21st Tunisia Chemistry Conference

TCC
2022

Organized by the

Tunisian Chemical Society

18-21 December 2022

Rosa Beach Hotel, Skanès Monastir, Tunisia

Abstracts of Lectures and Communications
List of Participants

Tunisian Chemical Society - Short Program of TCC 2022

Sunday 18 December 2022	
14.00	**Welcoming participants, distribution of documents and check in**
19.30	***Dinner***
Monday 19 December 2022	
09.00 – 09.15	**Opening Ceremony**
09.15 – 09.50	**Plenary Lecture 1 Lynne A. PILCHER** *University of Pretoria, South Africa*
09.50 – 10.05	**Intervention 1 Mohamed M. CHEHIMI** *Executive Editor-in-Chief of Chemistry Africa*
10.05 – 10.40	**Poster Session 1 (P 1 - P 40) Alphabetical Order**
10.45 – 12.30	**Oral Communications - Session 1 : OC 01 - OC 07**
13.00	***Lunch***
14.40 – 15.15	**Plenary Lecture 2 Mahmood JAVEED** *KAUST, Thuwal, Saudi Arabia*
15.15 – 15.30	**Intervention Sponsor 2 Mohamed Ali Zaouali** *AQUATUN*
15.30	***Gathering for the group photo***
15.45 – 16.45	**Oral Communications - Session 2 : OC 08 - OC 11**
16.45 – 17.30	**Coffee break + Poster Session 2 (P 41 - P 80) Alphabetical Order**
17.30 – 18.45	**Oral Communications - Session 3 : OC 12 - OC 16**
19.30	***Dinner***
Tuesday 20 December 2022	
09.00 – 09.35	**Plenary Lecture 3 Jalel LABIDI** *University of Basque Country (UPV/EHU), San Sebastián, Spain*
09.35 – 10.10	**Plenary Lecture 4 Philiswa Nosizo NOMNGONGO** *University of Johannesburg, Doornfontein Campus, South Africa*
10.10 – 10.25	**Intervention Sponsor 3 -** *HTDS*
10.25 – 11.00	**Poster Session 3 (P 81 - P 120) Alphabetical Order**
11.00 – 12.30	**Oral Communications - Session 4 : OC 17 - OC 22**
13.00	***Lunch***
15.00 – 16.00	**Oral Communications - Session 5 : OC 23 - OC 26**
16.00 – 16.45	**Coffee break + Poster Session 4 (P 121 - P 160) Alphabetical Order**
17.00 – 19.00	**General Assembly of the Tunisian Chemical Society**
19.30	***Dinner***
21.00	**Election of the new National Bureau of the Tunisian Chemical Society**
Wednesday 21 December 2022 (morning)	
09.00 – 09.35	**Plenary Lecture 5 Fabrice ANIZON** *Université Clermont Auvergne, CNRS, Clermont Auvergne INP, ICCF, Clermont-Ferrand, France*
09.45 – 10.45	**Oral Communications - Session 6 : OC 27 - OC 30**
10.45 – 11.15	**Poster Session 5 (P 161 - P 191) Alphabetical Order**
11.15 – 12.15	**Oral Communications - Session 7 : OC 31 - OC 34**
12.15 – 12.50	**Plenary Lecture 6 Michel BALTAS** *Laboratoire de Chimie de Coordination du CNRS, Toulouse, France*
12.50	**Closing Remarks and Poster Awards**
13.00	***Lunch, Check Out and Departure***

FOREWORD

On behalf of the the Tunisian Chemical Society, it is a great pleasure to welcome you to the 21st Edition of the Tunisian Chemistry Conference (TCC2022).

As the last editions, TCC is intended to cover all aspects of chemistry science from fundamental to applied chemistry.

The Organizing Committee has considered many issues to make TCC2022 an ideal forum to discuss recent progress and challenges in chemistry and to offer the delegates opportunities for cooperation and networking.

For this 2022 edition, we invited renowned Speakers by trying to take into account both disciplinary and geographical diversity. Invited Speakers come from South Africa (2), Saudi Arabia (1), Spain (1) and France (2). Various topics dealing with modern methods of teaching, the properties of new synthetic or bio-based materials, nanotechnology and environmental analytical chemistry or medicinal chemistry will be discussed.

TCC 2022 brought more than 379 participants, and the program promises to be rather busy with 133 oral communications and 191 poster communications, which will cover several topics.

we have selected the beautiful Rosa Beach Hotel in Skanes Monastir which we do hope will be an inspiring venue for all delegates.

Dear participants, we thank you in advance for coming all the way to Monastir to share your solid research. We hope you enjoy the science as well as your time in this beautiful coastal region of Tunisia.

Yours with kindest regards

Pr Hatem BEN ROMDHANE

President of the Tunisian Chemical Society
and Chairman of TCC2022

SCIENTIFIC COMMITTEE

BEN ROMDHANE Hatem	*FST - University of Tunis El Manar*
NOMNGONGO Philiswa Nosizo	*Univ. of Johannesburg, South Africa*
TRARI Mohamed	*USTHB University, Algiers, Algeria*
MEGRICHE Adel	*FST - University of Tunis El Manar*
CHAOUACHI Béchir	*University of Gabès, ENIG-Gabès*
EFRIT Mohamed Lotfi	*FST - University of Tunis El Manar*
BERGAOUI Latifa	*Univ. of Carthage, INSAT-Tunis*
MNIF Amine	*Univ. of Tunis El Manar, FST-Tunis*
LATROUS Latifa	*FST - University of Tunis El Manar*
AMMAR Houcine	*University of Sfax, FSS-Sfax*
BELLAKHAL Nizar	*University of Carthage, INSAT-Tunis*
BEN JANNET Hichem	*Univ. of Monastir, FSM-Monastir*
KHITOUNI Mohamed	*University of Sfax, FSS-Sfax*
REZGUI Farhat	*Univ. of Tunis El Manar, FST-Tunis*
ABIDI Rym	*University of Carthage, FSB-Bizerte*
BOUBAKER Taoufik	*Univ. of Monastir, FSM-Monastir*
BEN SALEM Ridha	*University of Sfax, FSS-Sfax*
ROMDHANE Mehrez	*University of Gabès, ENIG-Gabès*
MOUSSAOUI Younes	*University of Gafsa, FSG-Gafsa*
BEN DHIA Mohamed Taieb	*Univ. of Tunis El Manar, FST-Tunis*

ORGANIZING COMMITTEE

BEN ROMDHANE Hatem	*FST - University of Tunis El Manar*
MEGRICHE Adel	*FST - University of Tunis El Manar*
CHAOUACHI Béchir	*Univ. of Gabès, ENIG-Gabès*
EFRIT Mohamed Lotfi	*FST - University of Tunis El Manar*
BERGAOUI Latifa	*Univ. of Carthage, INSAT-Tunis*
MNIF Amine	*Univ. of Tunis El Manar, FST-Tunis*
LATROUS Latifa	*FST - University of Tunis El Manar*
ABDELKAFI Mohamed Mouldi	*Univ. of Tunis El Manar, FST-Tunis*
LAAJIMI Imed	*Tunisian Chemical Society*

	Sunday 18 December 2022							
14.00	**Welcoming participants, distribution of documents and check in**							
19.30	***Dinner***							
	Monday 19 December 2022							
09.00 – 09.15	**Opening Ceremony**							
09.15 – 09.50	**Lecture 1** **Lynne A. PILCHER** - Introduced by *Hatem Ben Romdhane* *Department of Chemistry, University of Pretoria, South Africa* Systems thinking in tertiary chemistry for sustainable development							
09.50 – 10.05	**Intervention 1** **Mohamed M. CHEHIMI** - Introduced by *Adel Megriche* *Executive Editor-in-Chief of Chemistry Africa* Chemistry Africa celebrating its 5th anniversary - Progress report and future prospects							
10.05 – 10.40	**Poster Session 1 (P 1 - P 40) Alphabetical Order** **Evaluators:** Nabil Zouari, Rafik Gatri							
	Oral Communications - Session 1							
	Room A - Chair: *Ridha Ben Salem* ***Organic Chemistry***		***Room B*** - Chair: *Houcine Naili* ***Inorganic Chemistry***		***Room C*** - Chair: *Latifa Bergaoui* ***Analytical Chemistry***		***Room D*** - Chair: *Hatem Majdoub* ***Catalysis & Polymer Science***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
10.45 – 11.00	**OC-01A**	ABID Hedia	**OC-01B**	AISSA Taissir	**OC-01C**	BELGACEM Chaouki	**OC-01D**	BOUYAHYA Chaima
11.00 – 11.15	**OC-02A**	ARAR Wafa	**OC-02B**	AMDOUNI Oumaima	**OC-02C**	BOUALLEGUE M^{ed} Chedly	**OC-02D**	BRIRMI Nour El Houda
11.15 – 11.30	**OC-03A**	AYACHI Amani	**OC-03B**	AGREN Soumaya	**OC-03C**	GUEDOUAR Rihab	**OC-03D**	CHALLOUF Oumayma
11.30 – 11.45	**OC-04A**	AYADI Nouha	**OC-04B**	BACCARA Sarah	**OC-04C**	LABIDI Aymen	**OC-04D**	HAJLAOUI Oumaima
11.45 – 12.00	**OC-05A**	BALLAGHA Najet	**OC-05B**	BEN JOMAA Mariem	**OC-05C**	TRABELSI Houyem	**OC-05D**	KHAIRI Rihab
12.00 – 12.15	**OC-06A**	BEN JABALLAH Oumayma	**OC-06B**	BEN SLIMEN Jihen	**OC-06C**	TORKHANI Rachel	**OC-06D**	SAKFALI Jamila
12.15 – 12.30	**OC-07A**	SOUII Ichrak	**OC-07B**	BEN SMIDA Youssef	**OC-07C**	MPUPA Anele	**OC-07D**	ALKISKAS Ismail
13.00	***Lunch***							

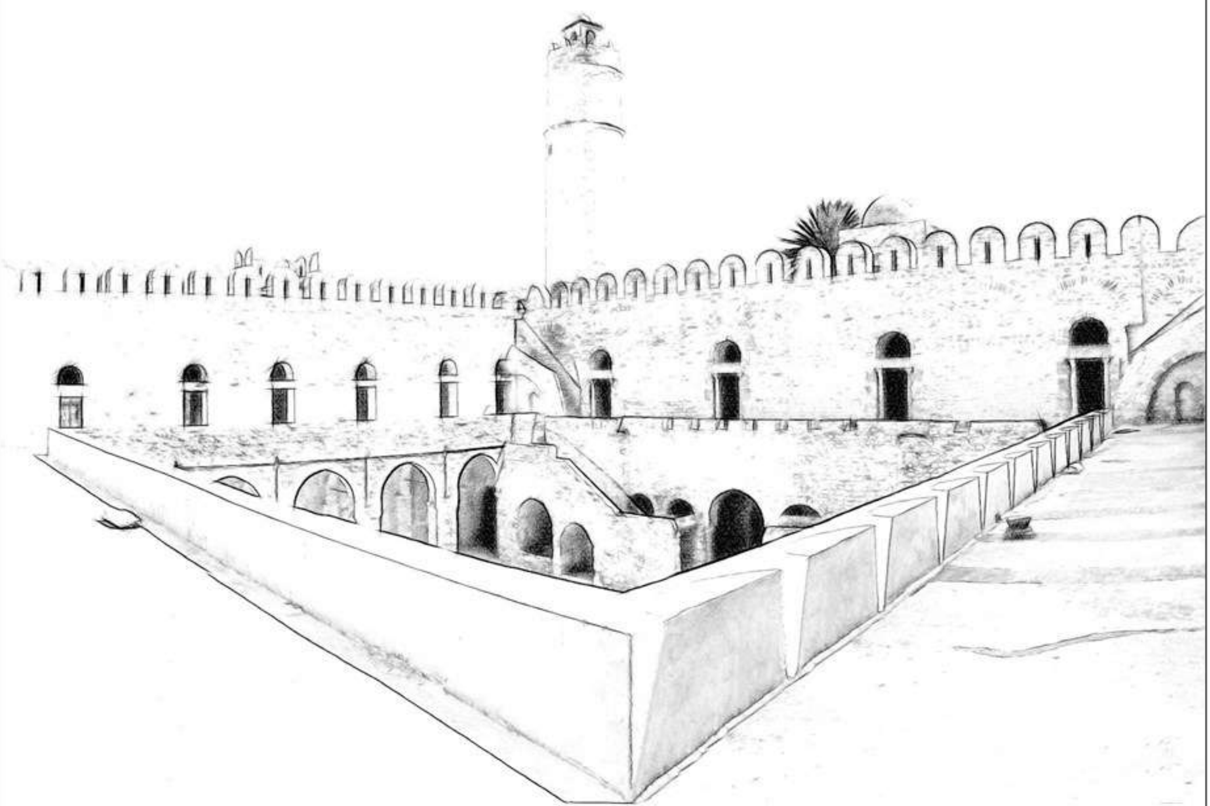
14.40 – 15.15	**Lecture 2** **Mahmood JAVEED** - Introduced by *Mohamed CHEHIMI* *King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia* Electronic properties of nitrogenated two-dimensional structures							
15.15 – 15.30	**Intervention Sponsor 2 - AQUATUN - Mohamed Ali Zaouali**							
15.30	**Gathering for the group photo**							
	Oral Communications - Session 2							
	Room A - Chair: Najib Mekni ***Organic Chemistry***		***Room B*** - Chair: *Halim Hammi* ***Inorganic Chemistry***		***Room C*** - Chair: *Mehrez Romdhane* ***Environment & Green Chemistry***		***Room D*** - Chair: *Wafa Essafi* ***Physical Chemistry***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
15.45 – 16.00	**OC-08A**	BEN MAAMER Chayma	**OC-08B**	CHAMAM Sabrine	**OC-08C**	AISSAOUI Yousra	**OC-08D**	BOUZAIENE Roua
16.00 – 16.15	**OC-09A**	BEN ROMDHANE Rabeb	**OC-09B**	ELHLELI Hanedi	**OC-09C**	AJARI Hanen	**OC-09D**	CHELLEGUI Mohamed
16.15 – 16.30	**OC-10A**	BOULILA Besma	**OC-10B**	FANDOULI Amna	**OC-10C**	AMRAOUI Amira	**OC-10D**	GABSI Mariem
16.30 – 16.45	**OC-11A**	BSAIHIA Mayssa	**OC-11B**	FERCHICHI Amal	**OC-11C**	ARFAOUI Oumayma	**OC-11D**	GARA Rayene

16.45 – 17.30	**Coffee break + Poster Session 2 (P 41 - P 80) Alphabetical Order** **Evaluators:** Raoudha Ben Ameur, Mohamed Belhouchet							
	Oral Communications - Session 3							
	Room A - Chair: *Thouraya Barhoumi* ***Organic Chemistry***		***Room B*** - Chair: *Ezzeddine Srasra* ***Inorganic Chemistry***		***Room C*** - Chair: *Khaled Alouani* ***Environment & Green Chemistry***		***Room D*** - Chair: *Mohamed Dammak* ***Physical Chemistry***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
17.30 – 17.45	**OC-12A**	FAIDI Abir	**OC-12B**	GANNOUNI Afef	**OC-12C**	BELHAMEID Ahmed	**OC-12D**	GHAZOUANI Anis
17.45 – 18.00	**OC-13A**	GHABI Amira	**OC-13B**	GARCI Fatma	**OC-13C**	BEN ABDALLAH Yosra	**OC-13D**	JEMILI Nouha
18.00 – 18.15	**OC-14A**	GRATI Nesrine	**OC-14B**	GHARBI Chaima	**OC-14C**	BOUBAKER Hana	**OC-14D**	MEDDEB-LIMEM Sondos
18.15 – 18.30	**OC-15A**	HABA Hamada	**OC-15B**	HAJJI Bassem	**OC-15C**	ETTEYEB Naceur	**OC-15D**	MRAD Sahar
18.30 – 18.45			**OC-16B**	GHILOUFI Mabrouka	**OC-16C**	GUESMI Rim	**OC-16D**	MESSAOUDI Boulanouar
19.30	***Dinner***							

	Tuesday 20 December 2022							
09.00 – 09.35	**Lecture 3** **Jalel LABIDI** - Introduced by *Farhat Rezgui* *University of Basque Country (UPV/EHU), Plaza Europa 1, San Sebastián, Spain* Chitin and Chitosan Based Materials							
09.35 – 10.10	**Lecture 4** **Philiswa Nosizo NOMNGONGO** - Introduced by *Latifa Latrous* *Department of Chemical Sciences, University of Johannesburg, Doornfontein Campus, South Africa* Nanotechnology and Environmental Analytical Chemistry: Current Status and Future Perspectives							
10.10 – 10.25	**Intervention Sponsor 3 - HTDS**							
10.25 – 11.00	**Poster Session 3 (P 81 - P 120) Alphabetical Order** **Evaluators:** Noureddine Raouafi, Azaiez Ben Akacha							
Oral Communications - Session 4								
	Room A - Chair: *Rafaa Besbes* ***Organic Chemistry***		***Room B*** - Chair: *Najoua Frini Srasra* ***Inorganic Chemistry***		***Room C*** - Chair: *Zouhair Ksibi* ***Environment & Green Chemistry***		***Room D*** – *Nizar Belakhal* ***Nanotechnology & Materials Sciences***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
11.00 – 11.15	**OC-17A**	HAJRI Azhar	**OC-17B**	HARZI Feriel	**OC-17C**	HAYDER Rassil	**OC-17D**	BAACHAOUI Sabrine
11.15 – 11.30	**OC-18A**	HASYEOUI Mohamed	**OC-18B**	HERMI Sabrine	**OC-18C**	KHLIFI Hiba	**OC-18D**	BAOUAB Med Hassen V
11.30 – 11.45	**OC-19A**	JEBARI Meriam	**OC-19B**	HOSNI Khaled	**OC-19C**	MANNAI Faten	**OC-19D**	BEN ABEDRABAH Nour El Houda
11.45 – 12.00	**OC-20A**	JEMAA Imen	**OC-20B**	KAAROUD Khadija	**OC-20C**	MIDASSI Sondos	**OC-20D**	BENARIOUA Younes
12.00 – 12.15	**OC-21A**	KAMOUN Madiha	**OC-21B**	MAAMER Rihem	**OC-21C**	MNAFKI Rim	**OC-21D**	HABLI Oumayma
12.15 – 12.30	**OC-22A**	KETATA Nahed	**OC-22B**	MARZOUGUI Basma	**OC-22C**	JANGHER Abdulhakim	**OC-22D**	HAJRI Imen
13.00	***Lunch***							

Oral Communications - Session 5								
	Room A - Chair: *Younes Moussaoui* ***Organic Chemistry***		***Room B*** - Chair: *Dalila Hellali* ***Inorganic Chemistry***		***Room C*** - Chair: *M^{ed} Taieb Ben Dhia* ***Physical Chemistry***		***Room D*** – *Fethi Touati* ***Nanotechnology & Materials Sciences***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
15.00 – 15.15	**OC-23A**	BEN HASSEN Manel	**OC-23B**	MISSAOUI Kahla	**OC-23C**	RAHALI Emna	**OC-23D**	MISSAOUI Besma
15.15 – 15.30	**OC-24A**	LAHMADI Ghofrane	**OC-24B**	MSAADI Idia	**OC-24C**	SOUIDI Emna	**OC-24D**	NASRI Olfa
15.30 – 15.45	**OC-25A**	RAISSI Hanen	**OC-25B**	MSAOURA Selma	**OC-25C**	ZARROUG Rim	**OC-25D**	SAAD Sara
15.45 – 16.00	**OC-26A**	SALHI Sirine	**OC-26B**	OUESLATI-OMRANI Refka	**OC-26C**	ZOUAGHI Med Oussama	**OC-26D**	NYABA Luthando
16.00 – 16.45	**Coffee break + Poster Session 4 (P 121 - P 160) Alphabetical Order** **Evaluators:** Haykel Galaï, Cheima Fersi							
17.00 - 19.00	**General Assembly of the Tunisian Chemical Society**							
19.30	***Dinner***							
21.00	***Election of the new National Bureau of the*** **Tunisian Chemical Society**							

	Wednesday 21 December 2022							
09.00 – 09.35	**Plenary Lecture 5** **Fabrice ANIZON** - Introduced by *Hichem Ben Jannet* *Université Clermont Auvergne, CNRS, Clermont Auvergne INP, ICCF, Clermont-Ferrand, France* Targeting kinases for the development of novel cancer and pain therapies							
	Oral Communications - Session 6							
	Room A - Chair: *Taïcir Ben Ayed* ***Organic Chemistry***		***Room B -*** Chair: *Lilia Ktari* ***Inorganic Chemistry***		***Room C -*** Chair: *Mohamed Boujelbene* ***Renewable Energy & Fuels***		***Room D -*** Chair: *Rym Abidi* ***Medicinal & Bio Chemistry***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
09.45 – 10.00	**OC-27A**	SLIMI Hanen	**OC-27B**	OUNALLI Chayma	**OC-27C**	AKROUT Hiba	**OC-27D**	BACCARI Wiem
10.00 – 10.15	**OC-28A**	TOUJ Nedra	**OC-28B**	ZIADI Med Amin	**OC-28C**	BELAKEHAL Rania	**OC-28D**	BENISSA Zina
10.15 – 10.30	**OC-29A**	ZAYENE Mayssa	**OC-29B**	BEN SLIMEN Aya	**OC-29C**	BOUSSELMI Ghada	**OC-29D**	CHIHAOUI Marwa
10.30 – 10.45	**OC-30A**	FATTOUM Hanna	**OC-30B**	BOUHAJEB Oumayma	**OC-30C**	HALLEK Tahani	**OC-30D**	ELAKREMI Manel
10.45 – 11.15	**Poster Session 5 (P 161 - P 190) Alphabetical Order** **Evaluators:** Béchir Chaouchi, Mohamed Ben Messaouda							
	Oral Communications - Session 7							
	Room A - Chair: *Mohamed Béji* ***Medicinal & Bio Chemistry***		***Room B -*** Chair: *Borhane Mahjoub* ***Water, Marine & Air Pollution***		***Room C -*** Chair: *Wided Kamoun* ***Renewable Energy & Fuels***		***Room D -*** Chair: *Habib Boughzala* ***Inorganic Chemistry***	
	Com.	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*	*Com.*	*Communicating*
11.15 – 11.30	**OC-31A**	KHEMIS Eya	**OC-31B**	BOUJELBANE Faten	**OC-31C**	SALHI Mansoura	**OC-31D**	BAROUNI Samira
11.30 – 11.45	**OC-32A**	MEHREZ Syrine	**OC-32B**	KHALED Fatma	**OC-32C**	SOLTANI Ilham	**OC-32D**	CHAHLA Sondes
11.45 – 12.00	**OC-33A**	MSEHLI Asma	**OC-33B**	OULED LTAIEF Olfa			**OC-33D**	JANDOUBI Alma
12.00 – 12.15			**OC-34B**	TALEB Fayrouz			**OC-34D**	ZOUAGHI Aymen
12.15 – 12.50	**Plenary Lecture 6** **Michel BALTAS** - Introduced by *Houcine Ammar* *Laboratoire de Chimie de Coordination du CNRS, Toulouse, France* Mechanochemistry as an alternative energy input: From fundamentals to medicinal chemistry							
12.50	**Closing Remarks and Poster Awards**							
13.00	***Lunch, Check Out and Departure***							



Speakers' Abstracts

Lynne A. PILCHER

Lynne Pilcher is an associate professor at the University of Pretoria. She graduated with a BSc degree in Chemistry and Biochemistry from Rhodes University, South Africa. After completing her BSc honours degree in Chemistry, she obtained an MSc degree at Rhodes University in marine natural products chemistry under the supervision of Mike Davies-Coleman. This was followed by a PhD in synthetic organic chemistry at Cambridge, UK under the supervision of Ian Paterson. She gained post-doctoral research experience in enzyme reaction mechanisms with David Cane at Brown University, USA before taking up an academic position at the University of Pretoria in 2003. She has led research projects in organic synthesis contributing to multidisciplinary projects in TB and Malaria, but her passion for research-informed quality teaching has shifted her research focus to that of tertiary chemistry education.

Systems thinking in tertiary chemistry for sustainable development

Lynne A. Pilcher

Department of Chemistry, University of Pretoria, South Africa

Recently there have been several calls to introduce systems thinking in chemistry education. Systems thinking has been identified as a key competence for sustainability[1] and meeting many of the sustainable development goals require an understanding of chemicals, their transformations and their interactions within the earth system.[2] Chemistry is a complex subject and has been made accessible to students through a reductionist approach to teaching. By incorporating systems thinking we can help students to see the bigger picture and consider the long-term implications of chemicals and how to redesign for a more sustainable future. We have developed and implemented two interventions at the first-year undergraduate level: one was designed for science students using the topic of surfactants and the other for engineering students using the stoichiometry of the synthesis of aspirin. Our designs were guided by the ChEMIST table that sought to characterize systems thinking in chemistry education.[3] We demonstrate how the systems thinking approach in both interventions did not lose the focus of the chemistry content that needed to be covered, exposed students to the concept of systems thinking, started to develop some systems thinking skills, and made a case for the contribution that chemistry can and should make to meet the UN sustainable development goals.

Key words: chemistry education, sustainability, curriculum, collaborative learning

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References

[1] Wiek A, Withycombe L, Redman CL. Key competencies in sustainability: a reference framework. Sustain Sci. 2011, 6, 203–218.

[2] Mahaffy PG, Matlin SA, Holme TA, MacKellar J. Systems thinking for education about the molecular basis of sustainability. Nature Sustainability. 2019, 2, 362–370.

[3] York S, Orgill M. ChEMIST table: A tool for designing or modifying instruction for a systems thinking approach in chemistry education. J. Chem. Educ. 2020, 97, 2114−2129.

Mahmood JAVEED

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PROFESSIONAL CAREER

RESEARCH INTEREST:

Exploring stable organic frameworks and their hybrids to address the global challenges in energy and environment.

EMPLOYMENT:

Senior Research Scientist
Advanced Membrane & Porous Materials Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia
July 26, 2021, to present

CTO at RuC2N Company
UNIST,104-709 50 UNIST, Ulsan 44919, Republic of Korea
September 2018 to July 2020

Research Assistant Professor
School of Energy & Chemical Engineering, Ulsan National Institute of Science and Technology, Ulsan Republic of Korea,
September 01, 2017, July 20, 2021

Post-Doctoral Research Fellow
With Prof. Jong-Beom Baek at Ulsan National Institute of Science and Technology, Ulsan Republic of Korea,
September 01, 2015, to August 31, 2017

EDUCATION

Ph.D. (2011-2015) in Energy and Chemical Engineering
Ulsan National Institute of Science and Technology
School of Energy and Chemical Engineering
Dissertation title: “Synthesis of Multifunctional Two-Dimensional Structures and Their Applications”
Advisor: Prof. Jong-Beom Baek

M.Sc.(2004-2007) in Chemistry (Specialization in Organic Chemistry)
University of Peshawar (Pakistan), Institute of Chemical Sciences.
Thesis: “Synthesis of N,N’-Disubstituted Acetamidines”
Advisor: Prof. Muhammad Arfan

B.Sc (2002-2004) in Chemistry
University of Malakand, Pakistan

RESEARCH FUNDING AS A PRINCIPAL INVESTIGATOR

NRF Project as a single PI (March 2019)
(Young Researcher program $500K)
National Research Foundation (NRF), Republic of Korea

Electronic properties of nitrogenated two-dimensional structures

Javeed Mahmood[a,b], Cafer T. Yavuz[a,b]

a) Oxide & Organic Nanomaterials for Energy & Environment (ONE) Lab, Physical Sciences and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955, Saudi Arabia
b) Advanced Membranes and Porous Materials Center (AMPMC), Physical Sciences and Engineering (PSE),King Abdullah University of Science and Technology (KAUST), Thuwal 23955, Saudi Arabia

Since the advent of graphene, the development of crystalline two-dimensional (2D) organic materials with semiconducting features have been extensively explored for their potential optoelectronic applications. Despite extensive progress in this field, it is still challenging to realize laterally extended organic materials with high electrical transport properties. To overcome these problems, two-dimensional network structures with uniformly distributed nitrogen atoms were synthesized.[1-5] The structures of network polymer were confirmed by scanning tunneling microscopy (STM) and powder X-ray diffraction (PXRD) pattern. These materials were used as active layers in a field-effect transistor (FET) study to check the semiconducting properties of the structures. The FET study using two-dimensional polymers thin flakes as the active layer in the bottom-gate top contact configuration revealed ambipolar charge transport and extraordinary high electron and hole mobilities surpassing most pristine organic materials without doping. These studies manifest a systematic approach to the design and synthesis of organic structures for electronic applications

Key words: Two-dimensional polymers, Semiconducting, FET, C_2N, C_3N, C_5N

References

[1] J. Mahmood, et al., Nature Communications, 2015, 6, 6486.
[2] J. Mahmood, et al., Proceedings of National Academy of Sciences, USA, 2016, 113, 7414-7419.
[3] J. Mahmood, et al., Advanced Materials, 2021, 33, 2004707
[4] J. Mahmood, et al., Communication Chemistry, 2020, 3, 31.
[5] H.-J. Noh, et al., CHEM, 2022, https://doi.org/10.1016/j.chempr.2022.08.001

Jalel LABIDI

Jalel Labidi has Chemical Engineering degrees from ENIG and PhD in Chemical Engineering from INPL-Nancy. He has developed his research career in several centers: Ecole Polytechnique de Montreal (Canada), CNRS (France), University of Girona and the University of the Basque Country. He has formed in 2012 the research group 'Biorefinery Processes' (BioRP). His research focuses on the development, optimization and integration of biorefinery processes, conversion of biomass components into building blocks, polymers and composite materials. He has been involved in numerous national and international projects.

