -pinène (32.2 %; 37.7 %) and β -pinene (27.8 % ; 30.7 %), respectively while β -phellandrene (17.2 % ; 11 %), α -phellandrene (14.1 % ; 7.2 %), α -pinène (11 % ; 8.9%), β -pinene (8.1 % ; 6.5 %) and p-cymene (5.8 %; 8.7 %) were found to be the major compounds in the stems oils of Boughrara and Naffatia, respectively. The antioxidant activities of essential oils were evaluated by reducing power assays and metal chelating activity. The obtained results revealed that the stems oils collected from Naffatia showed the highest reducing power with an EC₅₀ value of 192 μ g/ml. However, the great metal chelating activity was recorded for the stems essential oils collected from Boughrara (IC₅₀= 43 μ g/ml).

Key words: *Pituranthos chloranthus*, essential oil, chemical composition, antioxidant activity.

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**SYNTHESIS, CHARACTERIZATION, ELECTRICAL
PROPERTIES OF
HLnP₂O₇·xH₂O·yNH₃ AND Gd₂P₄O₁₃ (Ln = Gd, Ho), (x = 2,3; y = 0,1)**

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New diphosphates [HGdP₂O₇·2H₂O]·NH₃ and HHoP₂O₇·3H₂O were synthesized by slow evaporation method at room temperature. The obtained crystals, with prismatic morphology, were characterized by means of X-ray diffraction (XRD) and infrared (IR) spectroscopy. The results showed a high purity phases.

The calcination of [HGdP₂O₇·2H₂O]·NH₃ at 850°C and HHoP₂O₇·3H₂O at 300°C in a static air furnace, allowed us to obtain respectively the tetrphosphate Gd₂P₄O₁₃ and the anhydrous diphosphate HHoP₂O₇. X-ray powder diffraction and infrared spectroscopy were used to identify these materials.

The electrical properties of HHoP₂O₇ and Gd₂P₄O₁₃ were investigated through impedance complex analysis. Resistance, conductivity values and conduction mechanism within the materials are determined and discussed. Activation energies of 0.405 and 1.16 eV were deduced from the Arrhenius plots for HHoP₂O₇ and Gd₂P₄O₁₃ respectively.



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