He has published more than 300 articles in international journals, 4 patents and 25 book chapters (H-index: 58). He has supervised 26 PhD thesis. He is associate editor of 2 international journals: Industrial Crops and Product (Elsevier) and Frontiers in Energy Research: Bioenergy and Biofuel (Frontiers) and member of the editorial board of several journals.

Chitin and Chitosan Based Materials

Rut Fernandez, Asier Salaberria, Jalel Labidi

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Chitin is the earth's second most abundant carbohydrate polymer after cellulose. Despite being one of the most widespread natural polysaccharide, chitin was for a long time considered as an intractable polymer due of its lack of solubility in common solvents, which limits its processing and practical use. Due to the mentioned limitations, chitin is usually converted to chitosan by deacetylation. Chitosan is well-known biopolymer with extensive application in various fields' such material science, food, health, and agriculture.

However, recent studies have focused on chitin nanoparticles and their applications in different fields.

In nature, chitin occurs as micro/nanofibrils that form a composite together with proteins, pigments and calcium carbonate and has a structural role in the exoskeleton of crustaceans and insects. The unique properties of chitin nanoparticles – such as their renewable and biodegradable character, extremely small size, low density, chemical stability, biological activity, and non-cytotoxicity – make them excellent candidates for use in extensive range of medical applications, nanocomposite fields, water treatment, cosmetics, electronics devices, etc..

The diversity of properties of chitin nanoparticles (size, shape, crystallinity, aspect ratio and morphology) depend on the chitin source; and the isolation process of the nanoparticles.

The present work will give an overview of the research carried out by our research group related to chitin and chitosan.

Key words: Chitin, Chitosan, extraction, nanoparticles

Philiswa N. NOMNGONGO

Prof Philiswa N. Nomngongo is a full Professor of Environmental Analytical Chemistry at the University of Johannesburg, Faculty of Science (Department of Chemical Sciences). She holds a DSI-NRF SARChI in Nanotechnology for Water and NRF Y1 rating. Her scientific career has been dedicated in solving different environmental problems in the field of water quality and environmental protection. Prof Nomngongo is author/co-author of more than 130 peer-reviewed publications and has presented 50+ keynote and invited contributions at scientific conferences. Her research achievements have been recognized through prestigious fellowships and awards such as 2014 L'Oreal-UNESCO Sub-Saharan Women in Science Regional fellowship; 2017 South African Women in Science award in the Distinguished Young Woman Research in the Natural and Engineering Sciences category; 2017 Vice-Chancellor's Distinguished Award: Most Promising Young Researcher of the Year and 2020/2021 NSTF-South23 Award winner (Category: Emerging Researcher & Engineering Research Capacity Development. She has supervised/ co-supervised 35 MSc and 15 PhD students. She is currently, supervising several postgraduate students.

Nanotechnology and Environmental Analytical Chemistry: Current Status and Future Perspectives

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The global increase in the quality of life accompanied by demand for emerging pollutants such as pharmaceutical and personal care products, has introduced a new threat to an already scarce natural resource for humans, which is water. These also drew considerable attention over the last decades due to the number of emerging pollutants have detected in aqueous environment compartments. Environmental analytical chemistry has changed significantly in past decades. This is due to the rapid developments in technologies as well as emergence of various pollutants. Because of this, environmental analytical chemistry field has benefitted from the emergence of nanotechnology. Nanotechnological-based analytical processes such as nanoparticles (NPs) and nanostructured materials as well as nanotools have continuously attracted more attention of analytical chemists. To be more explicit, nanomaterials play a big role in the process of sample preparation method development for various applications, ranging from food and environmental analysis. This study covers the application of porous nanomaterials in various sample preparation for analysis of various selected of emerging contaminants (fluoroquinolone antibiotics, sulfonamides, tetracyclines parabens, anticonvulsants and β-blockers) in water systems.

Key words: Nanotechnology, Sample preparation, Emerging contaminants, Water bodies

Fabrice ANIZON

Fabrice Anizon obtained a Master in Chemistry in 1996 from Blaise Pascal University (Clermont-Ferrand, France), after carrying out research in the groups of Professors Georges Jeminet (Clermont-Ferrand) and Daniel T. Glatzhofer (Oklahoma University, United States).

In 1999, he received his PhD in organic and biological chemistry at Blaise Pascal University, under the supervision of Prof. Michelle Prudhomme, working on the synthesis of rebeccamycin derivatives as topoisomerase I or protein kinase inhibitors. He joined the group of Prof. Philip J. Kocienski at the Universities of Glasgow (Scotland) and Leeds (England) as a post-doctoral fellow. After being shortly appointed Lecturer at the University of Leeds, he moved to Blaise Pascal University in September 2001. He was appointed Professor in 2008, in the same University. Now Professor at Clermont Auvergne University, his research interests focus on the design synthesis of biologically active hetero-aromatic compounds.

Targeting kinases for the development of novel cancer and pain therapies

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The research projects developed in our group, at the Institute of Chemistry of Clermont-Ferrand, focus on the design and synthesis of original nitrogen hetero-aromatic scaffolds with biological potencies. Biological targets of synthesized molecules are mainly protein kinases involved in pathologies such as cancer or pain.

Two topics will be addressed during this presentation. First, the discovery of pyrazole derivatives with inhibitory potency toward Pim kinases. Among them, pyrazolo[4,3-*a*] phenanthridines (Figure 1) are of high interest for the development of acute myeloid leukemia drug candidates [1]. Second, we designed 3,5-disubtituted pyridin-2(1*H*)-one derivatives (Figure 1) that exhibit promising analgesic activity in rat models of mechanical allodynia, a frequent pain symptom of chronic pain [2]. The syntheses as well as biological activities will be presented.

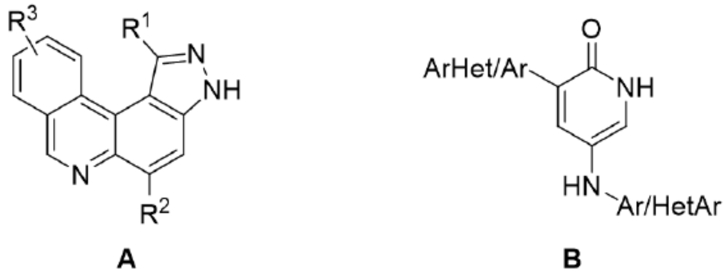

Figure 1. Structures of pyrazolo[4,3-a]phenanthridines (**A**) and pyridin-2(1H)-one derivatives (**B**).

Keywords: Nitrogen hetero-aromatic compounds, cancer, pain

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Michel BALTAS

Born in Athens-Greece; High School studies in Athens. University studies and career in France

Diplomas at University Paul Sabatier Toulouse

Doctorat d'État (1984-1987); Grant and work with the pharmaceutical industry : « Roussel Uclaf » and the Scientific Institute Roussel.

Doctorat 3ème cycle (1981-1984) ; and Associate Professor (teaching at the Licence).

DEA (Diplôme d'Etudes Approfondies) in Molecular Chemistry, section Organic Chemistry (1981, Major)

Maîtrise on Physical Chemistry (1980, Major)

Academic Foreign Mobility

Invited Scientist: Department of Chemistry, McGill Univesrity, Montreal, Canada (Pr. T. FRISCIC) «Organic Mechanochemsirty: synthesis of a-enones and oxidation/epoxidation studies» 19/09/2018-7/11/2018.

Visiting Scientist at:

Polytechnical School ETH Zürich (Pr Andrea VASELLA) «Synthesis of fused pyrrolo and triazolo sugars, potential inhibitors of glycosidases» 3/01/96-27/02/97.

UK/French ALLIANCE programme (1990-1992) : 2 x 3 months with Prof. K.T. DOUGLAS at University of Manchester (U.K.) «Three-dimensionnal reconstitution of the CAD2 enzyme's active site through molecular modelling».

CNRS career: 10/1986; Director of Research at CNRS 10/2004-

1986-2020: Laboratoire de Synthèse et Physicochimie de Molécules d'Intérêt Biologique LSPCMIB, UMR 5068, Toulouse

2020- : Laboratoire de Chimie de Coordination CNRS-UPR 8241, Toulouse **;** team V "New antimalaria compounds and pharmacological approaches" Inserm ERL 1289

Responsabilities

03/1998-09/2020 : Head of the team PNASM «Produits Naturels et Analogues : Synthèses et Mécanismes» at the LSPCMIB

01/2007-01/2016 Director of the Laboratory : LSPCMIB UMR 5068

02/2016-12/2020 Director of the Commitee Sciences de la Matière (14 laboratories on Chemistry, Materials Science, Physics and Theoritical Chemistry)

Founding member of:

The PICT platform: Plateforme Intégrée de Criblage de Toulouse https://www.chembioscreen.fr/en/facility/293/plateforme-integree-de-criblage-de toulouse.html

The GALA platform « Galénique Avancée » https://www.imt-mines-albi.fr/fr/plateforme-gala

The «Groupement d'Intérêt Scientifique » GIS-CNRS Chimiothèque Nationale ;
https://cat.opidor.fr/index.php/Chimioth%C3%A8que_Nationale

Two Laboratoires Internationales Associés (LIA): UPS/CNRS with Morocco, Ukraine)

PhD's Direction/co-Direction

22 Theses since 1987. The future of some PhD students : 2 integrated CNRS; 5 Associate Professors/Professors ; 8 in the Pharmaceutical, Fine chemicals, Analytical Industry in France, USA, Canada, China, Switzerland…

Production

Peer review Publications > 140; Conférences and congresses invited > 65; Poster communications > 150

Valorisation

Three patents; one of them initiated the creation of the start-up Syntivia (2010): 2 compounds in the market since 2014

Participation to European Programmes

Integrated European: NM4TB (New Medicines for Tuberculosis) FP6-LIFESCIHEALTH, (2006-2011). COST programmes: CM1307 (2013-2018) Chemotherapy towards diseases caused by endoparasites. CM1407(2014-2019) Challenging organic syntheses inspired by nature. From natural products chemistry to drug discovery.

Research Interests and activities

Design, syntheses, physico chemical and biological studies of natural and bioinspired compounds.

Design, syntheses enzymatic studies and biological evaluation of heterocyclic compounds.

Mechanochemistry: use of non conventional activation methods for elaborating biologically active acompounds. From fundamental studies to medicinal chemistry.

All research conducted are related to important diseases and to societal health problems; two related to mostly developed countries diseases (cardiovascular, cancer) and two to worldwide diseases affecting principally less developed countries (tuberculosis, malaria).

Mechanochemistry as an alternative energy input: from fundamentals to medicinal chemistry

Michel Baltas

Laboratoire de Chimie de Coordination du CNRS - UPR8241
Inserm ERL 1289 Equipe "Nouvelles molécules antipaludiques et approches pharmacologiques"
205 route de Narbonne - BP 44099 - 31077 Toulouse Cedex

One of the main goals in the area of organic synthesis is the research and development of efficient environmentally safe methods. In fact, since the 2000s many regulations for the chemical and pharmaceutical industries have appeared, especially in terms of efficiency, waste management and energy input. All these issues are now addressed and termed «Green Chemistry». In that respect, mechanochemistry, a domain that is developed actively the two last decades, treats on the influence of mechanical energy on chemical transformations. Many efforts were developed worldwide towards understanding of mechanochemical processes mechanochemical and on synthetic approaches for creating a variety of compounds. After a short introduction on the mechanochemistry now-days, I will focus on two topics: 1) fundamental mechanistic studies concerning the a) coupling between a 1,2-diamine system and a 1,2-dione one leading to phenazine or quinoxaline; b) Diels-Alder reaction. 2) Medicinal mechanochemistry: elaboration of nitrogen contained scaffolds and biological activities.

Key words: cycloadditions, mechanisms, hydrazones, 1,2,4-triazoles, biological activities.

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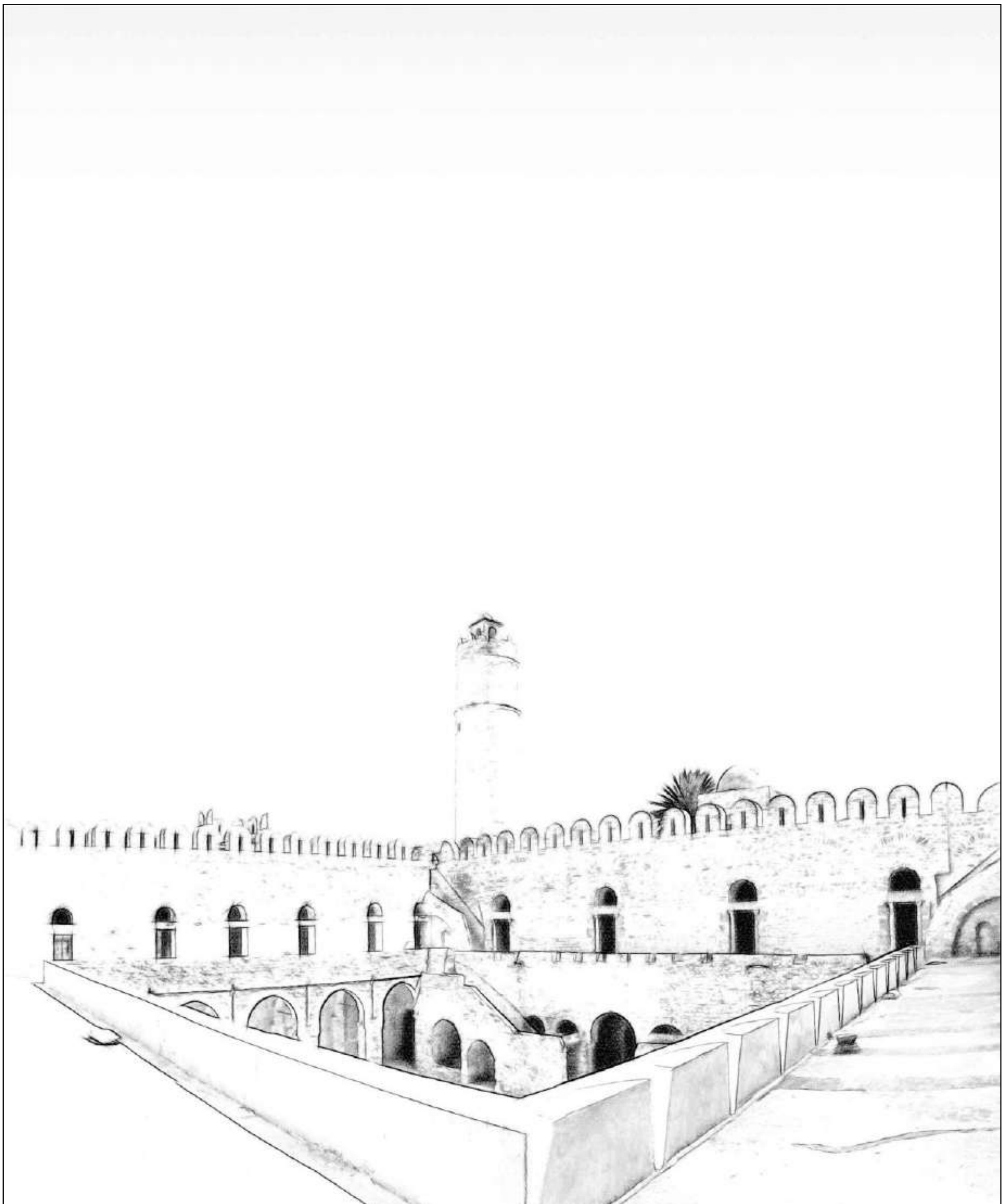

List of Oral Communications

Communicatings' Names	**Ref**
H. Abid, A. Mechria *FSG - Gabès* New copper(II) complexes supported by azomethine ligands: synthesis and characterization	**OC 01A**
S. Agren, J. El Haskouri, M.H.V Baouab *IPEIM - Monastir* Synthesis and study of structural and optical properties of fluorescent Boranils from their corresponding anils	**OC 03B**
T. Aissa, R. Ksiksi, D. Aissaoui, N. Srairi-Abid, M.F. Zid *FST - Tunis* Synthesis, physico-chemical characterizations, and antiproliferative activity on U87 human brain cancer cells, of a new vanadium complex (V), tetra-[methylimidazolium] dihydrogen decavanadate	**OC 01B**
Y. Aissaoui, M. Trabelsi-Ayadi, I. Ghorbel-Abid *FSB - Bizerte* Adsorption of Erythromycin from aqueous solution using Tunisian clay materials. Effect of operating parameters	**OC 08C**
H. Ajari, F. Khaled, H. Akrout, B. Chaouachi, A. Figoli *ENIG - Gabès* Effect of pore formers on the morphology and the proprieties of recycled low density polyethylene flat sheet hydrophobic membranes	**OC 09C**
H. Akrout, R. Benrejeb, B. Chaouachi *ENIG - Gabès* Design, modeling and simulation of a multi-concentrator solar water heater	**OC 27C**
I. Alkiskas *Misurata University, Misrata, Libya* Synthesis and characterization of novel thermotropic liquid crystalline poly(ether-ketone)s based on cyclopentanone moiety	**OC 07D**
O. Amdouni, R. Jimenez, I. Sobrados, J. Sanz, R. Ternane *FSB - Bizerte* Influence of rare earth elements incorporation on the structural and the ionic properties of NASICON type materials	**OC 02B**
A. Amraoui, S. Gamoudi, M.J. Periago, N. Baenas, E. Srasra *CNRSM - Borj Cédria* Interaction natural pigments-clay by solid-state reaction	**OC 10C**
W. Arar, R. Ben Ali, M.V. El May, A. Khatyr, I. Jourdain, M. Knorr, L. Brieger, R. Scheel, C. Strohmann, A. Chaker, A. Ben Akacha *FST - Tunis* Synthesis, crystal structures and biological activities of halogeno-(O-alkylphenylcarbamothioate)bis(triarylphosphine) copper(I) complexes	**OC 02A**

Communicatings' Names	**Ref**
O. Arfaoui, H. Sbihi *FSB - Bizerte* Chemical and fatty acid composition of crude and purified extracts obtained from Datura innoxia seeds extracted with different solvents	**OC 11C**
A. Ayachi, S. Samet, A. Ben Ammar, B. Bouzayani, M. Treilhou, M. Trigui, M. Siala, N. Tene, R. Mezghani-Jarraya *FSS - Sfax* Antioxidant and antimicrobial activities of Anthyllis henoniana stems extracts and direct identification of phenolic compounds from its ethyl acetate and methanol extracts	**OC 03A**
N. Ayadi, J. Deschamp, T. Ben Ayed, M. Lecouvey *Université Sorbonne Paris Nord, France* The emerge of a new bifunctional peptidic organocatalysts for the stereoselective Michael addition of aldehydes onto nitroalkenes	**OC 04A**
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S. Baccara, I. Sobrados, J. Sanz, R. Ternane *FSB - Bizerte* Structural and electrical properties of new Al-Gd doped lithium-phosphate NASICON type material	**OC 04B**
W. Baccari, I. Saidi, M. Znati, P. Waffo-Teguo, H. Ben Jannet *FSM - Monastir* Synthesis and molecular docking study of new sesquiterpene coumarin arylidene conjugates from the natural coladonin	**OC 27D**
N. Ballagha, M. Jmaï, M.L. Efrit, H. M'Rabet *FST - Tunis* A simple and efficient protocol for accessing to functionnalized pyrrolidine	**OC 05A**
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S. Barouni, B. Belgacem, R. Ben Hassen *FST - Tunis* Structural studies and electrical and optical properties of $LaSrSnInRuO_9$ simple perovskite prepared by the mechano synthesis route	**OC 31D**
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M. Ben Hassen, D. Msalbi, M.S. Ifa, F. Chabchoub *FSS - Sfax* Synthesis and antiproliferative breast cancer of new [1,2,4]triazolo[4,3-a]pyrimidines	**OC 23A**
O. Ben Jaballah, S. Azzouni, M.L. Efrit *FST - Tunis* New 1,2,4-triazoles derivatives from some N-functonnalized imidates	**OC 06A**
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C. Ben Maamer, P.C. Mpawenayo, B. Lecachey, N. Alouane, P. Mangeney, J. Marrot, A. Van Der Lee, S. Bouaouli, M. Guillaumont, R. Besbes, H. Gerard, E. Vrancken, J.M. Campagne *FST - Tunis* Dynamic kinetic resolution processes based on the switchable configurational instability of allenyl copper reagents	**OC 08A**
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A. Ben Slimen, H. Najjar, A. Megriche *FST - Tunis* Combustion synthesis of nanosized Ag-doped Co_3O_4 as organic dyes degradation catalysts	**OC 29B**

Communicatings' Names	Ref
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Y. Ben Smida, A. Boukhachem, D. C. Onwudiwe, A.H. Hamzaoui *CNRSM - Borj Cédria* Ab initio study of the ground state, electronic structure, and optical properties of α-Ba_2SnS_4	**OC 07B**
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G. Bousselmi, N. Khemiri, M. Kanzari *ENIT - Tunis* Synthesis of n-type Ag_2ZnSnS_4 thin films by thermally evaporated process for solar cell applications	**OC 29C**

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C. Bouyahya, N.D. Bikiaris, A. Zamboulis, A. Kyritsis, M. Majdoub, D.N. Bikiaris, P.A. Klonos *FSM - Monastir* Semicrystalline copolymers based on polycaprolactone and polyisosorbide: Synthesis, characterization, and degradation	**OC 01D**
R. Bouzaiene, S. Boughammoura *FSM - Monastir* Study of the effect of solvation on the formation and the mobility of TTAB micelles	**OC 08D**
N.E.H. Brirmi, R. Mercier, N. Jaffrezic-Renault, S. Chatti, H. Ben Romdhane *FST - Tunis* New polymeric adsorbents for benzene derivatives removal in wastewater	**OC 02D**
M. Bsaihia, N. Allouche, H. Ben Salah *FSS - Sfax* First natural isolation of a xanthenone from a local plant "Tricholaena teneriffae" cultivated in Tunisia	**OC 11A**
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S. Chamam, M. Salem, S. Azouz, A. Hannachi *ENIG - Gabès* Evaporation of desalination brines: Simulation vs. experimental	**OC 08B**
M. Chellegui, B. Champagne, V. Liégeois, M. Trabelsi *FSS - Sfax* Molecular modeling of reactivity in organic chemistry: A DFT study of the Diels-Alder reactions between 2,5-dimethylfuran and ethylene, thermodynamic and kinetics analysis	**OC 09D**
M. Chihaoui, H. Lazreg, A. Cheikh Mhamed, L. Chahed, I. Messaoudi, F. Chaubet, M. Ben Mansour, R.M. Maaroufi *ISBM - Monastir* Extraction, physicochemical characterization and biological activities of chondroitin sulfate	**OC 29D**
M. Elakremi, L. Sillero, J. Labidi, R. Ben Salem, Y. Moussaoui *FSG - Gafsa* UPLC-ESI-MS/MS polyphenolic profile and antioxidant activities of Pistachio female leaves extracts obtained by microwave assisted extraction	**OC 30D**

Communicatings' Names	**Ref**
H. Elhleli, F. Mannai, R. Khiari, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* Microencapsulation using polysaccharides extracted from Opuntia Ficus Indica	**OC 09B**
N. Etteyeb, N. Mouguech, P. Taillandier, J. Bouajila, M. Romdhane *ISBAM - Medenine* Kinetics of palm by-product fermentation using Kombucha starter culture	**OC 15C**
A. Faidi, N. Allouche *FSS - Sfax* Chemical and biological studies of a local medicinal plant	**OC 12A**
A. Fandouli, A. Houas, A. Rayes *FSG - Gabès* Synthesis, crystal structure, Hirshfeld surface analysis of a new hybrid compound bis(benzylammonium)tetrachlorocadmate(II)	**OC 10B**
H. Fattoum, A. Cherif, M. Abderrabba, M. Ben Massouda *FSG - Gafsa* Antioxidant properties of phenolic compounds extracted from olive mill wastewater using 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) ABTS •+	**OC 30A**
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A. Gannouni, R. Kefi *Université de Carthage* X-Ray diffraction, IR spectrum, optical properties, AIM, NBO, RDG, HS, Fukui function and biological analysis of a novel hybrid compound $(C_9H_{15}N_3)[CuCl_4(H_2O)]$	**OC 12B**
R. Gara, M.O. Zouaghi, Y. Arfaoui *FST - Tunis* Theoretical evaluation of the performance of photovoltaic cells based on crown ether porphyrins and phthalocyanines: Determination of optoelectronic properties	**OC 11D**
F. Garci, H. Chebbi, N. Rouzbeh, L. Rochels, S. Disch, A. Klein, M.F. Zid *FST - Tunis* Structure, optical and magnetic properties of the pyridinium cobaltate $(C_6H_9N_2)_2[CoCl_4]$	**OC 13B**
A. Ghabi, S. Souissi, T. Boubaker *FSM - Monastir* Nucleophilic reactivities of pyrazoles in 50% DMSO-50% MeOH and correlation nucleophilicity versus basicity	**OC 13A**

Communicatings' Names	**Ref**
C. Gharbi, C. Ben Nasr, L. Khedhiri *FSB - Bizerte* Efficient synthesis, crystal assembly, vibrational properties, theoretical calculations, molecular docking and Pharmacokinetic profiling of a novel 2D layered hybrid compound $(C_6H_{10}N_3O)_2Cu_2Cl_6$	**OC 14B**
A. Ghazouani, J. Mhalla *FSM - Monastir* Influence of dielectric friction on the dependency of the mobility of carboxymethylated cellulosic chains with the nature of their counterions	**OC 12D**
M. Ghiloufi, B. Trifi, S. Sahbani, O. Ghodbane, F. Touati, S. Kouass *INRAP - Sidi Thabet* $g\text{-}C_3N_4/CuO/TiO_2$ composite nanomaterial with performances of photocatalytic degradation of Levofloxacin and electrochemical properties	**OC 16B**
N. Grati, H. Galai, A. Alatrache *INRAP - Sidi Thabet* Influence of short uptake moisture on drug-excipient binary mixture: DSC and FTIR contribution	**OC 14A**
R. Guedouar, M. Abidi, M. Mhiri Kamoun, W. Tahri, S. Besbes Hentati *INSAT - Tunis* Relationship between electrochemical oxidation of 3-(4-fluorophenyl)-2-methyl-[1,2A] benzimidazolo-1,3,5-triazin-4-thione and its antimicrobial activity	**OC 03C**
R. Guesmi, M.R. Ben Romdhane, N. Benbettaieb, A. Assifaoui, T. Barhoumi-Slimi *FST - Tunis* Development and characterization of new packaging film based on vegetable and active essential oil and organoclay	**OC 16C**
H. Haba, M.I. Badaoui, A.A. Magid, L. Voutquenne-Nazabadioko, M. Benkhaled *University of Batna 1, Algeria* Alkaloids and polyphenols with antioxidant and anticholinesterase activities from Atractylis cancellata	**OC 15A**
O. Habli, J. Zaghdoudi, M. Kanzari *FST - Tunis* Study of the nonlinearity effect on the optical properties of a one-dimensional photonic crystal	**OC 21D**
B. Hajji, M. Chemingui *FSS - Sfax* Effect of two-step ageing treatment on microstructure and mechanical properties of a commercial Al–Zn–Mg–Cu alloy	**OC 15B**
O. Hajlaoui, H. Essaddam, L. Bergaoui *INSAT - Tunis* Effect of the polyaniline solvent on the properties of cellulose–PAni composites	**OC 04D**

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A. Hajri, D. Alimi, M. Jridi, H. Sebai *ISBB - Béja* Synthesis, biological activities and molecular docking studies of [1,2,4]triazolo[4,3-b][1,2,4,6]thiatriazine-1,1-dioxides	**OC 17A**
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T. Hallek, M. Montacer *FSG - Gabès* Occurrences and origin of oil seeps and new marks of petroleum impregnations in Northwestern Tunisia: Implications from aliphatic biomarkers and statistical modelling	**OC 30C**
F. Harzi, O. Zouaghi, N. Fakhar Bourguiba *FST - Tunis* Crystal structure, spectroscopy, DFT calculations, thermal analysis, Hirshfeld surface and magnetic properties of a new organic-inorganic hybrid material $(C_{12}H_{16}N_2O)[CoCl_4]$	**OC 17B**
M. Hasyeoui, A. Samarat, F. Mongin *FSB - Bizerte* Oxazolo[5,4-f]quinoxaline-type selective inhibitors of glycogen synthase kinase-3α (GSK-3α): Development and impact on temozolomide treatment of glioblastoma cells	**OC 18A**
R. Hayder, M.L. Efrit, N. Besbes, M. Kamoun *CNRSM - Borj Cédria* Contribution of the green synthesis of cetals and dioxolanes	**OC 17C**
S. Hermi, C. Ben Nasr, M.H. Mrad *FSB - Bizerte* Synthesis, crystal structure, vibrational spectroscopy, optical study and thermal analysis of a new complex based on 2,6-Dimethanolpyridine: $[(C_7H_{10}NO_2)CdCl_3]n$	**OC 18B**
K. Hosni, K. Mahmoudi, E. Srasra *CNRSM - Borj Cédria* Mechano-synthesis, characterization, and adsorptive properties of Mg-Al-LDH and Zn-Al-LDH for olive mill wastewater treatment	**OC 19B**
A. Jandoubi, M. Krimi, R. Ben Hassen *FST - Tunis* Natural cellulosic fiber from alfa (Stipa Tenacissima): Extraction and characterization	**OC 33D**
A. Jangher, S. M. Aghila, B. M. Mahara *UNIVERISTY OF TRIPOLI, Libya* Investigation the adsorption of Congo red dye on natural and acid activated Libyan bentonite from aqueous solutions	**OC 22C**
M. Jebari, K. Pasturaud, B. Picard, J. Maddaluno, F. Rezgui, I. Chataigner, J. Legros *FST - Tunis* "On water" reaction of deactivated anilines with 4-methoxy-3-buten-2-one, an effective butynone surrogate	**OC 19A**

Communicatings' Names	Ref
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N. Jemili, W. Essafi *FST - Tunis* Complexation of polyelectrolytes in aqueous solution. Application to wastewater treatment	**OC 13D**
K. Kaaroud, P. Smet, B. Badroui *FSM - Monastir* Synthesis, crystal structures and thermal properties of rare earth silicate oxyapatite	**OC 20B**
M. Kamoun, A. Hafiane, N. Besbes, M.L. Efrit *CNRSM - Borj Cédria* Ultrasound design and biological activities of new generation of [1,2-a] benzimid azolyl-1,3,5-triazines	**OC 21A**
N. Ketata, D. Atoui, R. Ben Romdhane, Y. Moussaoui, R. Ben Salem *FSS - Sfax* One-step access to new polycyclic aromatic hydrocarbons via C-H bond functionalization catalyzed by palladium	**OC 22A**
R. Khairi, S. Zaidi, A. Bougarech, M. Abid, A.J.D. Silvestre, A.F. Sousa, S. Abid *FSS - Sfax* Development of bio-based, chemical resistant, and semi-crystalline polyesteramides derived from FDCA and 5,5′-isopropylidene bis(2-furfurylamine)	**OC 05D**
F. Khaled, H. Ajari, H. Akrout, K. Hidouri, B. Chaouachi *ENIG - Gabès* A study of recycled low-density polyethylene membrane performance in vacuum membrane distillation unit powered by solar energy	**OC 32B**
E. Khemis, M. Ben Mustapha, I. Chaieb, R. Ascrizzi, G. Flamini, H. Ben Jannet, A. Zardi-Bergaoui *FSM - Monastir* Chemical investigation and insecticidal effect of Thapsia garganica L. essential oil against Tribolium castaneum	**OC 31A**
H. Khlifi, A. Houas, L. Elsellami, F. Parrino *FSG - Gabès* Novel approach for selective photocatalytic degradations using 4-Carboxyphenylboronic acid functionalized TiO_2	**OC 18C**
A. Labidi, M.C. Ben Rayana, L. Latrous El Atrache *LNCM - Tunis* Development of a RP-HPLC method for the quantification of GZP and ELB in human plasma: Application in a pharmacokinetic study	**OC 04C**

Communicatings' Names	**Ref**
<u>G. Lahmadi</u>, A. Romdhane, A.M. Lawson, A. Daich, H. Ben Jannet, M. Othman *FSM - Monastir* Design and semi-synthesis of novel oleanolic acid and isoindole 1,2,3-triazole conjugates	**OC 24A**
<u>R. Maamer</u>, G. Mikaelian, P. Benigni, D. Hellali *FST - Tunis* Heat capacities of AgCs $(NO_3)_2$ and $Ag_3Cs(NO_3)_4$	**OC 21B**
<u>F. Mannai</u>, M.N. Belgacem, Y. Moussaoui *FSG - Gafsa* Physicochemical, rheological and surface tension properties of polysaccharides extracted from Opuntia ficus-indica (Cactaceae)	**OC 19C**
<u>B. Marzougui</u>, Y. Ben Smida, M. Ferhi, K. Horchani-Naifer, A.H. Hamzaoui *CNRSM - Borj Cédria* Experimental and theoretical study of the luminescent properties of Pr doped $LaAsO_4$ nanoparticles	**OC 22B**
<u>S. Meddeb-Limem</u>, A. Ben Fredj *IPEIB - Bizerte* Glyphosate dimers: Structure, stability and solvation effects	**OC 14D**
<u>S. Mehrez</u>, S. Absi, A. Hamdi, Y. Kacem, J. Kraiem *FSM - Monastir* Synthesis of new chiral amino acid derivatives and study of their anti-inflammatory activity	**OC 32A**
<u>B. Messaoudi</u> *Higher School in Applied Sciences, Tlemcen, Algeria* A theoretical investigation of the rate constant of trichloroethylene reaction with $O(^3P)$ over the range of temperature 285-1035	**OC 16D**
<u>S. Midassi</u>, A. Bedoui, N. Ben Salah *FSG - Gabès* Efficient degradation of chloroquine drug by electro-Fenton oxidation: Effects of operating conditions and degradation mechanism	**OC 20C**
<u>B. Missaoui</u>, N. Hamdi, J. Mediouni Ben Jemâa, J.M. Krafft, S. Boujday, L. Bergaoui *INSAT - Tunis* Recycling of industrial tobacco waste to obtain bioinsecticide nanocomposite based on Nicotine to control Tribolium castaneum (Tenebrionidae)	**OC 23D**
<u>K. Missaoui</u>, K. Ferchichi, N. Amdouni *FST - Tunis* Development and characterization of materials for application as electrodes in energy storage systems	**OC 23B**
<u>R. Mnafki</u>, A. Morales, L. Sillero, R. Khiari, Y. Moussaoui, J. Labidi *FSG - Gafsa* Posidonia Oceanica balls: Chemical composition	**OC 21C**

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A. Mpupa, S. Kholofelo Selahle, B. Mizaikoff, P. Nosizo Nomngongo *University of Johannesburg - South Africa* Miniaturised liquid phase extraction of butyl and phenyltins in sediment samples using Deep eutectic solvent: Optimisation and HPLC-ICP-MS analysis	**OC 07C**
S. Mrad, M. Hichri, C. Lafuente *FST - Tunis* Surface and calorimetric behavior of N,N-dimethylacetamide with n-alkanols and 2-alkanols	**OC 15D**
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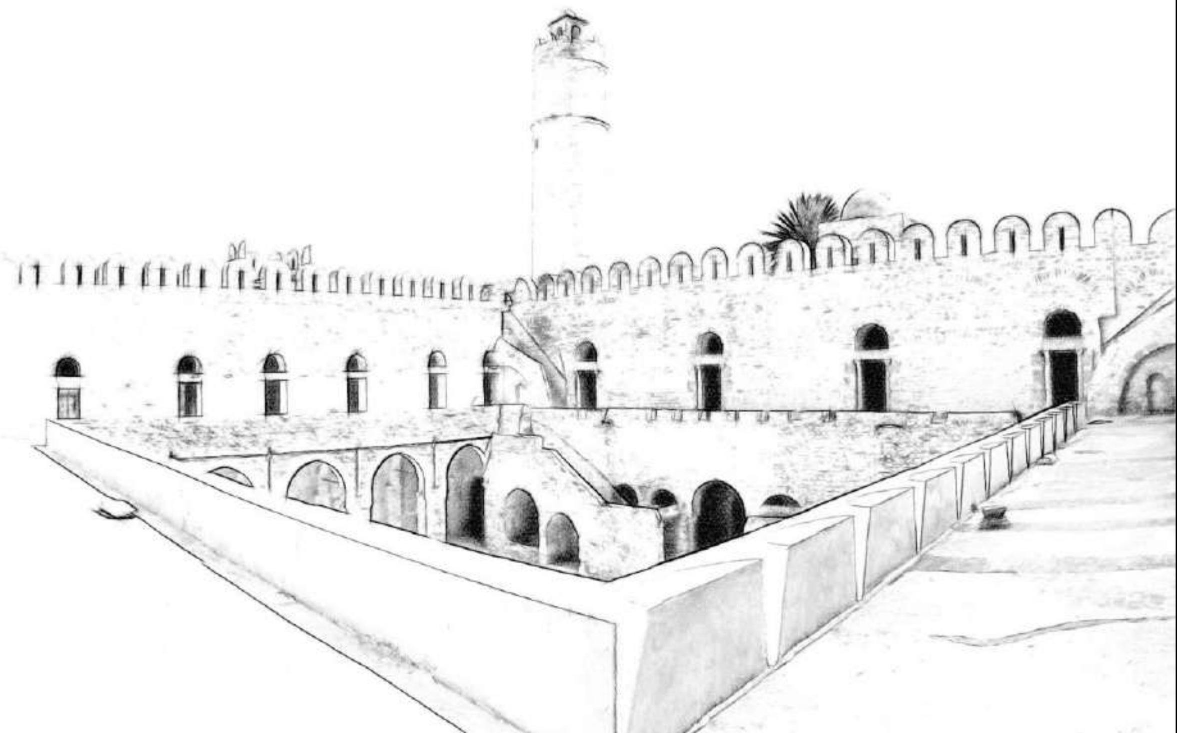
S. Msaoura, A. Houas, A. Rayes *FSG - Gabès* A new 0-D hybrid bismuth halide compound $(C_{13}H_{28}N_2)_4[BiCl_6]_2.2Cl.5H_2O$: Synthesis, crystal structure and physical properties	**OC 25B**
A. Msehli, S. Sayettat, A. Shekoory, L. Duquesne, I. Defer, A. Bouraoui, K. Senni, H. Majdoub *FSM - Monastir* Effects of marine polysaccharides from Tunisian and Brittany seashore biodiversity on dermal fibroblast proliferation and matrix metalloproteinases secretion	**OC 33A**
O. Nasri, J. Zaghdoudi, M. Kanzari *FST - Tunis* Temperature sensor based on one-dimensional hybrid photonic crystals	**OC 24D**
L. Nyaba, B. Prudence Khunou, P. Nosizo Nomngongo *University Of Johannesburg, South Africa* Application of $MOS4^{2-}$ intercalated magnetic layered double hydroxide for preconcentration of cadmium and lead from water samples	**OC 26D**
R. Oueslati-Omrani, I. Khattech, A.H. Hamzaoui *CNRSM - Borj Cédria* The influence of ZnO additions on the structural investigations and thermochemical behavior of M_2O-ZnO-P_2O_5 (M ≡ Na or Li) phosphate glasses	**OC 26B**
O. Ouled Ltaief, N. Fakhfakh, N. Dammak, S. Siffert, M. Benzina *ENIS - Sfax* Novel zeolite prepared using Tunisian raw clay: Study of C3H6 breakthrough dynamic adsorption onto zeolite material	**OC 33B**
C. Ounalli, M. Essid, S. Abid, Z. Aloui *FSB - Bizerte* Synthesis, crystal structure, vibrational and optical properties of a new Bi(III) halide complex: $(C_9H_{13}N_2O_2)_2Bi_2Cl_8$	**OC 27B**

Communicatings' Names	**Ref**
E. Rahali, Y. Arfaoui *FST - Tunis* Theoretical DFT insights into the nature of chalcogen bonding between SO_2, SO_3 and diazine: Noncovalent interactions involving σ and π holes	**OC 23C**
H. Raissi, T. Boubaker *FSM - Monastir* Nucleophilicities of cyclic secondary amines in methanol	**OC 25A**
S. Saad, I. Dávila, F. Mannai, J. Labidi, Y. Moussaoui *FSG - Gafsa* Effect of hydrothermal treatment on Zyziphus lotus's integral valorisation	**OC 25D**
J. Sakfali, S. Ben Chaabene, R. Akkari, F. Dappozze, G. Berhault, C. Guillard, M. Saïd Zina *FST - Tunis* High photocatalytic activity of wide band gap oxide nanoparticles induced by structural defects	**OC 06D**
M. Salhi, M. Romdhane, E. Berrich, F. Aloui *ENIG - Gabès* Performance and exhaust emissions of an internal combustion IC engine operated with olive pomace pyrolysis oil	**OC 31C**
S. Salhi, D. Kanzari-Mnallah, I. Jourdin, M. Knorr, C. Strohman, M.L. Efrit, A. Ben Akacha *FST - Tunis* Synthesis and structural study (^{31}P, ^{1}H, ^{13}C NMR and X-Ray crystallography) of some β-phosphonated thiosemicarbazones	**OC 26A**
H. Slimi, T. Ollevier, J. Kraiem *Faculty of Pharmacy - Monastir* Iron chloride-catalyst as a convenient route to provide a selective, practical and green homo and cross-etherification reactions	**OC 27A**
I. Soltani, M. Romdhane, E. Berrich, F. Aloui *ENIG - Gabès* Experimental investigation of date palm wastes by pyrolysis: Date palm leaves and date palm leaf stems	**OC 32C**
E. Souidi, S. Saîd, C. Autret-Lambert, A. Megriche *FST - Tunis* Influence of $Ba_{0.6}Sr_{0.4}TiO_3$ (BST) addition on the dielectric properties of $CaCu_3Ti_4O_{12}$ (CCTO) ceramics	**OC 24C**
I. Souii, J.M. De Los Santos, M.L. Efrit, H. M'Rabet *FST - Tunis* First and easy synthesis of a new family of Phenylene-bis-(allylic-α-aminophosphonates)	**OC 07A**

Communicatings' Names	**Ref**
F. Taleb, M. Ben Mosbah, Y. Moussaoui *FSG - Gafsa* Ibuprofen retention using biobased polymer from spent coffee grounds	**OC 34B**
R. Torkhani, M. Jebari, H. Galai *INRAP - Sidi Thabet* Physical stability study of candesrtan in co-amorphous system with amlodipine	**OC 06C**
N. Touj, L. Delaude *ISSTE - Borj Cédria* Synthesis and catalytic applications of bimetallic ruthenium-arene complexes bearing fluorinated imidazolium-2-dithiocarboxylates zwitterions	**OC 28A**
H. Trabelsi, K. Alouani *FST - Tunis* Electrochemical behavior of zinc and cadmium complexes in solution with bidentate organochalcogenophosphorus ligands	**OC 05C**
R. Zarroug, B. Ayed *FSG - Gabès* Synthesis, characterisation, stability and human serum albumin binding of a decavanadate complex $(C_4H_7N_2)_6[V_{10}O_{28}].8H_2O$	**OC 25C**
M. Zayene, F. Le Bideau, H. Ben Jannet, M. Alami, A. Romdhane, S. Messaoudi *FSM - Monastir* New synthesis of diaryl tropane derivatives by palladium(II)-catalyzed C(*sp*^{3})–H activation	**OC 29A**
M.A. Ziadi, D. Hellali *FST - Tunis* Mixing enthalpies of solid solutions $(Cs_{1-x}, Tl_x)\ NO_3$ at 298.15 K	**OC 28B**
A. Zouaghi, B. Belgacem, R. Ben Hassen *ISSBAT - Tunis* Investigation of optical, dielectric and conductivity studies of new $Sr_2Sn_{1.33}In_{0.33}Ni_{0.33}O_{6-\delta}$ double perovskite	**OC 34D**
M.O. Zouaghi, S. Hassen, I. Özdemir, N. Hamdi, Y. Arfaoui *FST - Tunis* Synthesis, X-Ray structure, optical and non-linear optical properties of rhodium-complex bearing N-heterocyclic carbene ligand: Molecular Docking and theoretical investigations	**OC 26C**



Abstracts of Oral Communications

Program of
Monday 18
December 2022

New copper(II) complexes supported by azomethine ligands: Synthesis and characterization

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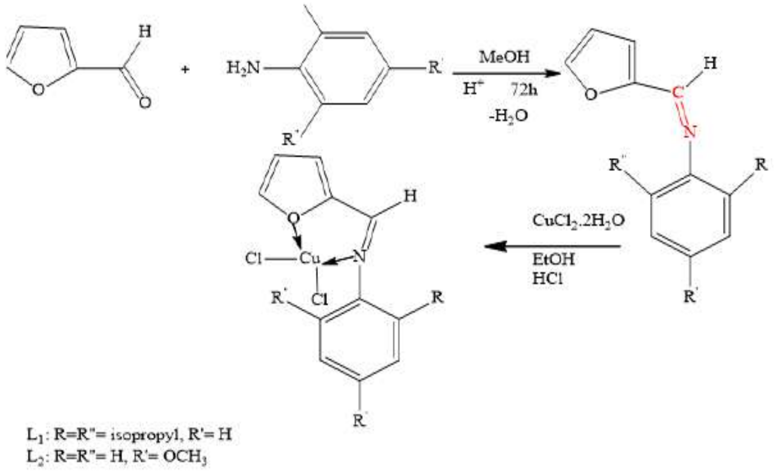
A series of azomethine ligands were prepared by condensation reactions of furfural with anilines[1, 2]. Ligands, 2-(N-2,6-diisopropylphenylformimino)furan(L1) and 2-(N-4-methoxyphenylformimino)furan (L2) were obtained by condensation reactions of the respective anilines with furfural. The reaction of copper (II) chloride dihydrate with one equivalent of the ligands L1 et L2 in ethanol at room temperature, always afforded the corresponding complexes $LCuCl_2$ (L= L1 or L2) with high yields. These new complexes have been characterized by IR spectroscopy, NMR spectroscopy, UV-VIS.



Key words: Bis(diimine), Copper (II) chloride dihydrate, IR spectroscopy.

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Synthesis, crystal structures and biological activities of halogeno-(*O*-alkylphenylcarbamothioate)bis(triarylphosphine) copper(I) complexes

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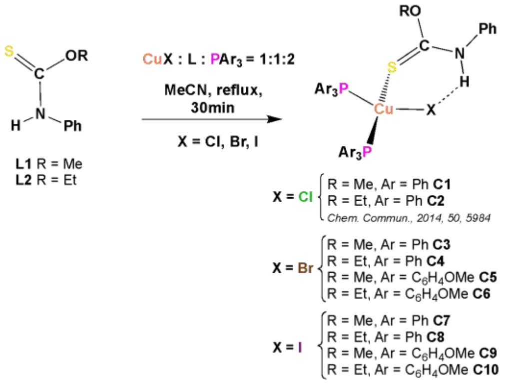
The reactions of *O*-alkyl *N*-phenylcarbamothioates **L** with copper (I) halides in the presence of two equivalents of PAr_3 allows the isolation and structural characterization of mononuclear thione complexes of type $[(Ar_3P)_2Cu\{ROC(=S)N(H)Ph\}X)]$ **C1-C10**. [1] According to X-ray diffraction analyses, all complexes adopt a distorted tetrahedral geometry and feature intramolecular N-H···Hal bonding, giving rise to six-membered cycles (Scheme).



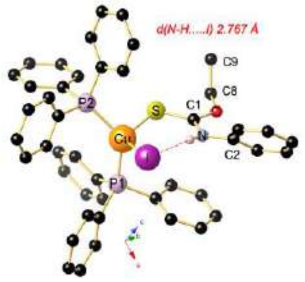


Figure. Molecular structure of **C8**.

The screening of the biological activity of these complexes reveals an antioxidant activity with a maximum activity for complexes **C7** and **C8** has been evidenced using the colorimetric DDPH method**.** This has been probed *in vivo* on Wistar rats for the preservation of hepatocytes integration after liver hypothermic conservation normal cellular state by addition of $[(Ph_3P)_2Cu\{EtOC(=S)N(H)Ph\}I]$ **C8**. The coordination chemistry of **L** towards other metal salts such as BiI_3 is currently under investigation [2].

Key words: Copper halide, *O*-alkyl-*N*-phenylcarbamothioate, complexes, biological activity.

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Antioxidant and antimicrobial activities of *Anthyllis henoniana* stems extracts and direct identification of phenolic compounds from its ethyl acetate and methanol extracts

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Nature has never encountered so much power. Today, the effectiveness of medicinal plants is recognized and scientifically demonstrated. Its undeniable benefits for our health have allowed phytotherapy to enter our daily lives. Plants collect metabolites, primarily phenolic compounds, which are a valuable supply of useful compounds for humans. In this work, we tried to investigate three stems extracts of *Anthyllis henoniana* (hexane, ethyl acetate and methanol) by determining their TPC, TFC, antioxidant activity using three *in vitro* assays (DPPH, FRAP and CAT) as well as their antimicrobial activity. We then proceeded with an LC-MS/MS characterization. The phytochemical composition of *Anthyllis henoniana* stems extracts was investigated to explain the results obtained in antioxidant and antimicrobial activities. The results showed that the methanol extract exhibited the highest antioxidant activity, while the ethyl acetate extract gave the sharpest antimicrobial effect. To explain these differences, we investigated the phytochemical composition of these two extracts, using liquid chromatography coupled with mass spectrometry. We therefore conclude that the difference in activities observed for the two extracts depends on the chemical composition of and on the percentage of each component in the extract.

Key words: *Anthyllis henoniana*, LC-HESI-MS^n, TPC, TFC, antioxidant and antimicrobial activities.

The emerge of a new bifunctional peptidic organocatalysts for the stereoselective Michael addition of aldehydes onto nitroalkenes

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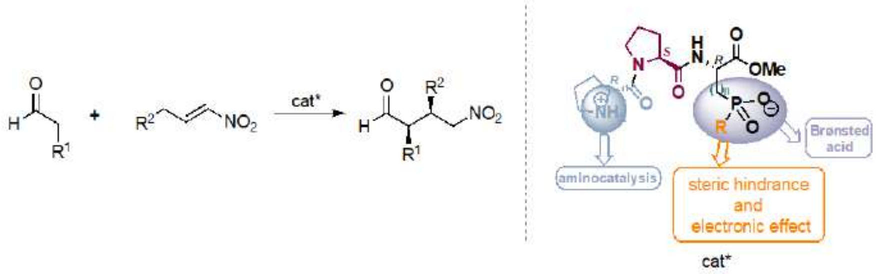
The biological activity of chiral substances and drugs often depends upon their structure, since their binding partners in the living body itself are highly stereoselective [1]. This crucial relationship between the configuration and the biochemical response of a particular molecule can be observed in the affinity of enantiomers for certain receptor in the living systems or in their toxicological properties. In this context, organocatalysis has emerged as a highly valuable tool for the construction of complex and enantioselective molecular frameworks from readily available starting materials [2]. In this communication, we will disclose an overview of a new efficient bifunctional peptides as organocatalysts [3] combining both aminocatalysis and an activation with a phosphinic acid moiety for the asymmetric Michael addition.



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A SIMPLE AND EFFICIENT PROTOCOL FOR ACCESSING TO FUNCTIONNALIZED PYRROLIDINE

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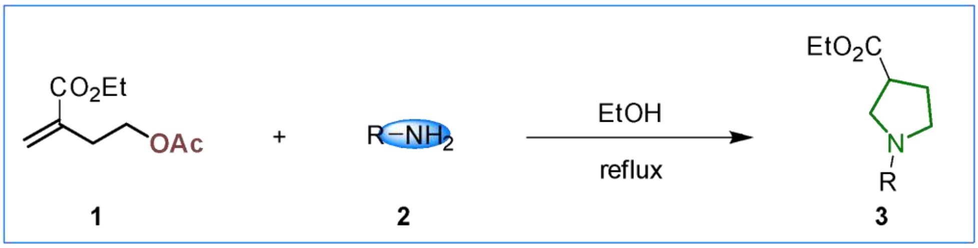
The pyrrolidine framework is a vital subunit widely found in many classes of organic aza-heterocycles. It makes part of the ten most common ring systems in tiny medicine molecules.[1] We describe in this work a simple and efficient protocol for accessing to functionalized pyrrolidine ring through two-steps (S_N2)-Michael addition on homoallylic living group (acetylated derivatives) **1** and primary amine **2** in reflux of ethanol.



Scheme: Aza-Michael addition of primary amines to homoallylic living group (acetylated).

Key words: Homo allylic living group (acetylated)**,** Aza Michael, Pyrrolidines.

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New 1,2,4-triazoles derivatives from some N-functonnalized imidates

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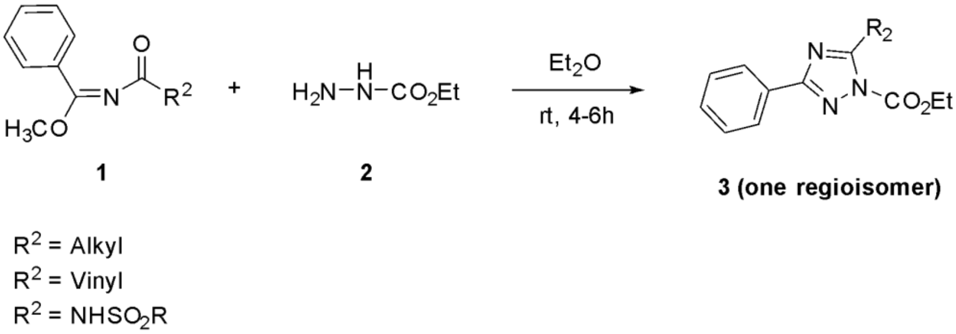
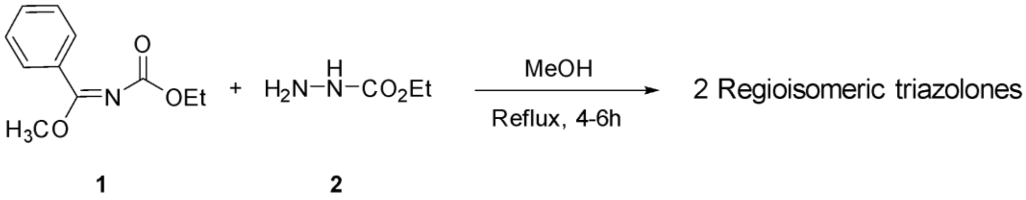
Due to the richness of five-membered heterocycles, especially 1,2,4-triazoles exhibit various biological activities such as antibacterial, antifungal, antioxidant, anti-inflammatory, antimoral[1-3] and pesticidal[4] properties. We were able to access new ranges of N-functionalized 1,2,4-triazoles by reacting ethyl carbazate with N-acylated, N-ethoxycarbonylated and N-sulfonamide imidates. Further study of the reaction allowed the interpretation of obtaining two regioisomeric triazolones, when the substrate is the ethoxycarbonyl imidate. This interpretation was supported by DFT calculations.

Key words: Imidate, Hydrazine, Triazole, DFT



In the case of R^2 = OEt :



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First and easy synthesis of a new family of Phenylene-bis-(allylic-α-aminophosphonates)

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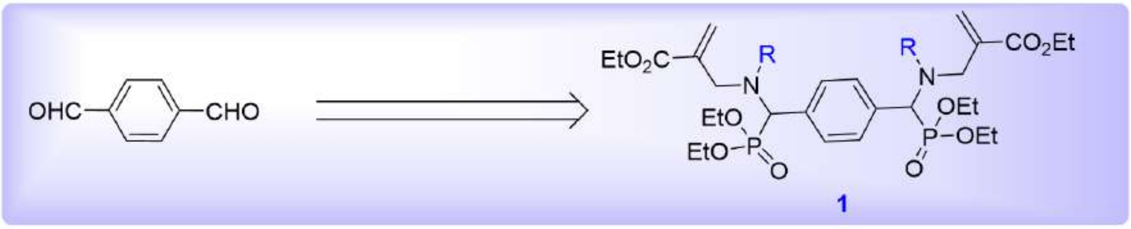
Allylic amines represent a significant class of compounds that gets an important interest in synthetic chemistry. This compound shows suitable building blocks for the synthesis of heterocycles and bioactive amines[1,2,3]. Herein, we report an easy and efficient synthesis of a new family of phenylene-bis-(allylic-α-aminophosphonates) **1** under mild conditions.

Keywords: Allylic amines, phenylene-bis-(allylic-α-aminophosphonates), mild conditions.



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Dynamic Kinetic Resolution Processes Based on the Switchable Configurational Instability of Allenyl Copper Reagents

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Pierre Mangeney,[3] Jérôme Marrot,[4] Arie van der Lee,[5] Samira Bouaouli,[3] Maya Guillaumont,[6]
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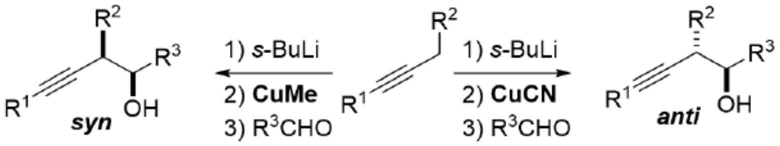
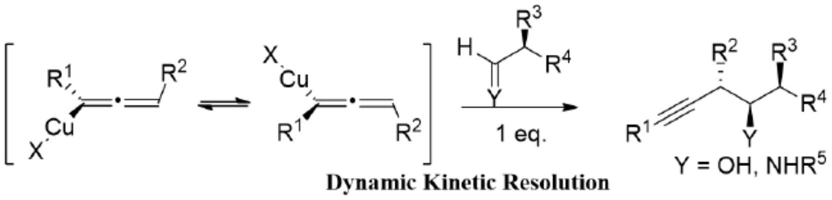
We focus herein on the stereodivergent behavior of cyano- and alkyl- allenylcuprates towards aldehydes. A coupled experimental and theoretical study shows that the ancillary copper ligand enables to control the spatial arrangement of the lithium cation with respect to the allenylcuprate moiety. Thus, a simple change of the nature of the copper substituent gives a straightforward and selective access to syn or anti homopropargylic alcohols. DFT calculations shown that in this system, the lithium counter-ion plays at the same time the role of an activator and a diastereoselective inductor: lithium has thus to be considered as the key for addition of allenylcuprates towards aldehydes. [1]



We also found that the transient allenyl copper reagents prove to be configurationally instable depending of the presence of lithium cation in the reaction media, which paved the way to efficient switchable dynamic kinetic resolution processes:



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Pd supported on locust bean gum as reusable green catalyst for Heck, Sonogashira coupling reactions and 4-nitroaniline reduction under ultrasound irradiation

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An easy and environmentally friendly method has been developed for locust bean gum extraction from carob seeds to be used as natural support of palladium. The reaction was carried out in water under ultrasonic irradiation for a short period of time (30 min). This catalyst was characterized by different analytical techniques such as ultraviolet–visible (UV-vis), Fourier transform infrared (FTIR), thermogravimetric analysis (TGA), scanning electron microscopy/ energy dispersive X-ray spectroscopy (SEM/EDX), elemental mapping analysis, and X-ray diffraction (XRD). The catalytic activity of Pd supported by locust bean gum was studied in Heck and Sonogashira cross-coupling reactions in different conditions under ultrasonic irradiation. Likewise, it was examined as green catalyst of 4-nitroaniline reduction at room temperature in water. The reusability of the catalyst was verified for five consecutive cycles, where excellent yields were obtained.

Key words: Catalyst, coupling reaction, ultrasonic activation, green chemistry

Graphical abstract.

Semi-synthesis of new triazole hybrid compounds from fluoroquinolone and isolated olive pomace triterpenic acids

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Anis ROMDHANE[b], Ata Martin LAWSON[a].

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Maslinic acid (MA) and oleanolic acid (OA) are two hydroxy pentacyclic triterpene acids (HPTAs) found as major compounds in *Olea europaea* L.. Due to their wide spectrum of biological activity, these compounds continue to attract great attention from the scientific community [1]. In this communication, we report an effective procedure for the selective isolation of MA and OA from olive pomace (*Olea europaea* L.) and the synthesis of new 1,4-disubstituted-1,2,3-triazoles (**3a, b**) derivatives. The last step of the synthesis is performed between MA and OA originated azides (**1a, b**) and a series of propargylated quinolones and fluoroquinolones throughout the Cu-catalyzed azide-alkyne cycloaddition (CuAAC).

Key words: *Olea europaea* L., Maslinic acid, Oleanolic acid, Fluoroquinolones, 1,3-Dipolar Cycloaddition, Triazoles.

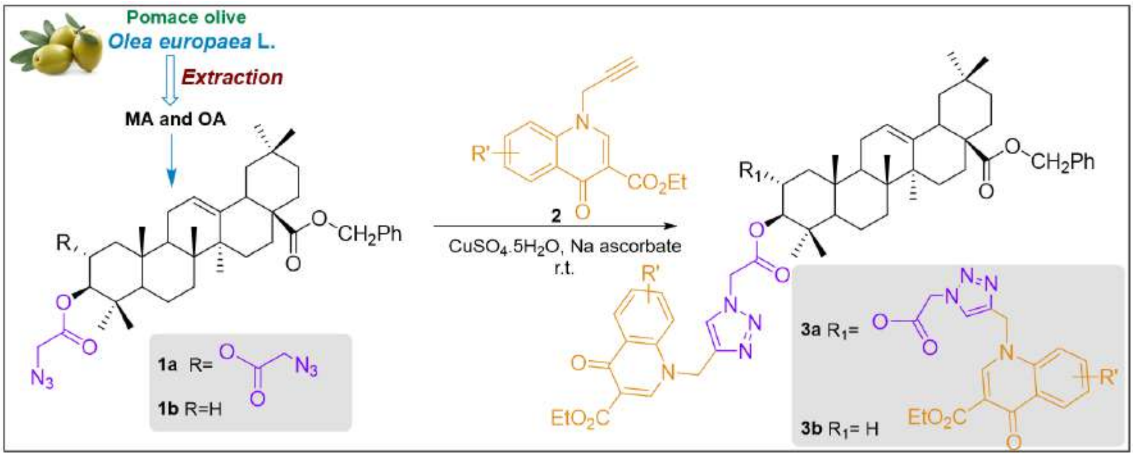

Figure 1: Synthetic pathway of triazoles **3**

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First natural isolation of a xanthenone from a local plant "*Tricholaena teneriffae*" cultivated in Tunisia

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Due to its geographical location and climate diversity, Tunisia is one of the richest Arab countries with 2100 plant species. This great floristic biodiversity has contributed to the development of scientific research in Tunisia, in several fields such as ethnomédecine, traditional pharmacopoeia and the valorization of natural substances.

As part of the research program of our laboratory on medicinal plants of the Tunisian flora, this work aims to carry out a chemical investigation and a biological evaluation of a local species «*Tricholaena Teneriffae*».

First, we extracted the aerial part of *Tricholaena Teneriffae* by cold maceration using solvents of increasing polarities (hexane, ethyl acetate and methanol). Then, a phytochemical screening showed that the methanol and ethyl acetate extracts had high levels of polyphenols and flavonoids. In addition, these extracts showed an interesting antioxidant activity and a significant antimicrobial activity thanks to their high content of phenolic compounds.

Second, the application of chromatographic techniques to the ethyl acetate extract allowed for the first natural isolation of a pure product identified with 12H-benzo[a]xanthen-12-one. Its structural elucidation was carried out using different spectroscopic techniques (NMR united and two-dimensional, UV).

Key words: *Tricholaena Teneriffae*, antioxidant activity, antimicrobial activity, NMR, 12H-benzo[a]xanthen-12-one.

Chemical and biological studies of a Local Medicinal plant

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Background and aim: Plants remain an important and inexhaustible source of biomolecules known by their interesting biological properties. In this work we were interested in the chemical investigation of organic extracts and essential oils from the aerial part (flowers, stems) of *enarthrocarpus clavatus* (Brassicaceae) as well as the evaluation of their antioxidant activity.

Methods: the extracts were prepared by means of a Soxhlet apparatus using different solvents with increasing polarity (hexane, ethyl acetate and methanol) while essential oils were obtained using hydrodistillation technique. The various components of the essential oils were identified by GC-MS (gas chromatography-mass spectrometry) analyze.

Results: The obtained extracts by Soxhlet from the aerial part (flowers and stems) of this plant have been chemically and biologically investigated. Ethyl acetate and methanol extracts showed the presence of various secondary metabolites. Moreover, these two extracts presented strong antioxidant activity which was evaluated by means of 2,2-diphenyl-1-picrylhydrazyl test (DPPH), reducing power (FRAP) and total antioxidant capacity (TAC) whereas the hexane extract had low antioxidant activity.

On the other hand, GC-MS analyze allowed the identification of various terpenes, sesquiterpenes and phenolic compounds in the essential oils. In addition, the essential oil from flowers presented a powerful DPPH scavenging activity ($IC_{50} = 0.2\ mg\cdot mL^{-1}$)

Conclusion: Ethyl acetate and methanol extracts as well as essential oil from *enarthrocarpus clavatus* flowers have interesting antioxidant activity which can be due to their richness in phenolic and terpenic compounds.

Key words: *enarthrocarpus clavatus***,** essential oil, antioxidant activity, GC-MS

Nucleophilic Reactivities of Pyrazoles in 50% DMSO-50% MeOH and Correlation Nucleophilicity versus Basicity

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Laboratoire de Chimie Hétérocyclique, Produits Naturels et Réactivité, Université de Monastir,
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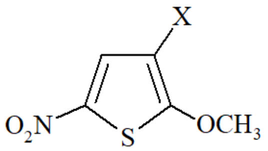
Pyrazoles have been the subject of intensive experimental and theoretical studies due to their importance in biological processes as well as synthetic applications. We now studied the reactions of 2-méthoxy-3-X-5-nitrothiophenes **1a-c** with a series of pyrazoles **2a-c** in 50% DMSO-50% MeOH at 20°C in order to determine the nucleophilicity parameters N and s_N of pyrazoles **2a-c** according to Eq (1) and to compare their reactivities with those of the homologous imidazoles.

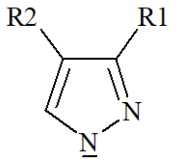
$$\log k\ (20\ °C) = s_N\ (E + N) \qquad (1)$$

On the other hand, structure-reactivity relationships of these pyrazoles are discussed in order to elucidate general relationship between nucleophilicities and basicities.



1

X = NO_2 , CO_2CH_3 and $CONH_2$



2

$R_1 = R_2 = H$
$R_1 = H, R_2 = Br$
$R_1 = CH_3, R_2 = Br$

Key words: Kinetics / Pyrazoles / Nucleophilicity / Mayr's Approach / L F E R.

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Influence of short uptake moisture on drug-excipient binary mixture: DSC and FTIR contribution

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This study aimed to evaluate a physicochemical stability between Acebutolol hydrochloride (ACB) and different common excipients: Polyvinylpyrrolidone (PVP), Magnesium Stearate (MgSt), Ascorbic acid (ASC), Citric acid (CIT), Butylhydroxyanisol (BHA) in freshly physical mixture and after exposure to short time under water vapour (2 hours at 38 °C and 90 % relative humidity (RH)). This compatibility study is performed out using mainly Differential Scanning Calorimetry (DSC) and Fourier Transform Infrared Spectroscopy in ATR mode (FTIR-ATR) for the binary physical mixtures of ACB-excipients in different ratio. Different thermal behaviours are illustrated for ACB in presence of various excipients in term of melting temperature (T_m). In the presence of all proportions of MgSt, the ACB stability is not affected, FTIR and DSC revealed no chemical interaction. However, in the presence of CIT, PVP and BHA, seriously ACB interaction was involved. Contrary to PVP, the mixture of ACB with ASC seems to lead to an improvement in the stability of the two components and a decrease in their interaction after storage under humidity. For all studied physical mixtures of ACB before and after exposure to humidity, FTIR spectra exhibited no significant changes suggesting no physical-chemical alterations. The result underlines that DSC was more relevant to FTIR analysis to highlight the incidence of slight uptake of moisture on Acebutolol in presence of ASC and PVP.

Key words: Acebutolol, Compatibility, Humidity, DSC, FTIR

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Alkaloids and polyphenols with antioxidant and anticholinesterase activities from *Atractylis cancellata*

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Atractylis plants belonging to the Asteraceae family are used in folk medicine against urinary retention, intestinal parasites and snakebite poisoning [1]. *Atractylis cancellata* L., is employed in folk medicine for the treatment of skin disorders [2], it is an herbaceous endemic plant growing in semi-arid zone of Mediterranean area [3]. We report herein the isolation and identification of one new alkaloid type pyrroloquinolone A, together with twelve known secondary compounds. Moreover, the antioxidant activity of extracts (PE, EtOAc and *n*-BuOH) and some phenolic compounds were detremined by DPPH, ABTS, CUPRAC, and reducing power methods. Furthermore, the acetylcholinesterase and butyrylcholinesterase inhibitory activities of extracts and the two alkaloids were tested. The ethanol extract (70%) of dried whole plant *A. cancellata* was partitioned by liquid/liquid chromatography into three extracts PE, EtOAc and *n*-BuOH. Purification of the PE, EtOAc and *n*-BuOH soluble parts using diverse chromatographic methods (VLC, CC, HPLC and TLC) afforded thirteen secondary metabolites **1-13**. Their structures were established using 1D- and 2D-NMR and HR-ESI-MS techniques, and comparison with data reported in the literature. These compounds are named pyrroloquinolone A, 4-methoxy-1-methyl-2-quinolone, chrysin, apigenin, tricine, quercetin, quercetin 3-*O*-β-D-glucopyranoside, isoorientin, diosmin, 4-*O*-caffeoyl-2-*C*-methyl-D-threonic acid, chlorogenic acid methyl ester, vanillin and 5-*O*-caffeoylshikimic acid. The antioxidant activity, evaluated by DPPH, ABTS, CUPRAC, and reducing power methods, showed that some compounds exhibit good antioxidant activity. Furthermore, the *n*-BuOH extract, and the two alkaloids pyrroloquinolone A**,** and 4-methoxy-1-methyl-2-quinolone displayed good AChE and BChE inhibitory activities. This study describes for the first time the occurrence of alkaloids in *Atractylis* genus.

Key words: *Atractylis cancellata*, Alkaloid, Polyphenol, NMR, Biological activity

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Synthesis, physico-chemical characterizations, and antiproliferative activity on U87 human brain cancer cells, of a new vanadium complex (V), tetra-[methylimidazolium] dihydrogen decavanadate

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The interest in decavanadate anions has increased in recent decades, since these clusters show interesting applications, particularly in the medical field as antibacterial, antiviral, and anticancer agents [1-2]. Here, we report a new decavanadate compound with organic molecules synthesized in an aqueous solution and structurally characterized by single-crystal X-ray diffraction, Infrared and UV-Vis spectroscopies, SEM coupled with EDX, and thermal analysis. The compound crystallizes in a monoclinic system, with the space group $P2_1/n$. The formula unit of the decavanadate compound consists of one dihydrogen decavanadate anion $[H_2V_{10}O_{28}]^{4-}$ and four organic 4-methylimidazolium cations $(C_4H_7N_2)^+$, linked through N-H…O hydrogen bonds and van der Waals interactions leads to a three-dimensional structure. In the crystal, organic cations are linked by π-π interactions. In this study, the cytotoxic and antiproliferative activities of $(C_4H_7N_2)_4H_2V_{10}O_{28}$ on human brain cancer cells U87 were investigated. This compound demonstrated a dose-dependent antiproliferative manner with an IC_{50} value of 0.22 µM. Therefore, we could consider that $(C_4H_7N_2)_4H_2V_{10}O_{28}$ as a future potential metallodrug in anticancer activity.

Keywords: Decavanadate, Synthesis, Infrared spectroscopy, SEM-EDX, Thermal analysis, Anticancer activity

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Influence of rare earth elements incorporation on the structural and the ionic properties of NASICON type materials

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NASICON materials are supposed to be used as alternative solid electrolytes for all solid-state Lithium-ion batteries [1-3]. In this work, a series of $Li_{1.3+x}Ti_{1.7-x}Al_{0.3}Ln_x(PO_4)_3$ compounds was synthesized using the solid-state reaction method at 900°C. Structural factors that affect Li conductivity were investigated with powder X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Nuclear Magnetic Resonance (NMR) and Impedance Spectroscopy (IS) techniques. The substitution of Ti^{4+} by Al^{3+} and Ln^{3+} allowed the incorporation of additional lithium, increasing Li-Li repulsions and improving Li conductivity in NASICON crystallites. A high "Bulk" conductivity ~ 8.91×10^{-4} $S.cm^{-1}$ was obtained for the x =0.2 composition, due to the creation of vacancies at the conduction paths intersection (M1-M3-M1). It was shown that the presence of secondary phases $AlPO_4$ and $LnPO_4$ increased the grain boundary conductivity from 4.27×10^{-8} $S.cm^{-1}$ (x = 0) to 6.46×10^{-7} $S.cm^{-1}$ (x = 0.2).

Key words: Solid electrolyte, NASICON, Solid-state method, Lithium-ion, Ionic conductivity

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Synthesis and Study of Structural and Optical properties of Fluorescent Boranils from Their Corresponding Anils.

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The synthesis of (A-F) BF_2 Boranils is described in this contribution. Importantly, from a synthesis perspective, Boranils A-BF_2, B-BF_2 and C-BF_2 can be obtained by low temperature only at 3 hours synthesis procedure While the rest of Boranils were synthetized at higher temperatures and longer reaction times. The synthesis of corresponding Boranils was straightforward and several grams were easily obtained. (A-F) BF_2 were subsequently characterized by using FTIR, NMR ^{1}H, NMR^{9}F NMR, EDX, TGA, UV-Vis and photoluminescence spectroscopy. All Boranils showed blue fluorescence emission under UV-Light after the restriction of Azomethine bond isomerization by BF_3. Et_2O treatment. Combined effect of substitution effect and B(III) complexation has a crucial role in structural, thermal, and mainly optical properties.

Key words: Boranils, Anils, Boranils, Green Chemistry.

Structural and electrical properties of new Al-Gd doped lithium-phosphate NASICON type material

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The commercial application of $LiTi_2(PO_4)_3$ NASICON (**Na S**uper **I**onic **CON**ductor) type material as solid state electrolyte is limited due to its low electrical conductivity. Recent several studies have shown the improvement of the ionic conductivity by substituting the titanium ions making the lithium conductors one of the best solid state electrolytes thanks to their great thermal and chemical stability offering to All-Solid-State-Batteries higher safety and energy [1,2]. In this work, the effect of gadolinium and aluminium substitution on $LiTi_2(PO_4)_3$ structure and its ionic conductivity have been studied. The doped NASICON-type phases have been prepared by solid-state reaction and characterized using the X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Nuclear Magnetic Resonance (NMR) and Impedance Spectroscopy (IS). XRD data indicated the formation of NASICON-type structure phases with rhombohedral symmetry with R-3c space group (n°167). The presence of $AlPO_4$ secondary phase was confirmed by the analysis of $^{6}Li/^{7}Li$, ^{31}P and ^{27}Al MAS-NMR spectra. Based on the Rietveld structure refinement (Fullprof software) and the impedance spectroscopy results, it was shown that the vacancy arrangement on the M(2) sites enhances the Li conductivity.

Key words: Solid-state electrolytes, Electrical properties, Rietveld structure refinement.

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Crystal structure, spectroscopic characterization, thermal behavior and Hirshfeld surface analysis of a new organic-inorganic hybrid compound $(C_{11}H_{10}N)_2[CuCl_4]$

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In this work, a novel organic-inorganic hybrid compound $(C_{11}H_{10}N)_2[CuCl_4]$ was synthesized by slow evaporation at room temperature. It was then characterized by different techniques: powder and single crystal X-ray diffraction, IR and UV-Vis spectroscopy, TGA-DTA thermal analysis, X-ray micrography and microanalysis (SEM / EDX) and Hirshfeld surface analysis. The molecular unit of the compound is formed by two independent phenylpyridinium, $(C_{11}H_{10}N)^+$, monoprotonated organic cations, and one tetrachlorocuprate(II), $[CuCl_4]^{2-}$, inorganic anion. The structure of the compound is formed by a succession of mixed layers parallel to the (010) plane; they consist of phenylpyridinium organic cations and tetrachlorocuprate(II) inorganic anions. The structural cohesion inside the layers is ensured by N-H···Cl hydrogen bonds. Van der Waals interactions ensure the cohesion between two adjacent mixed layers to form a 3D network. Three-dimensional Hirshfeld surface (3D-HS) **[1]** and two-dimensional fingerprints (2D-FP) **[2]** reveal that the structure is dominated by Cl···H/H···Cl; H···H and C···H/H···C contacts.

Keywords: Crystal structure; Hybrid compound; Tetrachlorocuprate(II); X-ray diffraction, 3D-HS; TGA-DTA.

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Sintering of Potassium Doped Hydroxy-Fluorapatite Bioceramics

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The present study describes the influence of potassium and hydroxyl substitutions on the structural, thermal and mechanical properties of fluorapatite bioceramics. A set of nonstoichiometric ion-substituted compounds, with a chemical formula of $Ca_{10-x}K_x(PO_4)_6F_{(2-2x)}$ $(OH)_x$ with $0 \leq x \leq 1$ synthesized by the wet precipitation method, were found to be single-phase apatites crystallizing in the hexagonal P63/m space group. The structural parameters, as well as the crystallite sizes, increased accordingly to the amount of added dopant-ions. The thermal behavior of these compounds, studied within the temperature range 500–1200˚C, indicated a partial decomposition of the apatitic phase and its transformation to tricalcium phosphate β-$Ca_3(PO_4)_2$ at temperatures exceeding 750˚C. A relative density of the sintered samples achieved the highest value with $x = 0.25$ and reached about 95% after sintering at 1050˚C for 1 h. The microstructures of the sintered samples were of a trans-granular aspect and experienced an increase in the radius of their pores as x increased. The prepared bioceramic materials were mechanically characterized by means of Young's modulus, flexural strength and fracture toughness measurements. The overall trend of these parameters evolved comparably to the relative density, and the maximum values obtained for $x = 0.25$ were measured to be 96 MPa, 47 MPa and 1.14 $MPa \cdot m^{1/2}$, respectively.

Ab initio study of the ground state, electronic structure, and optical properties of α-Ba_2SnS_4

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The DFT method has been used with success to predict the ground state, electronic structure, and optical properties of a ternary thiostannate compound (α-Ba_2SnS_4). The calculation has been performed using GGA-PBE approximation by the mean of CASTEP [1] software. The Charge distribution method (CHARDI) [2] shows a reduction in the coordination number of the barium atom after the structure optimization. The electronic structure shows that the studied compound is a semiconductor with a direct band gap and the calculated activation energy is about 2.469 eV. The electronic transition between the valence band and conduction band have determined based on the dielectric function, density of states and the selection rules [3]. Four electronic transitions have been determined: $Sn|p\rangle \rightleftarrows Sn|s\rangle$; $Sn|p\rangle \rightleftarrows Ba|s\rangle Sn|p\rangle \rightleftarrows Ba|s$; $S|p\rangle \rightleftarrows S|s\rangle$; $Sn|s\rangle \rightleftarrows Sn|p\rangle$. The absorption spectra shows that α-Ba_2SnS_4 could absorb both in the Visible and the UV lights region, and the highest absorption value reaches a value of about $3x10^5$ cm^{-1} along [010] direction which allows to suggest the compound as possible candidate for optoelectronic applications such as the photocatalysis. The phonon calculation shows the mechanical stability of the title compound.

Keywords: Thiostannate, ab initio calculation, electronic structure, optical properties, phonon.

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Evaporation of desalination brines: Simulation vs. experimental

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Sodium chloride is mainly produced either through an ancient process in which seawater gets concentrated by naturel evaporation or by forced water extraction processes, driving the precipitation of halite crystals. Traditionally, after salt harvesting from concentrated seawater brines, a residual by-product depleted in sodium chloride, known as bittern, is discharged into the sea [1]. This waste stream has severe negative environmental impacts on the receiving water body. On the other hand, both brines and bitterns are highly concentrated solutions rich in various minerals, some of which are on the top list of strategic compounds as demonstrated by the intensive research activity on the field [2]. In this work, seawater evaporation has been simulated using PHREEQC software, which is able to predisct the physico-chemical properties and species activities through the full Pitzer model. For each sparingly soluble salt during the evaporation process, once supersaturation is reached, the solution is allowed to deplete through precipitation of single or multiple species. Simulation will focus on the evolution with mass concentration factors of the following properties: density, electrical conductivity and the quantity of salts precipitated. Simulation results are compared to the experimental ones obtained by forced water evaporation using seawater and desalination brine.

Key words: Desalination process, seawater evaporation, brine, salts precipitation, PHREEQC simulation, experimental evaporation, physico-chemical properties.

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Microencapsulation Using Polysaccharides extracted from *Opuntia Ficus Indica*

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Microencapsulation of sunflower oil was performed using a complex coacervation method. Mucilages cactus extracted from *Opuntia ficus indica* (OFI) and Chitosane (Chi) were used as wall materials. The physicochemical characteristics of mucilage samples and obtained microcapsules were studied. The FTIR analysis showed the presence of galactose and pectin in mucilages. The XRD detected minerals as calcium salts. The SEM revealed particles with irregular shapes and forming particle aggregations. The microcapsules, formed by complex coacervation crosslinked with mucilage cactus and chitosane had sufficient stability to maintain their structure and existing good characteristics for cosmetic application, such as average diameter below 12 µm, low solubility and low hygroscopicity. Furthermore, the encapsulation efficiencies of the obtained microcapsules ranged from 83% to 87%. The obtained results can be considered as a promising and potential. Since the microencapsulation of sunflower oil using mucilages and chitosane as well materials will have more wide application in various fields such as food and cosmetic industry.

Key words: Microcapsules, Complex coacervation, Mucilage cactus, Chitosane.

Synthesis, crystal structure, Hirshfeld surface analysis of a new hybrid compound Bis(benzylammonium)tetrachlorocadmate(II)

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The synthesis of organic-inorganic hybrid materials represent one of the most active areas of materials science and chemical research [1] as there is a growing interest in developing materials with specific characteristics not found in a single constituent which can be a promising solution in a number of applications [2]. A new non-centrosymmetric hybrid material, $(C_6H_5CH_2NH_3)_2CdCl_4$, was synthesized, by slow evaporation method at room temperature (RT). Single-crystal X-ray diffraction (SC-XRD) analysis showed that the material crystallized at RT in orthorhombic system with space group Cmca and the following unit cell parameters a = 7.5047(5) Å, b = 33.070(2) Å, c = 7.5791(5) Å,V = 1881.0(2) $Å^3$ and Z = 4. The asymmetric unit of the crystal consists of an isolated anion $(CdCl_4)^{2-}$ and a protonated benzylamine disordered with two possible orientations around a crystallographic special position. Such crystallographic disorder phenomenon prompted us to determine the structure of this compound at low temperatures. The crystal structure does not retain the same space group symmetry over a wide temperature range, as shown by single crystal analyses performed at 100, 200 and 298 K. In fact, at 100 K this material crystallizes in the monoclinic system with space group Cc and the cation is found in two different positions in the asymmetric unit. At 200 K, this material crystallizes in orthorhombic system with space group Aba2. Each allotropic variety consists of corner-sharing distorted $CdCl_6$ octahedra forming two-dimensional layers stacked in a staggered fashion. Benzylammonium cations $C_7H_7NH^+$ are located in the interlayer spacing and link adjacent inorganic layers via charge-assisted weak hydrogen bonds between the ammonium $-NH_3^+$ moieties and Chloride ions. Hirshfeld surfaces and their associated 2D fingerprint plots were used to explore and quantify the intermolecular interactions in the crystal lattice of the title compound. The new title compound is also characterized by FT-IR spectroscopy and thermal analysis.

Key words: Organic-inorganic hybrid material; Crystal structure; thermal analysis; Hirshfeld surface analysis.

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Self-assembly of new cobalt thiocyanic complex based on 3,4-dimethylaniline

Synthesis, Empirical, Antioxidant activity, and Quantum theory investigations

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The reaction of 3,4-dimethylaniline with thiocyanic acid and the transition metal $CoCl_2.6H_2O$ leads to the production of a novel complex$\{[Co(SCN)_4]\ (C_8H_{12}N)_3\}\cdot Cl$, according to the slow evaporation process. The synthesized compound has been fully characterized by single-crystal X-ray diffraction. UV-Visible, FTIR spectroscopy, TGA analysis, and DFT circulations were also performed. The crystal structural analysis reveals that the solid $\{[Co(SCN)_4]\ (C_8H_{12}N)_3\}\cdot Cl$ crystallizes in the monoclinic system with the space group $P2_1/n$.

Metal cations are joined into corrugated chains parallel to the *b*-axis direction in $\{[Co(SCN)_4]\ (C_8H_{12}N)_3\}\cdot Cl$ by four thiocyanate anions. The crystal structure was calculated using XRPD data, indicating that it is closely connected to the DRX mono-crystal results. Different interactions pack the system into a ring formed by N-H···Cl and N-H···S hydrogen bonds. C–H···π and the π···π stacking of anilinuim ring and N–H···S intermolecular interactions for $\{[Co(SCN)_4]\ (C_8H_{12}N)_3\}\cdot Cl$ increase the crystals' robustness. Hirshfeld surface analysis cum 2D fingerprint plots visualize the main intermolecular interactions with their contributions in the solid-state phase. The molecular geometry of the complex obtained from the crystal structure was used for quantum chemical calculation. Here, frontier orbital analysis and electrostatic potential illustrate the chemical reactivities of the metal-organic complex. QTAIM and NCI analysis reveal the strength of interactions at the electronic level.

Keywords: Metal complex, Cobalt thiocyanate, Crystal structure, Physico-chemical study, Hydrogen bonds, Hirshfeld surface analysis, DFT studies.

X-Ray diffraction, IR spectrum, optical properties, AIM, NBO, RDG, HS, Fukui function and biological analysis of a novel hybrid compound $(C_9H_{15}N_3)[CuCl_4(H_2O)]$

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The paper reports the preparation and structural characterization of a novel hybrid complex $(C_9H_{15}N_3)[CuCl_4(H_2O)]$ grown by slow evaporation technique in aqueous solution at room temperature and characterized by X-ray diffraction, spectroscopy measurement, optical absorption, photoluminescence proprieties, Hirshfeld surface analysis, thermal and biological study. The crystal arrangement consists of $[CuCl_4(H_2O)]_n^{2n-}$ chains spreading alone c axis at x= 1/2 and y= 1/2. To build the three-dimensionality of the structure, the organic cations are linked to the chains through hydrogen bond type. The new prepared compound was screened for its antioxidant activity. The Photoluminescence proprieties were also reported. The nature and proportion of contacts and the rapport of enrichment in the crystal packing were studied by the Hirshfeld surfaces. The vibrational properties FT-IR and UV–VIS spectral analyses of present compound have been researched by theoretical calculations. Energy gap (Eg) of the molecule was found using LUMO and HOMO calculation. The local reactivity analyses (Fukui functions) were evaluated to identify the reactive sites in the protonated organic part. Intermolecular interactions were analyzed by molecular electrostatic potential surface (MEPS), the reduced density gradient (RDG), natural bond orbital (NBO) and topological AIM are reported. The NBO analysis of title compound shows that the maximum energy is equal to 37.61 $Kcal.mol^{-1}$ confirmed the charge transfer between organic and inorganic groups. The activation of thermodynamic parameters is calculated by DFT/ B3LYP/LanL2DZ. Finally, the biological activities of $(C_9H_{15}N_3)[CuCl_4(H_2O)]$ were investigated by DPPH and ABTS tests.

Keywords: X–ray single crystal diffraction, Hirshfeld surface analysis, Fukui, RDG, AIM, biological study.

Structure, optical and magnetic properties of the pyridinium cobaltate $(C_6H_9N_2)_2[CoCl_4]$

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X-ray diffraction of the blue crystalline material showed isolated $[CoCl_4]^{2-}$ tetrahedral in the structure, connected to the aromatic 2-amino-4-methylpyridinium cations through H bonding while the cations show π-stacking. FT-IR spectroscopy with Hirshfeld surface analysis confirmed the importance of the 2-amino function in the cations for the hydrogen bonding. The material is thermally stable up to 270 °C. Intense UV-vis absorptions in the range 200–400 nm were assigned to π–π* transitions in the pyridinium cation, weaker features in the range 600–750 nm were due to ligand-field transitions in the d^7 high-spin system $[CoCl_4]^{2-}$. The molar susceptibility measured over a range of 5–300 K reveals paramagnetic behavior at high temperature range with an effective magnetic moment of μeff = 4.74 μB indicating a significant spin-orbit coupling contribution adding to the spin-only value of 3.87 μB expected for Co(II) with 3d7 high spin configuration.

Key words: Co(II), 2-amino-4-methyl pyridinium, multifunctional ligands, hydrogen bond network, magnetic measurements

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Efficient synthesis, crystal assembly, vibrational properties, theoretical calculations, molecular docking and Pharmacokinetic profiling of a novel 2D layered hybrid compound $(C_6H_{10}N_3O)_2Cu_2Cl_6$

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The 2D hybrid compound bis(2-amino-4-methoxy-6-methylpyrimidinium) bis(μ_2-chloro)-tetrachloro-di-copper(II), $(C_6H_{10}N_3O)_2Cu_2Cl_6$,was successfully synthesized by slow solvent evaporation at room temperature. The structural properties were investigated using single crystal X-ray diffraction and reveals that the structure contains a centrosymmetric hexachlorodicuprate group where each Cu atom is coordinated to four Cl atoms in a slightly distorted square planar geometry. Nearby $[Cu_2Cl_6]^{2-}$ dimer units had short contacts with one another. The crystalline building stability is ensured by N–H…Cl and C–H…O hydrogen bonding as well as weak C–H$\cdots\pi$ intermolecular interactions. From the infrared spectroscopy analysis, the functional groups were identified.Simultaneously, the molecular docking of the studied compound with an HSP90/PDB: 5LRZ was performed by AutodockVina. Additionally, drug-likeness and ADME properties of $(C_6H_{10}N_3O)_2Cu_2Cl_6$ were performed in detail.

Keywords: 2D hybrid compound, X-ray diffraction, Molecular docking, Drug-likeness properties.

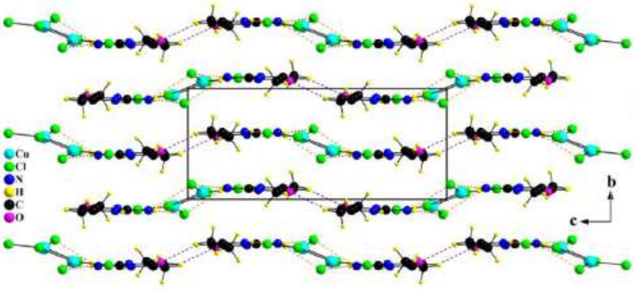

Figure.1: Projection along the *a*-axis of the structure of $(C_6H_{10}N_3O)_2Cu_2Cl_6$. Dotted lines show hydrogen bonds.

Effect of two-step ageing treatment on microstructure and mechanical properties of a commercial Al–Zn–Mg–Cu alloy

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To meet the expectations of the automotive and aeronautical industries, aluminum producers are constantly seeking to optimize existing alloys or develop new, more efficient ones. The aluminum alloys with the best mechanical characteristics are structurally hardened. This hardening is always to the detriment of plasticity. The purpose of the present work is to determinate the heat treatment that offers a better compromise between these two terms.

The study of the effect of the heating rate during two-step ageing treatment on the evolution of the microstructure and the mechanical properties of an industrial aluminum alloy (7075: Al-Zn-Mg-Cu) homogenized at 475 °C and matured for 84 hours was carried out using different experimental techniques.

Samples were aged after quenching first at 105 °C to obtain a well-developed structure of GP zones, and then in the second step at 140 °C. Two-step ageing treatment leads to the increase of yield strength and retention of good plastic deformability. These properties are obtained due to a finer dispersion of the GP zones and a high nucleation rate, which occur during the pre-ageing treatment (at 105 °C).

The decrease in the heating rate to reach the second stage, significantly increases the yield strength by obtaining comparable values of elongation, for example, the increase in the yield strength of 120.05 MPa is accompanied by a decrease of 0.68% in elongation only.

Key words: Al–Zn–Mg–Cu alloy, Two-step ageing treatment, Precipitation hardening, Mechanical properties.

g-C3N4/CuO/TiO2 composite nanomaterial with performances of photocatalytic degradation of Levofloxacin and electrochemical properties

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It is reported that metal doping is one of the most effective and conventional methods to elevate the separation rate of photogenerated electron-hole pairs. Doping of CuO in the crystal structure of TiO_2 improved the photocatalytic properties in the degradation of organic compounds due to the synergistic effect between CuO and TiO_2. The effect is further enhanced by the addition of third materials.

In this work, a TiO_2 photocatalyst is modified with CuO and g-C_3N_4 to obtain g-C_3N_4/CuO/TiO_2 nanocomposites with a different mass ratio of CuO. The best photocatalyst activity of the $CuO_x/TiO_{2(1-x)}$ composite is obtained for x=20%. The synergism of ternary composites exhibited greater photocatalytic activity than CuO/TiO_2. The highest degradation of Levofloxacin reached 99 % and 44 %, after 10 and 60min UV irradiation over ternary and binary composites respectively. g-C_3N_4/CuO/TiO_2 (20% in CuO) presented a better result and efficient degradation of LEVO under artificial UV with a concentration of 5.10^{-3} g/L of LEVO, a mass of 2.10^{-2} g and a very short treatment time (10 minutes). Under simulated solar irradiation, the degradation of g-C_3N_4/CuO/TiO_2 was 100% after only 20 minutes.

Keywords: Nanocomposites, photocatalytic degradation, levofloxacin, UV and sunlight.

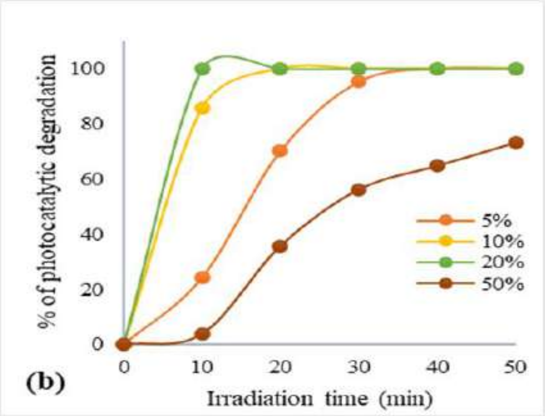

Figure 1: Effect of g-C_3N_4/CuO/TiO_2 (20% CuO) on the degradation of Levofloxacin

Development and Validation of Liquid Chromatography Tandem Mass Spectrometry (LC-ESI-MS/MS) Method for the Analysis of chloramphenicol residues in Biological Matrices

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This research involved the development of a Multi-Reaction-Monitoring (MRM) experiment in tandem Mass Spectrometry for the detection and quantification of Chloramphenicol in various biological matrices.

The resulted LC-MS/MS method showed high selectivity and sensitivity and was validated in accordance with ISO/EC 17025 requirements.

Validation criteria for the analysis of CAP in poultry and fish meat matrices included linearity, accuracy, specificity, precision, repeatability, limit of detection and Limit of quantification.

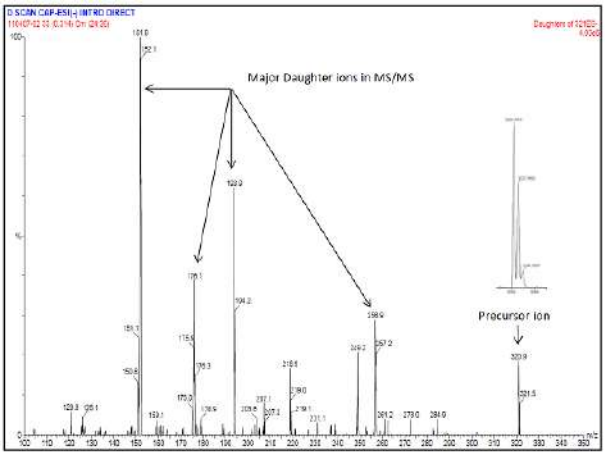

Fig. 1: MS/MS spectra of Chloramphenicol in Daughter Scan mode

For the developed method the linearity, accuracy and precision were found to be acceptable. Chloramphenicol limit of detection and limit of quantification values were respectively 0.152 µg Kg^{-1} and 0.206 µg Kg^{-1} and are below its minimum required performance level (MRPL) of 0.300 µg Kg^{-1} set out in the EU legislation; Commission Decision 2002/657/EC.

Key words: Tandem Mass Spectrometry, Chloramphenicol, chromatography, Validation

Study of the removal of emerging pharmaceutical pollutant, by adsorption onto pomegranate peels

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Every year large quantities of pharmaceutical compounds are used in human and veterinary medicine to treat symptoms, diseases and infections. Molecules of these compounds detected in groundwater and even in drinking water, have a harmful effect on human health and on environment. To face this situation of concern, many works are oriented towards the elimination of these emerging pharmaceutical contaminants by several physicochemical treatment processes. In this context, we focus the study on the elimination of a pharmaceutical product, sulfasalazine, by adsorption on a bio-adsorbent which also permitting the valorization of agro-food waste.

The bio-adsorbent is prepared from pomegranate peels. Then a structural and physico-chemical characterization was carried out by various analytical techniques such as: IR spectroscopy, SEM and BET... The adsorption study of sulfasalazine on bio-adsorbent was initiated by a study of the adsorption isotherms (Freundlich, Langmuir and Temkin) followed by kinetic and thermodynamic studies in order to understand the phenomenon of sulfasalazine adsorption on the surface of the bio-adsorbent.

KEY WORDS : adsorption, pomegranate peels, emerging pharmaceutical pollutant, isotherms kinetic; thermodynamic.

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RELATIONSHIP BETWEEN ELECTROCHEMICAL OXIDATION OF 3-(4-FLUOROPHENYL)-2-METHYL-[1,2A] BENZIMIDAZOLO-1,3,5-TRIAZIN-4-THIONE AND ITS ANTIMICROBIAL ACTIVITY

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Due to their chemical structure which includes a carbon-nitrogen double bond and electron-rich substituents, benzimidazole derivatives have significant biological and anticorrosive activities [1,2] Although several studies concerning the structure-activity relationship have been reported by several teams, the mechanism of action of these heterocycles remains to be clarified. We report in the present work, the study of the electrochemical behavior of 3-(4-fluorophenyl)-2-methyl-[1,2a] benzimidazolo-1,3,5-triazin-4-thione, by the approach of cyclic voltammetry with a platinum electrode, to bring clarifications to their antibacterial activities.

Key words: Benzimidazole, single-crystal X-ray diffraction, Cyclic Voltammetry, Antimicrobial activity.

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Development of a RP-HPLC method for the quantification of GZP and ELB in human plasma: Application in a pharmacokinetic study

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Hepatitis C is a contagious liver disease transmitted by blood. Unfortunately, 65 to 85% of patients will progress to chronic infection. Since 2014, several new direct-acting antivirals (DAAs) which selectively target HCV replication have been approved. These drugs allowed shorter treatment duration and impressive cure success rates of around 95%. The combination of Grazoprevir (GZP) and Elbasvir (ELB) is one of the newest therapies that had been shown to be highly effective for the treatment of adult patients chronically infected with genotype 1 or 4 as well as in some challenging cases. Pharmacokinetic evaluations are very requiring in both clinical studies and individual patient cases. Data obtained from such studies are useful to evaluate the efficacy and safety for new drug development and for ensuring the appropriate use of medicines by predicting the influence of pharmacokinetic drug interactions and the contraindications.

The development of a bioanalytical method to measure the concentration of a trial drug in human plasma samples is aiming to support pharmacokinetics evaluation for combination therapies in clinical studies. A chromatographic method for the quantification of GZP and ELB in human plasma is developed. The separation was carried out by using a Waters Spherisorb Phenyl brand column (150 mm x 4.6 mm ID, particle size of 5 µm) maintained at 40°C ± 2°C through which the mobile phase passes at a flow rate of 0.8 mL min^{-1}. The mobile phase consists of a phase A containing 90% acetonitrile and 10% of a 5 mM ammonium formate buffer (+0.1% v/v of trimethylamine, the pH is adjusted to 3.2) and a phase B containing 10% acetonitrile and 90% of buffer. The selected detection wavelength was 215 nm. Quantification is performed by internal calibration and compounds are recovered from plasma by liquid-liquid extraction with ethyl acetate solvent. This method is applied in the context of an in-vivo study of the bioavailability of ELB in rats by LC/MS in order to determine the pharmacokinetic parameters Tmax, Cmax of ELB. The applicability of the developed method for the quantification of ELB in the context of clinical studies has been successfully verified.

Key words: Grazoprévir, Elbasvir, LC/MS, Pharmacokinetic, human plasma

Electrochemical behavior of zinc and cadmium complexes in solution with bidentate organochalcogenophosphorus ligands

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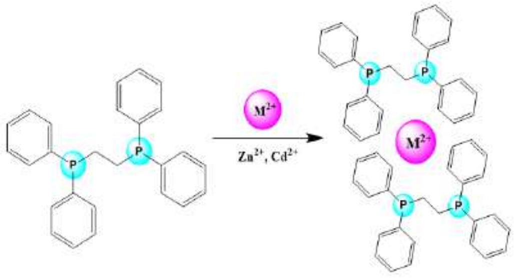
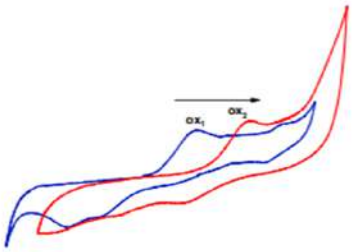
Organophosphorus ligands of the $R_2P(CH_2)_nPR_2$ type are good complexing agents for transition metals [1]. In fact, the complexes formed with the latter are widely used as catalysts and as anticancer agents [2]. This study is devoted to the electrochemical study of the complexation in solution of Zn^{2+} and Cd^{2+} cations with the organophosphorus ligands of type $Et[PPh_2]_2$ (L.1) and its sulfide analogue $Et[P(S)Ph_2]_2$ (L.2). We followed the electrochemical behavior of the two ligands with the latter by cyclic voltammetry. Indeed, the oxidation peak of free L.1 appears at Eox = 0.685 V, while that of the complex of Zn^{2+} and Cd^{2+} appear successively at 1.121 V and 0.966 V. Similarly, we noticed a difference in the electrochemical behavior of L.2, appears at Eox = 1.04 V, while the Eox of Zn^{2+} and Cd^{2+} complexes appear successively at 1.343 V and 1.247 V. By comparing the stability of the complexes with the two ligands, we noticed that they form more stable complexes with Zn^{2+} than with Cd^{2+}.

Key words: 1,2-bis(diphenylphosphino)ethane, metal complexes, cyclic voltammetry, ^1H and ^{31}P NMR





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Physical stability study of candesrtan in co-amorphous system with amlodipine

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Poor water solubility of many drugs has emerged as one of the major challenges in the pharmaceutical world. The crystalline form of a drug offers the advantage of high purity and physical or chemical stability. However the amorphous state that exhibits a disordered structure leads to a higher apparent water solubility, dissolution rate and oral absorption. Amorphization is a well-established strategy to enhance the dissolution properties. Nevertheless, the amorphous state is inherently unstable toward recrystallization. Co-amorphous system of a drug and a small-molecule excipient or of two complementary drug can offer a stability enhancement.

In this work, we study the physical stability of combination between an Angiotension receptor blocker "Candesartan Celexetil" and calcium channel blocker "Amlodipine besylate" obtained by ball milling and quench cooling and characterized using different technique; IR, XRD and DSC. In samples obtained by milling, AMB promotes the amorphization of CDS and impairs its recrystallization under humidity. While heating the co-amorphous system within DSC, a crystallization of co-crystal occurred and melted at a higher temperature in comparison to pure amorphous CDS. Depending on the preparation methods, mechanical process or heating-cooling, the crystallization kinetics might differ, leading to distinct behaviors upon heating on DSC. Milled induced disorder is less stable than that of quench cooling. Furthermore, by involving PVP as third component into CDS-AMB system, a shift of glass transition temperature toward higher temperature is exhibited and the cold crystallization event is disappeared. The higher PVP content results in stronger interaction leading to more stable association. This research can open the path to improve the development of CDS and AMB fixed-dose combination as generic formulation with enhancing delivery and reducing dosage of such poorly soluble drugs to get better curative benefits.

Keywords: Anti-hypertensive Drugs, FDC, Physical stability, co-amorphous, ball milling, Quench cooling

Miniaturised liquid phase extraction of butyl and phenyltins in sediment samples using Deep eutectic solvent: Optimisation and HPLC-ICP-MS analysis

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Organotins are persistent organic pollutants that were used to be of high importance as biocides in polymers and antifouling agents in ship paints. However, due to their toxic effects, bioaccumulation and endocrine disrupting properties, their extensive application has been banned. However, due to their persistence nature, traces of organotins are still present in the environment especially in sediments. In the present study, A rapid and environmentally friendly analytical method was developed for simultaneous extraction of tributyltin (TBT), diphenyltin (DPhT), dibutyltin (DBT), monophenyltin (MPhT), monobutyltin (MBT) and triphenyltin (TPhT) s from sediments. The extraction efficiencies of hydrophobic deep eutectic solvents were investigated. and the extracted organotins were quantified using high-performance liquid chromatography–inductively coupled plasma-mass spectrometry (HPLC-ICP-MS). The experimental parameters affecting the extraction process were optimized using response surface methodology. Under optimized conditions, the limits of detection and limits of quantification ranged from 0.2 -1.1 ng g^{-1} and 2.3-6.0 ng g^{-1} respectively. The accuracy expressed in the form of percentage recoveries ranged between 89.2 % and 105 %. The developed extraction method was applied for the extraction of organotins in freshwater and seawater sediments. The results obtained demonstrated that TBT and TPhT were present in seawater sediments.

Key words: Deep eutectic solvents, high performance liquid chromatography, organotins, tributyltin

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Adsorption of Erythromycin from aqueous solution using Tunisian clay materials - Effect of operating parameters

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Nowadays, all the countries of the world are aware to protect the quality of the environment, as many studies have been carried out to find economically, socially and environmentally viable solutions. Our work is part of this context, which aims to investigate the capacity of raw Tunisian clays to remove the residues antibiotic drugs used for human and veterinary from wastewater. In this study, batch equilibrium experiments were conducted to explore the efficiency of the sorption behavior of Erythromycin (ERY) molecule from aqueous solution. The optimum conditions for ERY removal were established such as contact time, the effect of pH and the varying of the concentration. The results claim that the pH =5 was optimum for the highest ERY removal, the highest removal efficiency R% = 39.8% and the equilibrium for the contact time is reached at 45 min. Additionally, Freundlich model was best fitted to ERY sorption data (R2 = 0.9872) and the ERY adsorption kinetics on the natural clay follows the pseudo-second order kinetic model.

Key words: Adsorption, Antibiotics, clay, Kinetics, Isotherm.

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Effect of pore formers on the morphology and the proprieties of Recycled Low Density Polyethylene flat sheet hydrophobic membranes

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Recycled Low Density Polyethylene (R-LDPE) hydrophobic membranes were prepared using thermally induced phase separation (TIPS) method, thus helping to lighten plastics load on the environment. Butyl acetate (BA) was used as solvent which is more sustainable solvent, Hexane as a non-solvent. In this study, the effect of pore formers on the proprieties of the flat sheet membrane was investigated. Moreover, three different additives: LiCl, PEG and alumina were used as pore-formers in order to improve polymer processability. Therefore, we are interested to see how this parameter affects the proprieties of the membrane. The crystalline property of the polymer was studied via Fourier transform infrared spectroscopy (FT-IR) in hopes of revealing differences in functional groups between the various membranes. In addition, the characterization of the obtained membranes was carried out in terms of thickness, contact angle, pore size, porosity, mechanical test, bubble point pressure. The microstructure of the obtained membranes was analyzed by scanning electron microscopy (SEM). It has been noticed that the addition of PEG and LiCl pore formers had an important role in improving the porosity and decreasing the contact angle. Although, the results of R-LDPE membrane revealed good porosity, more hydrophobic and improving the mechanical properties when LiCl used as pore former.

Keywords: Recycled Low Density Polyethylene; membrane; hydrophobic; pore formers; TIPS

Interaction natural pigments-clay by solid-state reaction.

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The aim of this study was to synthesize new colored hybrids based on Tunisian purified clay and natural powders of flowers: *Malva sylvestris, Chrysanthemum coronarium, Silene dioica, Anagallis monelli, Pelargonium x hortorum*. The identification of floral pigments in Tunisian flowers was studied. The chlorophylls (a and b), total flavonoids (TF), total phenolic compounds (TPC), and carotenoids have been analyzed using UV-Vis spectrophotometry and high-performance liquid chromatography (HPLC-DAD). In addition, the antioxidant capacity was determined by using the oxygenated radical absorption capacity assay (ORAC) and the antioxidant power to reduce ferric ion assay (FRAP)**.** The properties of the studied clay have been evaluated by using pharmaceutical and microbiological tests. The colored hybrids are prepared by solid-solid reaction and analyzed using X-ray diffraction (XRD) and Fourier transform infrared (FTIR). The chlorophyll a is present in large quantities in the *Malva* flower which presents the lowest antioxidant capacity. Chlorophyll b, and the TPC are more abundant in the *Pelargonium x hortorum.* The TF appeared in high quantities in the *Anagallis* flower. The carotenoids present the highest value in *Chrysanthemum* flower. The results of the clay characterization justify its use as pharmaceutical and cosmetic agents. The colored hybrids obtained by green synthesis can be used as biocosmetic products.

Keywords: floral pigments; clay; green synthesis; colored hybrids.

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Chemical and Fatty Acid Composition of Crude and Purified Extracts Obtained from Datura innoxia Seeds Extracted with Different Solvents

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Oils play a key role as raw materials in a variety of industries. The aim of this study was to evaluate the potential of Datura innoxia seed oil cultivated in Tunisia for industrial purpose and to study the effects of hexane, chloroform, and isopropanol as extraction solvents on the compositions of the extracts. The results showed that the hexane and chloroform extracts were mainly neutral oils which were rich in linoleic (≈46%) and oleic (≈31%) acids. However, the isopropanol extract contained large amount of neutral oil and organic acids. Neutral oil contained mainly palmitic acid (40.2%) and some important and valuable epoxy (15.4%) and cyclopropane (13.2%) fatty acids. Analysis of the sterol and tocopherol levels of the crude and purified oil extracted revealed that they were significantly affected by the extraction solvent used.

Key words: seed oil, extraction, tocopherol

Photonic materials in environmental applications

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The contamination of environmental compartments due to industrial activity is an issue of concern, the removal of these pollutants being an area of intensive research in the last decades. On the one hand, the use of sorbent materials for the retention of pollutants is an alternative, while photocatalysis is also suitable for removing organic compounds from water and air by harvesting sunlight. In this sense, TiO_2 semiconductor is a reference catalyst active in photocatalysis, which benefits from the advantages of low cost, high activity, stability, and non-toxicity **[1]**. The use of nanocomposite materials prepared by combining polymers and nanoparticles is a good alternative for the degradation of organic compounds [2].

In this context, this study describes the modification of conventional paper with polyamide-TiO_2 nanostructures combined with plasmonic nanoparticles to form nanocomposite materials which depicts both sorbent as well as photocatalytic activity. Until now, we have investigated the photocatalytic activity under sunlight irradiation and the role of different components with two model analytes, i.e., methyl orange and crystal violet, observing that the extraction capability of the materials for their use as sorbent is provided by the polymer, while the presence of the semiconductor nanoparticles enables further photocatalytic activity, which can be combined for decoupling the extraction under dark conditions and the subsequent degradation of the dyes under sunlight. In this sense, the reusability of the nanocomposite paper substrate upon modification with the photonic materials has been evaluated as compared to polymeric modified paper.

Key words: Photocatalysis, TiO_2 nanoparticles, plasmonic nanoparticles, polymers/cellulose, dyes

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Eco-friendly Esterification of carboxylic acids via dimethyl carbonates catalyzed by ferric salts

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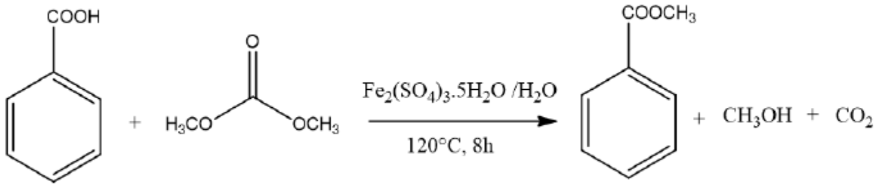
Esterification reaction is very widely used in the industrial applications. However, there is a great need to versatile and simple processes that can reach higher yields by the greener means.

Hence, we have initiated a method to develop a new methylation reaction that relies upon safe, green reagents such as dimethyl carbonate (DMC) [1], which is regarded as an environmentally friendly alternative for methyl esterification in stead of methanol [2].

An ecological esterification of carboxylic acids in which $Fe_2(SO_4)_3.5H_2O$ [3] is used as green catalyst due to their benefits for the environment, human health, and safety.



Key words: green chemistry, esterification, dimethyl carbonate, iron-based catalyst.

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Amine treated *Phragmites australis* based beads for simultaneous removal of hazardous Congo Red and Cr(VI) from aqueous solutions

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In the present study, pentaethylenhexamine (PEHA) modified *phramites australis* based beads (BPA-M) were developed as a potential biosorbent for the simultaneous adsorption and regeneration of Congo Red (CR) and Hexavalent Chromium Cr(VI) from aqueous solutions.
Beads based on *Phragmites Australis* (BPA) were prepared using the Boubaker et al method [1, 2]. The dependency of Cr(VI) and CR adsorption efficiency on the variables such as pH, initial pollutants concentration, and contact time was studied by central composite design (CCD) coupled with response surface methodology (RSM). The characteristics of BPA-M before and after adsorption have been widely evaluated by FTIR and SEM/EDX. This study showed that the most favorable conditions for the simultaneous elimination of Cr(VI) and CR were the following: pH 4.5, 30 mg L^{-1} for Cr(VI), 40 mg L^{-1} for Congo Red and a contact time of 120 min with a mass fixed by 1 g L^{-1} and temperature fixed by 25°C with a maximum adsorption percentage of 96.34% for CR and 83.95% for Cr(VI). The thermodynamic results revealed that the simultaneous adsorption of CR and Cr(VI) was spontaneous, physical and endothermic with increased randomness at the solid/liquid interface. The study of the equilibrium isotherms showed that the Sips model corresponded well to the experimental data, which reflects the heterogeneous nature of the BPA-M surface. Adsorption-desorption experiments revealed that BPA-M could be reused for up to ten cycles with constant percentage recovery values.

Key words: Beads based on *Phragmites Australis*, Amine treated, simultaneous adsorption, Congo Red, Hexavalent Chromium, regeneration

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Kinetics of palm by-product fermentation using Kombucha starter culture

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The date palm is the main wealth of southern Tunisian. It offers a wide range of agricultural by-products consisting mainly of cellulose, hemicellulose, lignin and sugar. This waste could be used in many industrial and biological processes. This work aims to study the fermentation of palm by-products. Fermentation was done following the Kombucha production procedure. The crushed by-product left to infuse for 15 min at 80°C. After cooling, the infusion is inoculated with 20 g of SCOBY culture and fermentation was carried out at 25°C for 15 days. All fermentations were performed in duplicate. The final biofilm was weighed (14g). The pH values of the samples were measured using an electronic pH meter. The results showed that the pH value goes from 6.7 to 2.7. This is due to the increase in acidity by organic acids derived from bacterial metabolites. HPLC analyzes were used to determine fermentation kinetics.

Key words: date palm, Fermentation, Kombucha, HPLC.

Development and characterization of new packaging film based on vegetable and active essential oil and organoclay

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In addition to their use in food, vegetable and essential oils have always found applications in several fields such as cosmetics [1], paint [2] and biofuels [3]. Recently, they have been used in the development of composite packaging materials [4]. However, poor mechanical properties and water/gas barrier properties remain the main obstacles to the development of bio-based materials. In this work, new composite films based on active natural extracts were synthesized by in-situ intercalation polymerization in organoclay layers. The synthesized composite films are characterized by various techniques such as thermal gravimetric analysis (TGA), differential scanning calorimetry (DSC), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM). Water and gas barriers, surface and mechanical properties of the composite film and antioxidant activity were tested.

Keywords: film-packaging, organoclay, vegetable and essential oils, antioxidant.

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Semicrystalline Copolymers based on Polycaprolactone and Polyisosorbide: Synthesis, Characterization, and Degradation

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During the past decades, the quest for sustainable chemicals, polymers, and materials has intensified. Recently, interest has focused on the use of isosorbide and its polymers as substitutes for fossil-based materials [1]. In this regard, a series of newly designed block copolymers based on two biodegradable polymers, poly(ε-caprolactone), PCL, and poly(isosorbide), PIS, with PIS fractions of 5, 10, 25 wt%, are studied here. The aim is to evaluate the effects of the amorphous PIS phase on the properties of semi-crystalline (majority) PCL. The synthesis strategy implies the polymerization of caprolactone onto initial PIS of low molar mass, yielding gradually shorter PCL blocks when increasing the starting amount of PIS. A comprehensive evaluation of degradation in phosphate buffer solution (PBS) and enzymatic environment indicated that the insertion of PIS prepolymer into the PCL chain promotes noticeable degradation in the presence of enzymes, resulting in a weight loss up to 21%, after only 20 days, for the PCL(75%)_*b*_PIS(25%) copolymer. Based on the results obtained in this work, these biodegradable block copolyesters were found to be ideal materials in which physical properties and biodegradation rates can be tailored to fit particular applications.

Key words: poly(*ε*-caprolactone), poly(isosorbide), block copolymers, (bio)degradability

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New polymeric adsorbents for benzene derivatives removal in wastewater

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Benzene derivatives are the most important organic water pollutants. [1] They are discharged in the liquid effluents from domestic, industrial, and agricultural activities. [2] These chemical compounds are the major hazardous wastes and have been enlisted by European Union and U.S Environmental Protection Agency (USEPA), [3] because of their high toxicity even at low concentrations, poor degradability and high reactivity causing several health problems for humans and aquatic organisms. [4, 5] Therefore, the elimination of these pollutants from wastewater constitutes a major challenge. In this context, we have focused our efforts on optimizing adsorption process by development of new aromatic polymers derived from biobased byproducts for high adsorption efficiency of organic pollutants

The aim of this study is to design triazole-containing pyridinic polymers as new synthetic adsorbent phases for pollutants removal in water. The obtained polymers were fully characterized using NMR spectroscopy, GPC, DSC and ATG. Their uptake performance to eliminate organic compounds was determined using High performance liquid chromatography (HPLC).

Key words: Benzene derivatives, adsorption, pyridine, biosourced

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On the way to greener furanic-copolyesters:
Synthesis, properties, water Sorption study and degradation behavior

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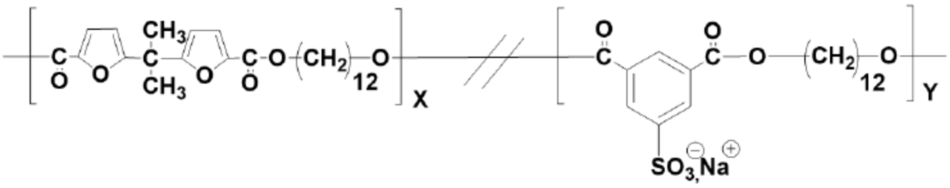
The intensive use and production of conventional polymers of petrochemical origin have enhanced the greenhouse effect and "white pollution", which has attracted increasing public attention [1]. Furans from biomass origin are considered as key chemicals to ensure the sustainability of the polymer industry [2]. Over the last decades, our laboratory has been engaged in the preparation of polyesters from biobased monomers bearing the furan heterocycle into their backbone through polycondensation, of ethyl 5,5'-Isopropylidene bis (2-furoate (DEF) from ethyl 2-furoate [3]. In this work, we propose to study the synthesis and properties of a new biobased copolyesters containing in their structure's furan rings and ionic groups through a very long chain aliphatic diol, dodecan-1,12-diol. The verification of their structure is carried out by IR-TF, RMN^{1}H, RMN^{13}C. Liquid water sorption, hydrolytic degradation and crystallinity are studied in order to evaluate their potential applications.



Key words: Dodecandiol, Ionic Copolyesters, Degradation

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Effect of the polyaniline solvent on the properties of cellulose–PAni composites

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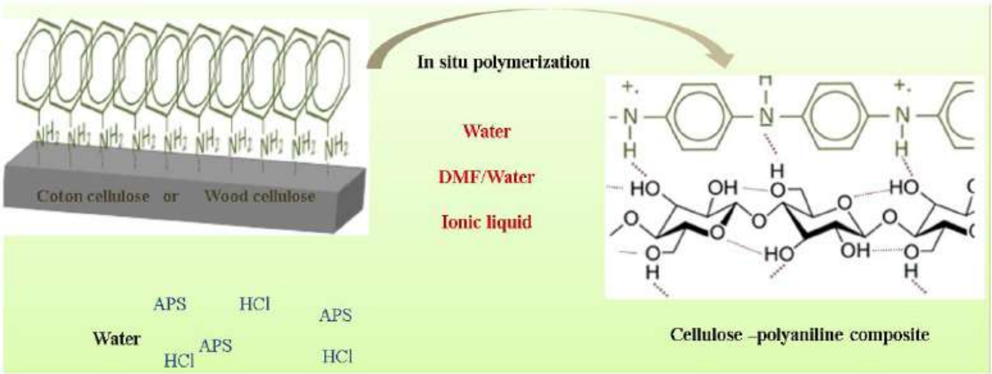
The properties of cellulose-polyaniline composites are strongly linked to several factors. This study deals with the effect of the solvent and the cellulose crystallinity on the cellulose-polyaniline composite properties. The composites were prepared using a simple *in situ* oxidative polymerization of aniline in the presence of commercial cotton cellulose fibers and cellulose fibers extracted from wood. Three solvents were used: water, ionic liquid or N, N-dimethylformamide (DMF).

The morphological study of composites was studied by scanning electron microscopy. Elemental analysis was determined by EDX. The XRD was used to measure the crystallinity of cellulose. The thermal stability of composites was checked by thermo-gravimetric analyzes. The measurement of electrical conductivity was performed using the four points technique.

The electrical conductivity measurements and the elemental analysis show that the higher the nitrogen content in the composite, the greater the electrical conductivity. The best conductivities were obtained when the DMF/water mixture was used.

Keywords: Cellulose, polyaniline, ionic liquid, conductive composite.



Development of bio-based, chemical resistant, and semi-crystalline polyesteramides derived from FDCA and 5,5′-isopropylidene bis(2-furfurylamine)

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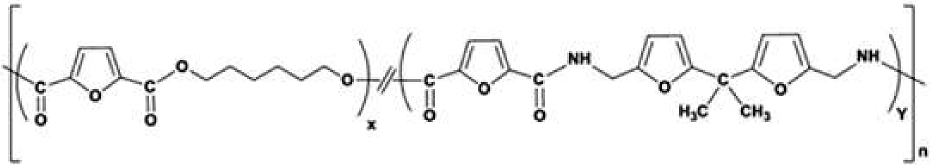
The quest for biobased polymers with enhanced thermal and mechanical properties, along with chemical stability, has witness the interest on polyesteramides, including those based on furans. However, the incorporation of 2,5-furandicarboxylic acid (FDCA)[1] or furan diamines[2] in such kind of polymers has been never reported before. In this work, we report a new series of bio-based polyesteramides from FDCA and 5,5′-isopropylidene bis(2-furfurylamine) (DAF) synthesized by a bulk polycondensation. The incorporation of DAF units significantly improved the thermal properties of the linear polyesteramides with FDCA units and endowed them with chemical resistance properties towards hydrolytic and oxidative conditions. Furthermore, these polyesteramides were semi-crystalline displaying a glass transition and a melting temperature of up to 28 and 136 °C, respectively, thus opening new perspectives for the preparation of high-performance polymers suitable for high-tech applications.



Keywords: bio-based polyesteramides, bulk polycondensation, degradation.

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High photocatalytic activity of wide band gap oxide nanoparticles induced by structural defects

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ZrO_2 nanoparticles were investigated for the photodegradation of formic acid under UV irradiation for the first time. The aerogel photocatalysts were prepared by an efficient sol-gel method and calcined at different temperatures. The samples showed the introduction of intermediate states in the wide band gap of ZrO_2, which may explain its photoactivity. These intermediate states are related to structural defects on the surface of the catalyst. It has been shown that photocatalysts calcined at lower and higher temperatures are the most efficient. This catalytic activity is mainly governed by the propensity to form structural defects whose density is partially controlled ; by the ability to form high surface area ZrO_2 nanomaterials by a new preparation method using supercritical conditions, and by the nature of the ZrO_2 phase involved. Thus, this study shows that proper preparation of oxide materials allows fine-tuning of the creation of bandgap intermediate sites by thermal post-treatments, rendering ZrO_2, a wide bandgap material, capable of photocatalytic operation under UV irradiation.

Key words: Wide band gap photocatalyst, mid-gap, structural defects, aerogel.

Synthesis and Characterization of Novel Thermotropic Liquid Crystalline Poly(ether-ketone)s Based on Cyclopentanone Moiety

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A series of poly(ether-ketone)s based on cyclopentanone moiety were synthesized from *2,5*-bis(3-ethoxy-4-hydroxybenzylidene)cyclopentanone and various dibromoalkanes by solution polycondensation technique. *FT-IR*, ^{1}*H-NMR* and Mass Spectroscopy were used to characterize the structure of the new monomer and poly(ether-ketone)s. The resulting polymers had inherent viscosities in the range of *0.69-1.12 dl/g* and the obtained polymer is easily soluble in aprotic organic solvents. Thermogravimetric analysis *TGA*, differential scanning calorimetric *DSC* analyses were made for all the synthesized polymers in order to study their thermal behaviour and liquid crystalline properties. The temperatures of *10%* weight loss occurred above *295 °C*, and the glass transition temperature T_g was in the range of *58-113* °C. *DSC* profiles of poly(ether-ketone)s with aliphatic spacer length *6,8* and *10* revealed both melting transition T_m and isotropization transition T_i peaks. It implies that these polymers exhibited thermotropic liquid crystalline behaviour. Polarised optical microscopy *POM* study confirmed the liquid crystalline characteristic of these polymers. Schlieren textures with some pores at *189* ºC (*Ti*) were visually observed under *POM*.

Keywords: thermo tropic liquid crystal, poly(ether-ketone)s, flexible spacers, polycondensation, polymerization.

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Study of the Effect of Solvation on the Formation and the Mobility of TTAB Micelles

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The conductivity of TTAB cationic surfactant: Tetradecyltrimethylammonium Bromide ($C_{17}H_{38}NBr$) in aqueous solution, was measured at 25°C and 1atm, in a large range of concentration: $1.2 10^{-3}$ $mol.l^{-1}$ $C°_{TTA^+} \leq 2.5 10^{-2}$ $mol.l^{-1}$.

Above the critical micellar concentration CMC H 3.62 10^{-3}M, $[(TTA^+)_{Zs}]^{Zapp}$ micelles are formed. TTAB aqueous solution is therefore an ionic mixture of free counterions Br^-, free monomers TTA^+, and micelles of apparent charge number $Z_{app} = Z_S$(〈 - ®)/(1 - ®), where Z_S is the structural charge number (=73), (1- 〈) the degree of the ionic condensation and (1-®) the degree of micellisation.

Experimental results were analyzed according to a proposed coherent model[1], based on the electro neutrality, the mass-action law, and on a generalization of the Fuoss ionic-association model[2] and of the Onsager–Kim–MSA conductivity theory of mixed electrolytes[3], in order to determine Z_{app}, α and β and to evaluate the electrophoretic and ionic relaxation friction effects on all the ionic species. The weak dielectric friction effect on micelles is also determined[4].

On the other hand, the equivalent conductivity at infinite dilution $\lambda°_{TTAB}$ of micelles is obtained by *adjusting*, at each concentration, the theoretical specific conductance to its corresponding experimental value.

From $\lambda°_{TTAB}$, we calculated the hydrodynamic stokes radius R_{app} of the micelles after taking into account the dielectric correction. This radius allows evaluating the number of water molecules N_{H2O} in the first shell of solvation around the $[(TTA^+)_{Zs}]^{Zapp}$ micelles.

The results are: 22.08 $Z_{app} \leq 23.02$; $\lambda°_{TTA^+}$ = (19.1 ± 1.8); $\lambda°_{TTAB}$ = (75 ± 3) $S.cm^2.equiv^{-1}$.

R_{app} = (24.1 ± 0.9) A°, and $N_{H2O} \approx 357$.

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Molecular Modeling of Reactivity in Organic Chemistry: A DFT Study of the Diels-Alder Reactions between 2,5-Dimethylfuran and ethylene: Thermodynamic and kinetics Analysis

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The promising potential of using biomass as a renewable resource to reduce dependence on petroleum-based resources has wetted considerable attention in terms of developing sustainable processes for the production of sustainable aromatic chemicals, such as p-xylene (PX), a basic chemical precursor for the synthesis of terephthalic acid (TA), mainly derived from petrochemicals [1]. As an alternative to the conventional petrochemical route, a biomass-based route has been demonstrated to display a very high potential for the production of renewable PX. It consists of a Diels-Alder (DA) reaction between a bio-based diene such as 2,5-dimethylfuran (2,5-DMF) and as ethylene, with subsequent dehydration. This reaction has been extensively studied, both experimentally and using quantum chemical modeling [2]. In particular, frontier molecular orbital (FMO) theory and density functional theory (DFT) have been used to explain the reactivity, the reaction mechanism, and the selectivity of for this type of reaction. In this seminar, I will present A DFT study of the solvent effects on the thermodynamics and kinetics of the uncatalyzed and Lewis acid-catalyzed DA reactions between 2,5-DMF and ethylene [3].

Key words: Biomass, 2,5-dimethylfuran, Diels-Alder Reaction, DFT calculations.

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Modeling of Ionic Condensation and Solvation of SDS micelles from semi-analytical calculations of Radial distribution Functions

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Above the critical micellar concentration CMC H 8$10^{-3}$M, $[(DS^-)_{Zs}]^{Zapp}$ micelles are formed. Sodium dodecyl sulfate (SDS) in aqueous solution is therefore an ionic mixture of free counterions Na^+, free monomers DS^-, and micelles of apparent charge number: Z_{app} = Z_S(〈 - ®)/(1 - ®), where Z_S is the structural charge number (=54), (1- 〈) the degree of the ionic condensation and (1-®) the degree of micellisation.

In previous works, we proposed a coherent simple model[1], based on the electro neutrality principle, the mass-action law, and on a generalization of the Fuoss ionic-association model[2] taking into account all the MSA cross charge-radius corrections, in order to determine Z_{app}, 〈 and ®. However, this model considers the solvent as a dielectric continuum.

We present in this work a new semi-analytical molecular statistical approach in order to describe thermodynamically both the phenomena of ionic condensation and solvation of SDS micelles. It consists in the calculation of respectively the counterion-micelle radial distribution function $g_{mic\text{-}Na}{}^{+}$(r) and the H_2O-micelle- radial distribution function $g_{mic\text{-}w}$(r) in solution, and then the number of water molecules N_{H2O} into the first solvation shell of micelle.

The approach needs the determination of the Potential of Mean Forces, PMF ($W_{mic\text{-}Na}{}^{+}$; and $W_{mic\text{-}w}$) by resolving the BBGKY integral hierarchy equation[3].

It was done by transforming BBGKY to a relatively simple differential equation analogue to the linear Boltzmann-Debye equation, which takes into account the co-volumes[4] of the different species, the local polarization of solvent molecules and therefore the variation of the permittivity around the micelles[5]. Integration of $g_{mic\text{-}Na}{}^{+}$(r) and $g_{mic\text{-}w}$(r) functions allows to obtain (1- α), Z_{app}, and N_{H2O}.

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Theoretical evaluation of the performance of photovoltaic cells based on crown ether porphyrins and phthalocyanines: Determination of optoelectronic properties

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The density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations have been performed for the estimation of different key parameters governing the intramolecular charge transfer (ICT) and photo-injection processes for photovoltaic devices such as frontier molecular orbital analysis (FMOs) [1], maximum absorption (λ_{max}) [2], density of states (DOS), charge transfer dipole (μ_{CT}) and open-circuit voltage (V_{oc}) [3] were calculated to evaluate the performance of a serie of phthalocyanines and porphyrins . Our computational findings revealed that all calculated energy gap values are lower than 3.5 eV. Better optoelectronic properties are achieved from ZnPrO4 with a highest value of LHE [4]. Besides, a remarkable jump in the amount of charge transfer q_{CT} values going from $ZnPcO_4$ to $ZnPrO_4$.

Keywords: Porphyrins, phthalocyanines, BHJ solar cells, density functional theory, electronic and optical properties

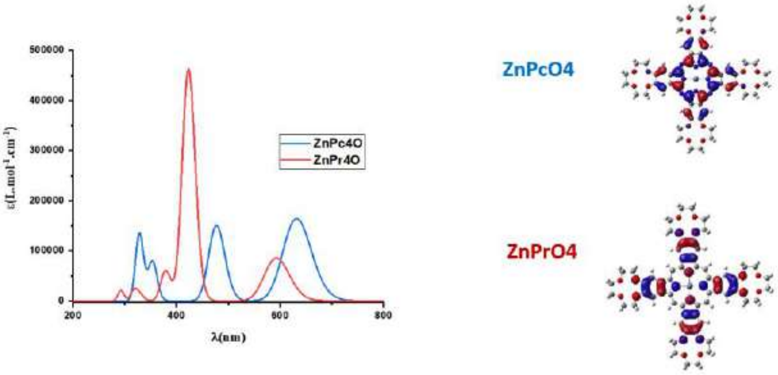

Fig. UV/vis absorption spectra of ZnPcO4 and ZnPrO4 as simulated at the TDDFT/B3LYP/ Def2-TZVP level of approximation

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Influence of Dielectric friction on the dependency of the Mobility of Carboxymethylated cellulosic chains with the nature of their counterions.

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We present a new general modelling of different carboxymethylated cellulosic polyelectrolytes XCMC of various degrees of substitution DS, in water at 25°C, in order to interpret the dependency of their conductibility, with their alkali counterions ($X \equiv Li^+$, Na^+, K^+ and Cs^+) in a concentration range between $5\ 10^{-4}$ to $5\ 10^{-2}$ equiv l^{-1}.

Coiled CMC chains are represented by a general ellipsoidal configuration. For stretched chains, we compare Manning's corrected model[1] to the Pearl-Necklace-like chain model[2]. The first model assumes polyelectrolyte chains as an infinite electric charged thread, with linear charge density equal to $e/b_S = (|Z_S| e/L_S)$; $|Z_S| = 750$ and $L_S = 3877$A° are respectively the structural charge number and length. In the second model, chains are assumed as a succession of $|Z_S|$ electrical charged groups or N_b blocks enclosing DS groups.

Calculation for each model of the degree of counter-ion condensation, and hydrodynamic, electrophoretic, ionic relaxation and dielectric friction effects, allows the comparison between experimental[3-4] and calculated[5] conductivities of KCMC, NaCMC, LiCMC and CsCMC aqueous polyelectrolytes.

The main conclusions of this study are: - 1/ The stretched chain configuration is predominant. - 2/ The Manning's model cannot fit completely the experimental data; - 2/ The degree of ionic condensation is quasi constant, independent on the nature of the counterions X, but it increases with DS; – 3/ Electrophoretic friction is important; it varies slowly with DS and not with X. However, the ionic relaxation friction effect is always about 12%; - 4/ The dielectric friction effect varies between 25% to 60% depending on DS and the nature of the counterions.

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Complexation of polyelectrolytes in aqueous solution. Application to wastewater treatment.

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In this work, the electrostatic complexation of strong polyelectrolytes (PEs) in aqueous solution was studied as a function of different parameters, such as the chemical charge density of the polyanion, hydrophobicity, the chain length of both polyelectrolytes and the polymer concentration. Two PE systems were investigated and characterized by a set of complementary experimental techniques, namely DLS, zetametry, ITC, viscometry and SAXS. A first system consists of a hydrophilic polycation, PDADMAC, and a hydrophobic polyanion, PSSNa (or P(St-co-SSNa)), prepared at different sulfonation rates and adopting a pearl necklace conformation in aqueous solution at intermediate sulfonation rates. A second system consists of the hydrophilic PDADMAC and a hydrophilic polyanion, PAMAMPS (or P(AM-co-AMPS)), at different chemical charge densities. Concerning the PSSNa – PDADMAC complexes, it was put forward that: i) the strength of the electrostatic interaction between PSSNa and PDADMAC overcomes the hydrophobic effect responsible for the formation of pearls, therefore all the anionic charges of PSSNa are accessible to complexation whatever the rate of sulfonation of the latter and the stoichiometry of the system is equal to 1 ; ii) the complexation of PSSNa by PDADMAC is a two step process: the formation of small (~ 50 nm) primary complexes firstly (exothermic reaction), followed by the aggregation of these primary complexes to form larger secondary complexes (endothermic reaction) ; iii) complexation is favored and colloidal complexes are more stable as a strong chain size dissymmetry is exhibited between the two PEs, i.e. when the titrated PE (PSSNa) has longer chains than the titrating PE (PDADMAC). For the PAMAMPS – PDADMAC system, it was suggested that : i) a colloidal complex formation step takes place prior to (or even concomitantly with) a coacervation step and the overall complexation reaction between PAMAMPS and PDADMAC is endothermic, indicating that the system is weakly interacting ; ii) the chemical charge density of PAMAMPS has no significant effect on the complexation stoichiometry (~ 1.4), neither on the sizes of the complexes. On the other hand, the potential application of the resulting polyelectrolyte complexes in environment and particularly for the retention of dyes and heavy metals in contaminated water was highlighted, due to the possibility of incorporating the contaminant into the polyelectrolyte complexes, of a relatively big size, being an advantage point of vue application.

Keywords: polyelectrolytes ; polyelectrolyte complexes ; pearl necklace conformation ; hydrophobic/hydrophilic ; colloids ; coacervates ; contaminant removal/retention.

Glyphosate Dimers: Structure, Stability and Solvation effects.

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We report a study on different ionization states and conformations of the glyphosate (N-phosphonomethylglycine) dimer system by means of quantum mechanical calculations. Optimized geometries for energy minima of the glyphosate dimer, as well as relative potential and free energies are computed in the gas phase and in aqueous solution. The density based solvation model (SMD) is employed to account for solvation effects. Energy calculations were done at B3LYP-D3/6-311++G(2d,2p) level. Ionized forms (anion/cation and either zwitterion–zwitterion or neutral–zwitterion) of the glyphosate dimer are predicted to exist in the gas phase and in aqueous solution, in contrast to glyphosate monomers [1]. In aqueous solution, the dimerization of glyphosate is found to be an exergonic process (ΔG_s=-8.6 kcal.mol^{-1}). Our computations predict that zwitterion-zwitterion glyphosate dimers might be abundant in supersaturated glyphosate aqueous solutions.

Key words: Glyphosate, Structural analysis, Dimerization, DFT, Empirical dispersion correction, SMD Solvation Model

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Surface and Calorimetric Behavior of N,N-Dimethylacetamide with n-Alkanols and 2-Alkanols

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The surface tension at the liquid-air interface of n-alkanols (from methanol to 1-pentanol) and 2-alkanols (from 2-propanol to 2-pentanol) was studied at three different temperatures (283.15, 298.15 and 313.15 K) and a pressure of 0.1 MPa. Surface tension deviations were also calculated. Moreover, the excess molar enthalpies for these mixtures were measured at T=298.15 K and a pressure of 0.1 MPa. The surface tension deviations are found to be positive for the system containing methanol, sigmoidal for the ethanol and negative for the rest of the alkanols. With regard to excess molar enthalpies, negative values are found for the system containing methanol, sigmoidal values for ethanol, and positive values for the rest of the alkanols.

Key words: Surface tension deviation, Excess molar enthalpy, n-Alkanols, 2-Alkanols, N,N-Dimethylacetamide.

A theoretical investigation of the rate constant of trichloroethylene reaction with O(^{3}P) over the range of temperature 285-1035

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There is a considerable demand for alkenes in a variety of daily life domains. In the atmosphere, alkenes can react with different reactants such as OH, Cl and O(^{3}P) [1]. For instance, the reactions of O(^{3}P) with chlorinated alkenes such trichloroethylene (TCE) are dangerous and highly toxic pollutants [2, 3]. The reaction of TCE with O(^{3}P) has a very complex multichannel mechanism [4-6]. So, the kinetics of this reaction is of importance to the specialized readership. Using CBS-QB3 method, we have calculated rate constant for the entitled reaction over a range of temperature 285-1035 K to be compared with the experimental outcomes.

Key words: CBS methods, Halogenated alkene, Rate constant, O-addition, H-abstraction.

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Program of
Tuesday 20
December 2022

Synthesis, biological activities and molecular docking studies of [1,2,4]triazolo[4,3-*b*][1,2,4,6]thiatriazine-1,1-dioxides

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A new series of [1,2,4]triazolo[4,3-*b*][1,2,4,6]thiatriazine-1,1-dioxides (**3a-g)** were synthesized, characterized, and evaluated for their acaricidal activity against the larvae and adults of *H. scupense.* The title compounds were obtained via the reaction of *N*-alkyl(aryl)-*N′*-(4*H*-1,2,4-triazol-3-yl)amidines and sulfuryl chloride in the presence of pyridine. The structure of the synthesized compounds was confirmed by FTIR, ^{1}H and ^{13}C NMR, and mass spectra and elemental analyses. Adult immersion test (AIT) was performed to determine the mortality of ticks and inhibition of oviposition and hatching after application of these compounds. Larval packet test (LPT) was performed on the larvae produced from the collected ticks. All tested compounds displayed a potent acaricidal activity. Among them, 2-benzyl-3-phenyl-2*H*-[1,2,4]triazolo[4,3-*b*][1,2,4,6]thiatriazine 1,1-dioxide **(3d)** showed the most potent ixodicide activity with an LC50 value of 0.19 mg/mL against 0.06 mg/mL for the standard drug amitraz. Furthermore, after 24 h of exposure, this compound caused a high mortality on *H. scupense* larvae, as it induced 100% mortality at the highest tested concentration (1 mg/mL). Molecular docking was investigated to determine the interaction between compound (**3g**) and eight crystal structures of bacterial and yeast proteins associated with virulence activity and antimicrobial resistance (figure 1).

Key words: Triazole, amidine, molecular docking, acaricidal effect, dioxide

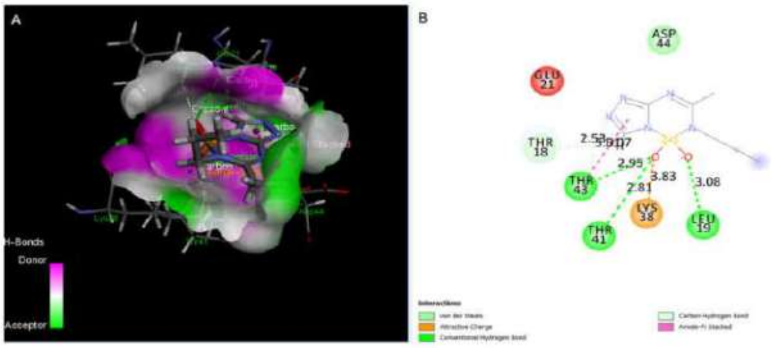

Figure 1. Discovery studio visualization of 3D and 2D of the interaction of TetM-mediated tetracycline resistance (3J25) with compound (**3g**).

Oxazolo[5,4-*f*]quinoxaline-type selective inhibitors of glycogen synthase kinase-3α (GSK-3α): Development and impact on temozolomide treatment of glioblastoma cells

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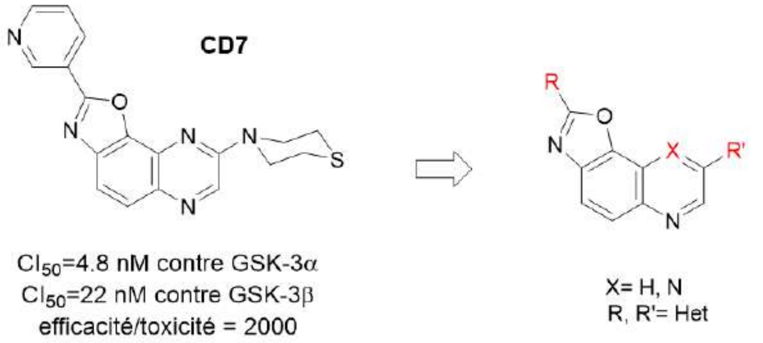
The serine/threonine kinase glycogen synthase kinase-3 (GSK-3) functions in wide range of cellular processes. It is therefore implicated in many human pathologies including diabetes, bipolar disorder, schizophrenia, Alzheimer's, Parkinson's diseases, cancer, and others[1]. However, two isoforms exist namely GSK-3α and GSK-3β and they don't play the same roles in these processes. Here we report the synthesis, design and evaluation of a novel series of inhibitors of the α-isoform of GSK-3. The starting point of these studies was an oxazolo[5,4-f] quinoxaline CD-07, which was previously identified by our group as a selective inhibitor towards the α isoform of GSK-3 (with IC 50 of 4.8 nM and 22 nM against GSK-3α and GSK-3β, respectively)[2]. Analogues of CD7 that could increase affinity for GSK-3α were designed through docking studies in a model of GSK-3α. By taking account of the suggested structural modifications, we prepared derivatives of the heterocycle oxazolo[5,4-f]quinoxaline that were evaluated for their activity on a panel of protein kinases.



CI_{50}=4.8 nM contre GSK-3α
CI_{50}=22 nM contre GSK-3β
efficacité/toxicité = 2000

X= H, N
R, R'= Het

Keywords: GSK-3α; oxazolo[5,4-f]quinoxaline; kinase inhibition; co-crystallization; molecular modelling; glioblastoma

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“On water” reaction of deactivated anilines with 4-methoxy-3-buten-2-one, an effective butynone surrogate

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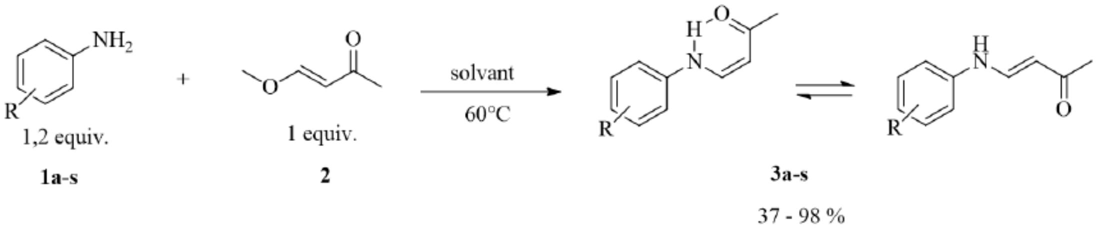
The aza-Michael addition reaction has been extensively studied and various researchers have reported the utility of this reaction towards the synthesis of various pharmacological active compounds [1] as well as natural products [2]. The conjugate addition of poorly nucleophilic aromatic amines such as aniline derivatives onto trans-4-methoxy-3-buten-2-one was easily carried out in specific polar protic solvents, without any promoting agent.



Scheme 1 : Aza-Michael additions of anilines onto 4-methoxy-3-buten-2-one

The aza-Michael reactions were found to be highly stereoselective and provided a series of enaminones in excellent yields. The reactions were accelerated under the « on water » conditions proceeded equally well or better than under other solvents « TFE, HFIP, etc.) or under neat conditions.

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Supramolecular chemistry:
Design and behavior study of entrelaced molecule

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Supramolecular chemistry is a field of chemistry, inspired by the organization of biological environments where the assembly of molecules involves mechanical interactions between molecular units[1]. Rotaxanes are interlocked molecules, comprising a linear section crossing at least one macrocyclic part and possessing terminal groups large enough to prevent unthreading[2]. Mechanical bond interactions characterize these structures. As a result, we are interested in the synthesis of [1] rotaxane by active recognition by a metal (or AMT). The reaction between an alkyne and an azide is catalyzed by copper (I) to generate the 1,4 isomer of triazole. a macrocycle with a cavity capable of chelating Cu(I). For the "click" reaction, a macrocycle with a side chain containing a terminal alkyne reacts with a stopper that has an azide function. A molecular brake with an asymmetric carbon was added at the bottom of the structure to prevent the structure from deinterlacing. As a result, we were eager to identify new critical aspects impacting and improving the construction of the interconnected structure. The number of copper equivalents has a significant impact on the selectivity of molecular lasso creation. Similarly, the existence of another macrocycle influences molecular lasso creation yield. We contemplated using a substitution reaction to provide a platform that allows for alternative lasso topologies. Unfortunately, only no interlaced structures were produced. Furthermore, we attempted to create a lasso using a shorter chain to investigate the effect of chain length on lasso formation.

Key words: click chemistry, [1] rotaxane, Supramolecular chemistry

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Ultrasound design and biological activities of new generation of [1,2- a] benzimid azolyl-1,3,5-triazines

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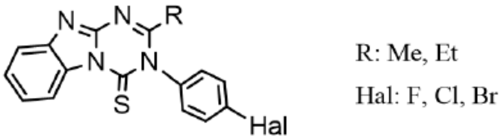
New 1,3,5-triazine derivatives showed excellent activity as anti-insulin resistance and anti-inflammation [1]. In our previous work the biological activities of benzimidazolo-triazine derivatives has been evaluated as anti-diabetic and anti histamine [2]. The N-halogenated benzimidazolo-triazine had shown interesting biological activities.

Ultrasound assisted reaction is important in green organic synthesis for their shorter time reaction and their higher yields products. The present work aim to synthesize and characterize under ultrasound irradiation a various N- halogen phenyl [1,2- a] benzimidazolyl-1,3,5-triazine and benzimidazolyl-iminoester. All derivatives has been evaluated for their anti-microbial and anti-aging activities.



Keywords: benzimidazolo-1,3,5-triazine, iminoester, Ultrasound

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One-step access to new polycyclic aromatic hydrocarbons via C-H bond functionalization catalyzed by palladium

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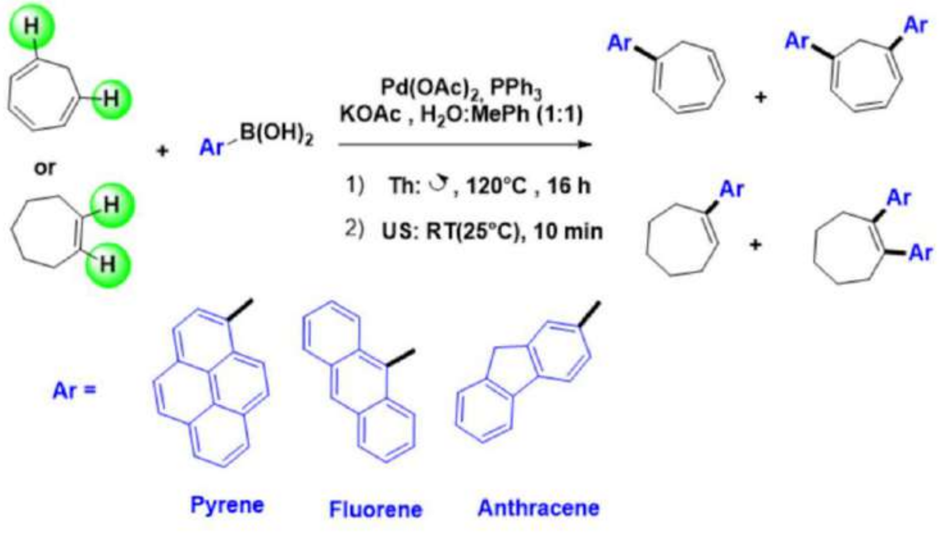
The cycloheptene and cycloheptatriene coupling with polycyclic aromatic hydrocarbons proved to be promising as it allowed to isolate new compounds, which is scientifically significant in terms of its potential application in various chemical fields. These compounds were synthesized relying upon a new methodology whre some principles of green chemistry were adopted. Thus, the reaction occurring in one step via a C-H bond functionalization, was catalyzed by a small amount of palladium acetate associated with potassium acetate as an inexpensive base under ultrasonic activation in a two-phase medium using water with the presence of an organic solvent where a significant yields ware obtained remarkably without using any ligand. In addition, we managed to reduce the reaction time from 16h during thermal activation to 7-10 min under ultrasonic irradiation to isolate six novel fluorescent semiconductor compounds whose CIE chromaticity coordinates displayed different colors. These compounds are of primary interest in the synthesis of blue high emitters performance with high stability and purity of color.

Key words: C-H functionalization, green chemistry, palladium, polycyclic hydrocarbon



Graphical abstract.

Synthesis and antiproliferative breast cancer of new [1,2,4]triazolo[4,3-*a*]pyrimidines

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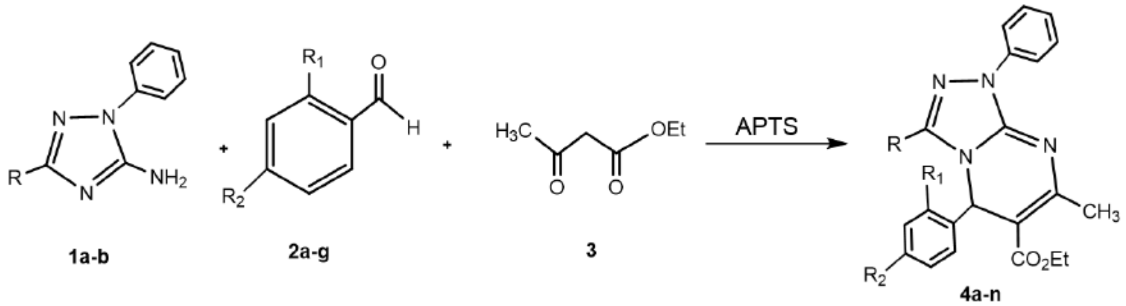
In this work, we study the reactivity of 5-amino-1-phenyl-1*H*-1,2,4-triazoles, simultaneously with aldehydes and ethyl acetoacetate according to the MCR method to form a new family of [1,2,4]triazolo[4,3-*a*]pyrimidines **4a-n**. The optimal reaction conditions consist to heat under the reflux of ethanol and using the APTS as a catalyst.

In addition, these triazolopyrimidiniques compounds were evaluated by anticancer activity against breast cancer tumor lines (MDA-MB-231 and MCF-7), especially the most potent inhibitory molecules are those that have a more significant decrease in IC_{50} against each type of MDA-MB-231 and MCF-7 tumor cells with IC_{50} values equal respectively 17.83µM and 19.73µM for **4c** and **4j** molecules, respectively compared to cisplatin.



Scheme 1: Synthesis of [1,2,4]triazolo[4,3-*a*]pyrimidines **4a-n**

Design and semi-synthesis of novel oleanolic acid and isoindole 1,2,3-triazole conjugates

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Oleanolic acid (OA) [1], a naturally occurring hydroxy pentacyclic triterpenoid that abound in the industrial olive-oil waste, has been reported several times for its interesting biological activities. Herein, we report an efficient method for the semi-synthesis of novel 1,2,3-triazole derivatives of OA (**3**). Triazole coupling compounds were obtained by treating azide (**1**), prepared from OA, with different isoindole alkynes (**2**) [2] through regioselective Cu(I)-catalyzed Huisgen 1,3-dipolar cycloaddition reaction [3]. The reaction afforded good yields for all the synthesized products.

Key words: Oleanolic acid, isoindole alkynes, semi-synthesis, 1,3-Dipolar cycloaddition, triazoles.

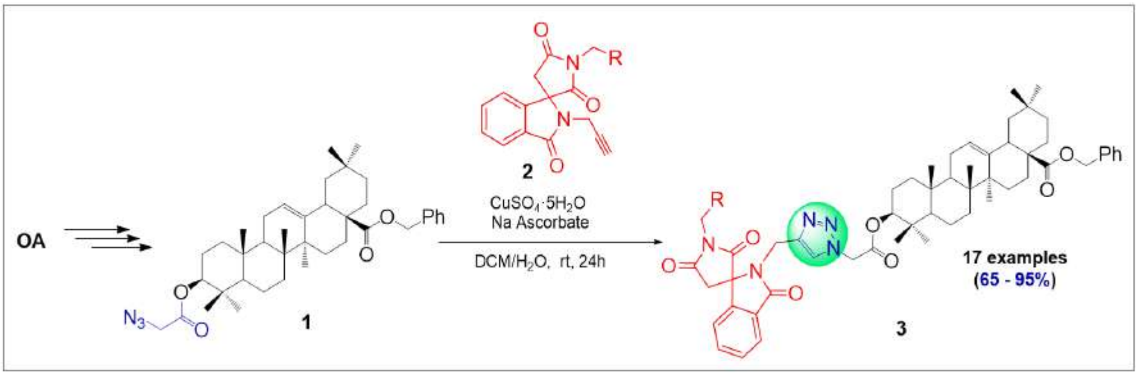

Figure 1. Semi-synthesis of novel 1,2,3 triazole-substituted oleanolic acid derivatives

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Nucleophilicities of cyclic secondary amines in Methanol

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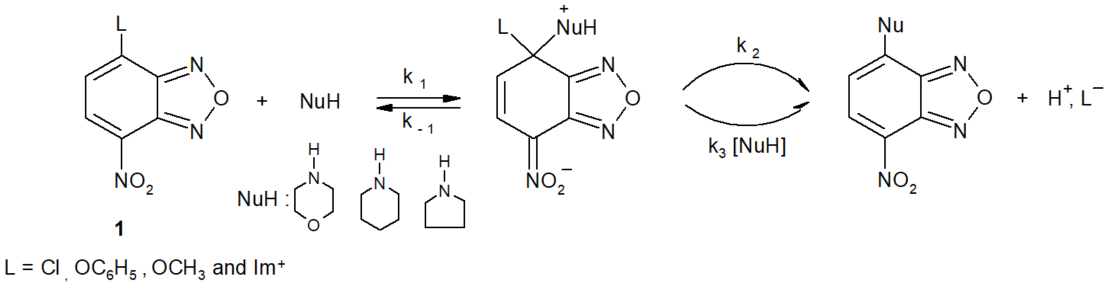
The kinetics of the S_NAr reactions of four 7-L-4-nitrobenzofurazans **1a-d** (L = Cl, OC_6H_5, OCH_3, Im^+) with three cyclic secondary amines (morpholine, pyrrolidine and piperidine) in methanol at 20 °C were reported. The second-order rate constants (log k) correlated linearly with the electrophilicity parameters E of electrophiles **1a-d** according to the linear free energy relationship **(1)** (Angew.Chem., Int.Ed.Engl. **1994**), allowing us to determine the nucleophile-specific parameters N and s_N for these series of amines.

$$\log k\,(20\ °C) = s_N\,(N + E) \qquad \textbf{(1)}$$

In addition, theoretical nucleophilicity index (ω^{-1}) for these series of amines has been calculated using a density functional theory (DFT) method and demonstrated that these values are linearly related to the experimental nucleophilicity parameters (N).



Reaction Mechanism of Nitrobenzofurazans **1a-d** with Secondary Cyclic Amines in Methanol at 20°C.

Key words: Kinetic / Equation of Mayr / Nucleophilicity Parameter *N* / 7-L-4-nitrobenzofurazans / Nucleophilicity Index (ω^{-1}) / Secondary Cyclic Amines.

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Synthesis and structural study (^{31}P, ^{1}H, ^{13}C NMR and X-Ray Crystallography) of some β-phosphonated thiosemicarbazones

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Thiosemicarbazone derivatives[1] and their complexes with metals have significant antiviral, antituberculous, antibacterial and antitumor activities[2]. Therefore, it is of great theoretical and practical significance to synthesize new thiosemicarbazone ligands.
The phosphonated thiosemicarbazone ligands **2** were prepared by reacting β-phosphonated hydrazones[3] **1** with isothiocyanate derivatives.

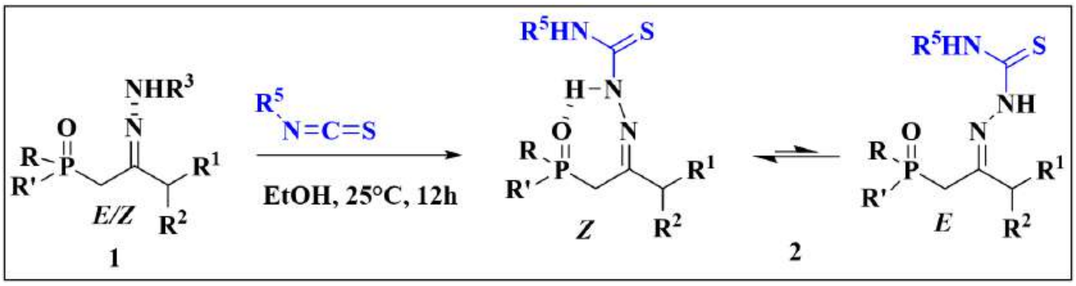

Fig I: Synthesis of phosphonated thiosemicarbazone ligands

The structures of all the synthesized products were characterized by NMR (^{31}P, ^{1}H, ^{13}C) and X-ray crystallography.

Key words: Phosphonated thiosemicarbazones, hydrazones, NMR, X-ray

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Crystal structure, spectroscopy, DFT calculations, thermal analysis, Hirshfeld surface and magnetic properties of a new organic-inorganic hybrid material ($C_{12}H_{16}N_2O$)[$CoCl_4$]

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In this work a novel organic-inorganic hybrid compound ($C_6H_{16}N_2O$)[$CoCl_4$], was obtained by slow evaporation method at room temperature and characterized by single-crystal X-ray diffraction. Powder X-ray, thermal analysis, UV-Vis, FT-IR and FT-Raman spectroscopies as well as magnetic measurements were carried on. The entitled compound crystallizes the monoclinic system with the space group $P2_1/c$. Single-crystal X-ray diffraction analysis indicates that the asymmetric unit in this compound is formed by a biprotonated organic cation of 2-Morpholinoethylamine $(C_6H_{16}N_2O)^{2+}$ and a tetrachlocobaltate(II) anion $[CoCl_4]^{2-}$. The atomic arrangement can be described as a succession of alternated organic/inorganic layers running along b axis. The different components are interconnected by N–H····O and N–H····Cl hydrogen bonds. The thermogravimetric analysis (TG) of the title compound gave an idea about the thermal stability of the latter showing three weight loss steps between room temperature and 1000°C. The room temperature IR spectrum was recorded and analyzed on the basis of literature to gain more information about the entitled compound and showed results in a good agreement with DFT calculations. The Hirshfeld surface analysis was conducted and associated to 2D fingerprint plots to investigate inter-molecular interactions and quantify their relative contribution in the crystal structure. The magnetic susceptibility measurements in the temperature range 2–300 K shows that the complex exhibits a weak antiferromagnetic exchange between the neighboring cobalt ions.

Key words: hybrid compound, crystal structure, DFT calculations, magnetic susceptibility

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Synthesis, crystal structure, vibrational spectroscopy, optical study and thermal analysis of a new complex based on 2,6-Dimethanolpyridine: $[(C_7H_{10}NO_2)CdCl_3]_n$

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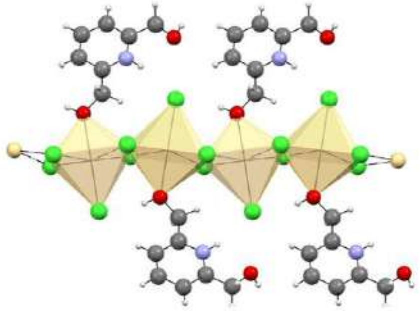
To better understand the ligand’s structural properties and with the aim of developing a new class of coordination polymers using 2,6-dimethanolpyridine as a coordinative building block, we present the crystal structure of catena(2,6- dimethanolpyridiniumtrichloro-cadmate(II)) of crude formula $[(C_7H_{10}NO_2)CdCl_3]_n$. Single crystal X-ray diffraction revealed that the 2,6-dimethanol pyridinium acts as a monodentate ligand through the oxygen atom of the hydroxyl group, showing that the compound crystallizes in the monoclinic system and $P2_1/c$ space group. The structure’s intermolecular interactions were studied using contact enrichment ratios and Hirshfeld surfaces. The crystal packing is maintained by several hydrogen bonds and ionic interactions. Powder XRD measurements confirmed the purity of the crystalline sample phase. SEM confirmed the surface homogeneity, whereas EDX semi-quantitative analysis corroborated the composition. IR spectroscopy identified vibrational absorption bands, while optical UV-visible absorption spectroscopy investigated optical properties. The thermal stability was tested using TG-DTA.

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



Representation of extended 1D polymeric chain showing the μ2 -Cl bridges.

Mechano-Synthesis, Characterization, and Adsorptive Properties of Mg-Al-LDH and Zn-Al-LDH for Olive Mill Wastewater Treatment

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Industrial olive oil production is of fundamental economic importance for many Mediterranean countries. However, this industry generates huge amounts of toxic olive mill wastewater (OMW) that could represent a serious threat to human health and environment biodiversity. In the current study, calcined layered double hydroxide (LDHs) were synthesized through mechanochemical process involving a manual grinding of magnesium or zinc - and aluminum nitrates salts in an agate mortar followed or not by a peptization process. The experimental results showed that the non-peptized LDHs have characteristics of a layered structure but with a relatively low crystallinity. At contrary, The peptization process allowed getting LDHs with regular particles having high crystallinity and good thermal stability. These LDHs achieved significant improvement in the quality of OMW. Indeed, after 44 hours of contact time, the removed amounts of chemical amounts of oxygen demand (COD) and biological oxygen demand BOD were assessed to about 300 and 100 mg.g^{-1}, respectively. Moreover, the discoloration rate of this effluent was more than 90%.

Keywords: Layered double hydroxides; Mechano-chemistry, Peptization; Olive mill wastewater; treatment

Synthesis, crystal structures, and thermal properties of rare earth silicate oxyapatite

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A novel series of apatite phosphors with a formula of $Na_{1-2x}La_9(SiO_4)_6O_2$:$xEu^{3+}$ were synthesized through a solid-state method. The crystal structures, photoluminescence, cathodoluminescence, and XANES were investigated systemically. In this work, the approach is demonstrated the efficient reduction of Eu^{3+} doped $Na_{1-2x}Eu_xLa_9(SiO_4)_6O_2$ apatite and evaluates if the structure and composition of the apatite host matrix can influence the luminescent properties of Eu^{3+} activator regarding the structure of these apatites [1], the concentration of the dopant and the annealing temperature may affect the distribution of Eu^{3+} ions at the M_1 and M_2 sites with the C_3 and C_s local symmetries, respectively. The results of the XRD analysis show an oxyapatite structure with the space group P63/m. Europium can occupy crystal matrices simultaneously in the form of Eu^{3+} and Eu^{2+} and enter nonequivalent crystallographic positions in a lattice, thus forming various optical centers. The increasing substitution of Eu^{3+} in the sodium site in the crystal favors the reduction from Eu^{3+} to Eu^{2+} ions, resulting in phosphors with a strong green emission at 520 nm and a small green-yellow-red emission of Eu^{3+} [2]. Cathodoluminescence (CL) measurements evidenced however the existence of a large fraction of unreduced and reduced europium activators. The Eu^{3+} and Eu^{2+} emissions were almost fully suppressed in CL and as a consequence, the reduction of Eu^{3+} to Eu^{2+} is obtained.

Keywords: Synthesis, Characterization, X-ray diffraction, emission.

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Heat capacities of AgCs $(NO_3)_2$ and $Ag_3Cs(NO_3)_4$

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Alkali nitrates are promising phase change materials for the development of thermal storage systems. Silver nitrate is often associated with them in many industrial and technological fields due to their physical and chemical similarities.

So, we have investigated, in a previous work, the phase diagram of the $AgNO_3$-$CsNO_3$ binary system [1]. This latter presents, in particular, two intermediate stoichiometric compounds: $Ag_3Cs(NO_3)_4$ and $AgCs(NO_3)_2$. The thermodynamic properties of these compounds are important information to determine their behavior as thermal energy storage materials. Their phase transition (solid/solid and solid/liquid) temperatures and enthalpies and their enthalpies of solution have been measured in previous investigations [2, 3]. This work focuses on the experimental determination, for the first time, of their heat capacities in the temperature range [298.15 – 503.15 K] by differential scanning calorimetry (DSC).

Key words: Heat capacities, intermediate compound, phase diagram, differential scanning calorimetry.

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Experimental and theoretical study of the luminescent properties of Pr doped $LaAsO_4$ nanoparticles

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Pr-doped $LaAsO_4$ nanoparticle samples have been synthesized using the combustion method. The purity of as prepared samples has been confirmed using the X-ray powder diffraction which shows that all the powders crystallize in the monoclinic system space group $P2_1/n$ with a shift of the pics to the low theta angles. The microstructure of the title compounds has been studied by the Debye Scherrer method and scanning electrotonic microscopy with both shows particle with nanometric size of about 70 nm. The measured excitation and emission spectrum have been obtained for λ_{em}= 460 nm and λ_{ex}=618 nm respectively. The electronic structure and the optical properties of the undoped and doped $LaAsO_4$ have been performed by the DFT method via the GGA+PBE and GGA+PBE+U approximations for the undoped and doped compounds. The bond structure and the density of the states show the intercalation of the states 4f of the Praseodymium in the forbidden band of $LaAsO_4$ which allows the decrease of the optical gap. The different electronic transition in the doped and undoped compounds have been deducted from the dielectric function curves and the density of states and confirm the emission in the visible region.

Key words: combustion method, DFT, bond structure, density of states, dielectric function, photoluminescence Properties.

Development and characterization of materials for application as electrodes in energy storage systems

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The NASICON "$Na_3V_2(PO_4)_2F_3$ (NVPF)" is the most beneficial material for use as a positive electrode for sodium-ion batteries. In addition, its structural modification that limits the insertion-disinsertion phenomenon motivated us to design and synthesize a new composite material «Polymer/NNPF» whose capacity of oxide alone was tried to improve which is about 128 $mAhg^{-1}$, by the presence of a conductive polymer; Polyaniline (PANI).

Great interest is given to the PANI which have found their applications in different industrial fields thanks to their typical stabilities, their simple and inexpensive syntheses, as well as its structure which provides a maximum degree of conjugation hence the ability to give high electrical conductivities.

Our work aims to improve the electrochemical performance of materials used as cathode in the sodium-ion battery, using the polyaniline that serves to protect the spray electrode during electrochemical reactions. The NASICON NVPF was synthesized by the soil-gel method[1] using a complex agent. Polymerization was produced by oxidative polymerization of the monomer and ammonium persulphate in a HCl[2] solution. Polymerization was carried out by varying the amount of starting monomer in order to modify the thickness of the polymer layer on the oxide surface.

Various characterization techniques such as X-ray diffraction (DRX, Fourier transform spectroscopy (FTIR), and Raman. The analyses showed that all the materials developed have the same structure including the P42/mnm space group. All materials also showed similar morphology.

Electrochemical performance was studied by galvanostatic. These good materials also showed good sodium reversibility during charge/discharge cycle.

Keywords: conductive polymers, PANI/ $Na_3V_2(PO_4)_2F_3$ composites, sodium-ion batteries.

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Enhancement with Hirshfeld surface analysis of structural, optical and luminescent performance of new V-substituted polytungstates

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Novel polyoxometallate, $(C_7NH_9F)_4(V_2W_4O_{19})\cdot 6H_2O$, based on V-substituted Lindqvist-type $[V_2W_4O_{19}]$ was synthesized and characterized by single-crystal XRD, IR and UV-Vis spectroscopies and photoluminescence measurements. X-Ray diffraction studies reveal that the title compound crystallizes in the triclinic space group $P\bar{1}$ with cell parameters: a = 8,6180 (16) Å, b = 8,9682 (17) Å, c = 16,656 (3) Å, α = 85,939 (4) °, β =75,247 (3) °, γ = 68,524 (3) °. The crystal packing displays 3D-supramolecular assembly confirmed by a detailed Hirshfeld surface analysis and their associated fingerprint plots. This letter analysis indicates that the most significant contacts in packing are O···H/O···H (42.9%) followed by H···H (22.2%) and H···F/F···H (11.4%). The optical band gap is determined, well confirming the semiconductor behavior of reported material. Furthermore, it exhibits photoluminescence emission in the solid state [1].

Keywords: Polyoxometallate, Lindqvist, X-ray Diffraction; IR, UV-visible Spectroscopies, photoluminescence property.

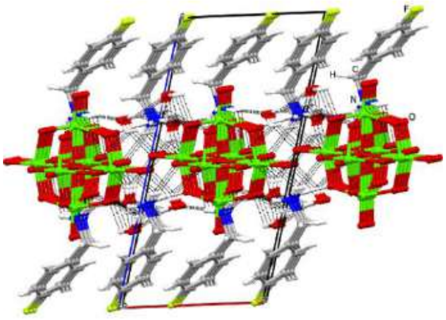

Figure 1 : Selected relevant hydrogen bonds structure within the crystal packing

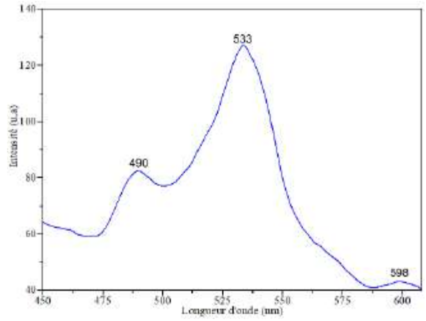

Figure 2 : Photoluminescence spectrum of $(C_7NH_9F)_4(V_2W_4O_{19})\cdot 6H_2O$

Reference

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A new 0-D hybrid bismuth halide compound $(C_{13}H_{28}N_2)_4$ $[BiCl_6]_2$ .2Cl.5 H_2O: Synthesis, crystal structure and physical properties

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Zero dimensional (0-D) hybrid bismuth halide materials have aroused high interest due to their hopeful emission properties [1-2]. Here, we report the synthesis by slow evaporation method and the characterization by single-crystal X-ray diffraction (SC-XRD), thermal analysis and optical measurements of a novel hybrid material 0-D $(C_{13}H_{28}N_2)_4[BiCl_6]_2.2Cl.5H_2O$. The structure of the title compound was determined by single-crystal X-ray diffraction (SC-XRD) at 296 K. Crystal data: Orthorhombic crystal system, space group $Pna2_1$, a = 6.587(2) Å, b = 11.697(4) Å, c = 14.625(5) Å, α = 90°, β = 92.514(6)°, γ = 90° and V = 2662.5(9) $Å^3$. The asymmetric unit of the structure contains four 4,4'-methylenebis(cyclohexylammonium) organic cations, two hexachlorobismuthate anions, two chlorine atoms and five water molecules. The crystal packing of the obtained compound is governed by the formation of various non-covalent intermolecular forces (H-bonding, Coulomb interactions, Van der Waals interactions) between $BiCl_6^{3-}$ anions and organic cations, assisted by water molecules. Hirshfeld surface analysis denotes that the most important contributions to the crystal packing are Cl···H/H···Cl and H···H interactions. The DSC/TGA curves presents two bands at 79 °C and 200 °C attributed to dehydration and to the decomposition of the material respectively. The diffuse reflectivity of powder sample was measured to obtain the band gap energy (Eg). The Eg of compound is calculated by the Kubelka-Munk method to be 3.36 eV, indicating that the compound can be classified as a semi-conductor. The photoluminescence analysis indicates that compound emits the strong yellow-orange light at 639 nm, which should be attributed to the charge transfer between Bi^{3+} and Cl^-.

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THE INFLUENCE OF ZnO ADDITIONS ON THE STRUCTURAL INVESTIGATIONS AND THERMOCHEMICAL BEHAVIOR OF M_2O-ZnO-P_2O_5 (M ≡ Na or Li) PHOSPHATE GLASSES

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Over the several decades, phosphate glasses have received significant attention due to their particular properties which makes them suitable for numerous applications such as: solid state lasers, optoelctronic devices, biomaterials…

In order to understand the effect of ZnO incorporation on the structural, physical properties and calorimetric dissolution of sodium and lithium based metaphosphate glasses.

Series of glasses with a general formula: (1-x)MPO_3-xZnO ($0 \leq x \leq 0.25$mol%) (M ≡ Na or Li) have been prepared using the conventional melt-quenching technique. Samples were investigated by means of X ray diffraction, density measurements, differential scanning calorimetry (DSC), ^{31}P NMR-MAS spectroscopy.

The variations of density and molar volume of glasses were attributed to the structural changes of the structure due to the formation of P-O-Zn ionic bonds.

The increase of glass transition temperature (T_g) values reflects an increases of the rigidity of the glass network when ZnO oxide is gradually introduced.

Thermochemical study of the glass series shows that the dissolution phenomenon is endothermic for lower ZnO content and becomes exothermic when ZnO oxide is gradually incorporated. The change in thermal sign can be explained by the depolymerization of metaphosphate chains (Q^2) which induces the formation of diphosphate groups (Q^1). These results were correlated to the spectroscopic investigations revealing the cleavage of P-O-P bridges.

Key words:

Phosphate glasses, ^{31}P NMR-MAS spectroscopy, depolymerization, thermochemical study.

Contribution of the green synthesis of cetals and dioxolanes

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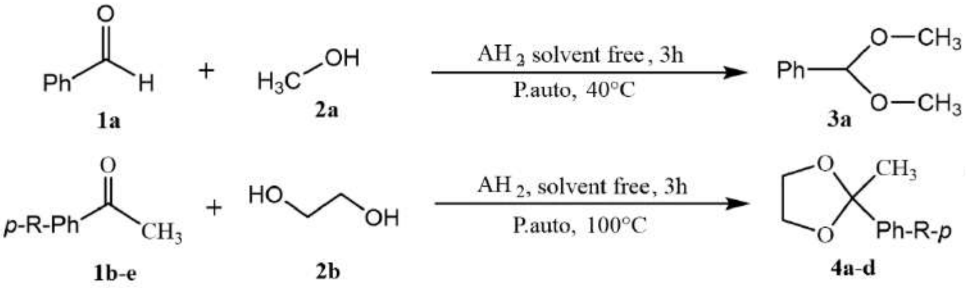
We are interested in 1,3-dioxolanes which are part of the skeletons of a large variety of organic and biological molecules which gives a very interesting applications in the biological and industrial fields. The reaction of benzaldehyde **1a** and aromatic methyl ketones **1b-e** with methanol **2a** and ethylene glycol **2b** are carried out in the presence of the Tunisian acid activated clay **AH$_2$**, under green experimental conditions, leads to the corresponding cetal **3a** and dioxolanes **4a-d**. The results obtained confirm then the acid activation of clay **AH$_2$** and its role in the catalysis of this acetalization reaction. Moreover, the nature of the substituents of the carbonyl compound has also a significant effect on the yield of products obtained.



1	**4**	**R**
b	**a**	CH_3O
c	**b**	H
d	**c**	HO
e	**d**	Br

Scheme: Synthesis of cetal **3a** and 1,3-dioxolanes **4a-d** from carbonyl compounds **1a-e**.

Key words: Acid activated clay, acetal, dioxolane, heterogeneous catalysis.

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Novel approach for selective photocatalytic degradations using 4-Carboxyphenylboronic acid functionalized TiO_2

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The surface of TiO_2 was linked to 4-carboxyphenylboronic acid to form 4-carboxyphenylboronic acid functionalized TiO_2 which was used as photocatalyst for selective photocatalytic degradations. The 4-carboxyphenylboronic acid molecules possess the ability to covalently link with vicinal diols [1,2]. This was proved in our work as the presence of boronate groups at the surface of the modified TiO_2 in a reacting medium containing two pollutants, enables the photocatalytic degradation of one pollutant and prevents the photocatalytic degradation of the second pollutant. The obtained results open in perspective the route for a process optimization towards the practical application of this green reaction.

Key words: Selective degradation, TiO_2, functionalization, 4-carboxyphenylboronic acid.

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Physicochemical, rheological and surface tension properties of polysaccharides extracted from *Opuntia ficus-indica* (Cactaceae)

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

Key words: polysaccharides, cladode, rheological properties, surface tension.

Efficient degradation of chloroquine drug by electro-Fenton oxidation: Effects of operating conditions and degradation mechanism

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The degradation of chloroquine (CLQ), an antiviral and antimalarial drug, using electro-Fenton oxidation was investigated. Due to the importance of hydrogen peroxide (H_2O_2) generation during electro-Fenton oxidation, effects of pH, current density, molecular oxygen (O_2) flow rate, and anode material on H_2O_2 generation were evaluated. H_2O_2 generation was enhanced by increasing the current density up to 60 mA/cm^2 and the O_2 flow rate up to 80 mL/min at pH 3.0 and using carbon felt cathode and boron-doped diamond (BDD) anode. Electro-Fenton-BDD oxidation achieved the total CLQ depletion and 92% total organic carbon (TOC) removal. Electro-Fenton-BDD oxidation was more effective than electro-Fenton-Pt and anodic oxidation using Pt and BDD anodes. The efficiency of CLQ depletion by electro-Fenton-BDD oxidation raises by increasing the current density and Fe^{2+} dose; however it drops with the increase of pH and CLQ concentration. CLQ depletion follows a pseudo-first order kinetics in all the experiments. The identification of CLQ degradation intermediates by chromatography methods confirms the formation of 7-chloro-4-quinolinamine, oxamic, and oxalic acids. Quantitative amounts of chlorides, nitrates, and ammonium ions are released during electro-Fenton oxidation of CLQ. The high efficiency of electro-Fenton oxidation derives from the generation of hydroxyl radicals from the catalytic decomposition of H_2O_2 by Fe^{2+} in solution, and the electrogeneration of hydroxyl and sulfates radicals and other strong oxidants (persulfates) from the oxidation of the electrolyte at the surface BDD anode. Electro-Fenton oxidation has the potential to be an alternative method for treating wastewaters contaminated with CLQ and its derivatives

Key words: Chloroquine, electro-fenton, H_2O_2 génération, Boron-doped diamond

Posidonia Oceanica balls: Chemical Composition

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Posidonia oceanica balls are the dominant sea grass in the Mediterranean Sea. This biomass has great potential for use as a novel lignocellulosic material on an industrial scale. The rational valorisation of these available renewable resources fits very well with the recent sustainable approach, commonly established everywhere. During this paper, the chemical composition of *Posidonia oceanica* balls was established according the TAPPI standard methods. The obtained results show clearly that the marine biomass present a high polysaccharide i.e. 68% and it can be justified to investigate in many applications and specially to produce fibre.

The delignification step was done by using soda-anthraquinone process. The obtained fibre was characterized by several methods by determination their mechanical, chemical, thermal and morphological behaviours.

Key words: *Posidonia oceanica balls,* fibre, surface morphology, characterizations.

Investigation the Adsorption of Congo red Dye on Natural and Acid Activated Libyan Bentonite from Aqueous Solutions

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Adsorption of Congo red (CR) from aqueous solutions by batch adsorption experiments onto natural Libyan bentonite (NLBn) and acid activated Libyan bentonite (ALBn) was investigated. Optimum sorption conditions were identified by varying solution pH, initial dye concentration, contact time, adsorption dosage and temperature. Chemical characterization of Libyan bentonite was carried out by Fourier Transform Infrared Spectroscopy (FT-IR), X-ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The isotherm data were investigated according to Langmuir, Freundlich and Temkin equations. Based on R^2, the equilibrium adsorption data was better fitted to Langmuir isotherm model than any other model. The kinetics data were analyzed using pseudo first-order and pseudo second-order models. The adsorption processes conformed to the pseudo second-order rate kinetics. Maximum adsorption capacity was found to be 4.3 mg/g for NLBn and 4.9 mg/g for ALBn at pH 9, 0.30g/L adsorption dosage, 60 min contact time and 303K for dye initial concentration of 50 mg/L. Thermodynamic parameters $\Delta G°$, $\Delta H°$ and $\Delta S°$ were calculated for the adsorption of CR dye on NLBn and ALBn, it was found that the adsorption of the CR dye by NLBn and ALBn was a spontaneous process and endothermic in nature.

Keywords: Adsorption, Libyan Bentonite, Congo red, Isothermal, Kinetic, Thermodynamics.

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Theoretical DFT insights into the Nature of chalcogen Bonding between SO_2, SO_3 and diazine: Noncovalent interactions involving σ and π holes

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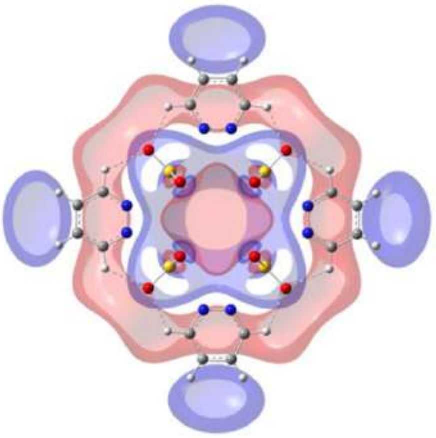
The irritant gases SO_2 and SO_3 can be the cause of certain health problems, especially in sensitive people such as asthmatics and children[1]. Short exposures can cause bronchial spasms, coughing spells, impaired respiratory function and eye irritation. By attaching to fine particles, a small part of this pollutant can even penetrate to the lower respiratory tract. Too high concentrations of SO_2 and SO_3 can cause acidification of the environment[2]. Once emitted into the air and in the presence of water, SO_2 and SO_3 are transformed into sulfuric acid H_2SO_4 which contributes to the phenomenon of acid rain. The consequences of such rains are acid deposits on building materials which can cause damage to the architectural and cultural heritage, the acidification of surface waters leading to the death of fish and soil deterioration which can have harmful effects on the vegetation and plants. DFT calculation of the capture of SO_2 and SO_3 via σ and π holes is performed with diazine molecules. The charge transfer interactions is highlighted by the wiberg indices calculation and the NBO analysis[3]. The IRC calculation is performed to connect the reactants SO_2 and SO_3 with the H_2SO_4 product via the transition states.



Keywords: chalcogen-bonding, σ and π-hole, noncovalent interaction, density functional theory.

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Influence of $Ba_{0.6}Sr_{0.4}TiO_3$ (BST) addition on the dielectric properties of $CaCu_3Ti_4O_{12}$ (CCTO) ceramics.

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CCTO/BST composites with x = (: x=0; x=0.01; x=0.02; x=0.03; x=0.05 and x=0.15) were synthetized by simple solid state reaction and were sintered at 1050°C, 1080°C and 1100°C for 12 h . The high dielectric loss associated with CCTO-based ceramics limits applications and drives the development of new solutions for example formation of ceramic composite. The microstructures of the sintered ceramics were observed and analyzed by scanning electron microscopy. The influences of different composition on the dielectric and electrical properties of the composites were investigated.

Key words: Composite materials; Dielectric properties; Permittivity, Grain boundary, Electrical properties.

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Synthesis, characterisation, Stability and Human Serum Albumin Binding of a decavanadate complex $(C_4H_7N_2)_6[V_{10}O_{28}].8H_2O$

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Polyoxometalates (POMs) as early-transition-metal oxide clusters have received much attention in various fields such as catalysis, ion exchange, electrochemistry, biological and medicine for their enormous variety of structures and unique properties [1-2]. Because of this importance, it was of interest to synthesize a new member of decavanadate complex $(C_4H_7N_2)_6[V_{10}O_{28}].8H_2O$ and to investigate it's structural characterization by single crystal X-ray diffraction, IR, ^{51}V NMR.

We also check the stability of the decavanadate anions in aqueous solution in the absence and presence of Human Serum Albumin (HSA), and evaluate the interactions of material with Circular Dichroism and Fluorescence spectroscopy.

The title compound was crystallized in the monoclinic system, space group $P2_1/n$ with a= 11.0603 (15) Å, b= 16.454 (2) Å, c= 14.7861 (17) Å, β= 94.853 (4)°, Z = 2.

Keywords: decavanadate, X-ray diffraction, HSA, binding interaction.

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Synthesis, X-Ray structure, optical and non linear optical properties of rhodium-complex bearing *N*-heterocyclic carbene ligand: Molecular Docking and theoretical investigations

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We performed a comparative DFT[1] theoretical study in order to investigate the impact of the iridium on the optoelectronic and non-linear optical properties of the complex. The new rhodium(I) N-heterocyclic carbene complex was synthesized in good yields by the reactions of rhodium dimer with benzimidazolium salts in tetrahydrofuran and the coordination mode of Rh-complex was confirmed by single crystal XRD analysis [2]. The M06-2X functional with the mixed basis set (6-31G(d): def2tzvp) was found to be the best method for optimizing the studied complex since it displayed close geometric data to the experiment. As a novelty in this work, iridium was found to be a performer for NLO applications over rhodium. The Rh-complex was used as a catalyst in the hydrosilylation of acetophenone derivatives with triethylsilane at 80 °C for 1h and was tested against *MCF7* and *MDA-MB-231* cancer cells, Micrococcus luteus LB 14110, Listeria monocytogenes ATCC 19117, Salmonella Typhimurium ATCC 14028, Staphylococcus aureus ATCC 6538, Pseudomonas aeruginosa and Candida albicans microorganisms.

Keywords: Rhodium(I) N-heterocyclic carbene complex, DFT, TD-DFT, NLO, Docking

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Prussian blue- and carbon black-improved performances of flexible laser-scribed graphene supercapacitors

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Laser-scribed graphene electrodes are currently used for the energy storage in 2D flexible supercapacitors with high energy density (~ mWh/cm^2) and power density and (~ mW/cm^2) [1-2]. Several approaches are used to further improve these parameters for use in sensors and powering small devices [2-4]. We showed that the energy density and power density of PI-derived graphene flexible interdigitated electrodes can be improved by the electrochemical modification of the electrode surface with carbon black and Prussian blue nanoparticles. To this end, we used a CO_2 laser (10,6 μm) to scribe graphene-based supercapacitors. Our results show that the modification of the surface interdigitated electrodes (8.16 mF/cm^2 @0.2 mA/cm^2) with carbon black nanoparticles (Vulcan XC-72R) and Prussian blue redox nanoparticles ($Fe_3(Fe[(CN)_6]_2)$ or both improves the storage performances respectively by 52%, 153% and 277%. The stability of the different devices was examined by galvanostatic charge-discharge cycling, @1.5mA/cm^2 for at least 3000 cycles, to show that the supercapacitors retained more 90% of their initial capacitance. Thus, cost-effective laser-induced graphene electrodes could be a viable alternative to metal oxides for high density supercapacitors.

Keywords: Laser-scribing; LIGIDEs; Prussian Blue; Vulcan XC-72R; Supercapacitors; Enhanced Performances

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Synthesis and Characterization of Conductive Nanocomposites Based on "Graphene" and Polysaccharides

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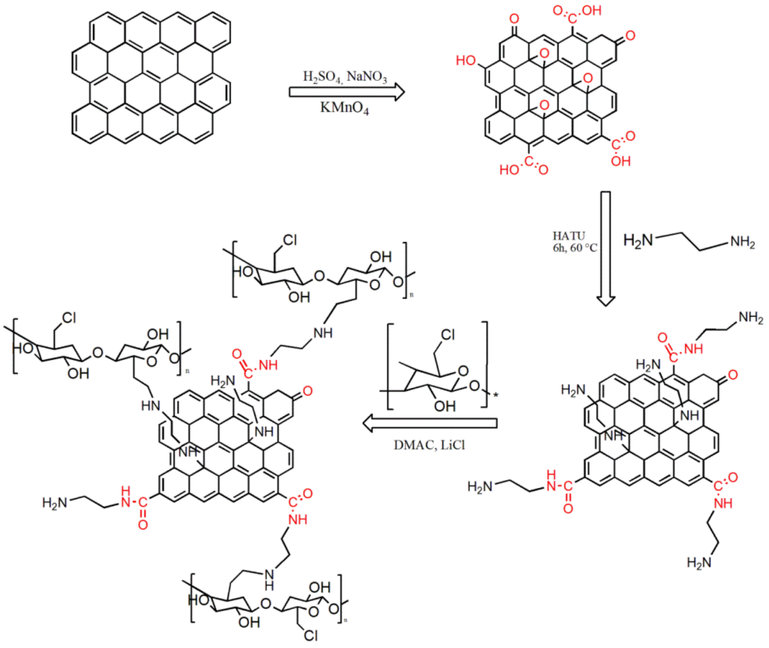
The main objective of this work has been to experiment a new ways of exfoliation of graphene sheets in polysaccharide matrices such as cellulose and chitosan doped with gold nanoparticles (Au). Our strategy was to explore new routes for the grafting of molecules and macromolecules onto graphene oxide (GO). First, we have oxidized commercial graphite by the method of Hummers which is a priori the simplest method to implement to produce a stable suspension of graphene oxide sheets totally exfoliated in water. The advantage of this oxidation is the formation of carboxylic acid and epoxy functional groups onto the graphite surface that can be functionalized in two stages by ethylenediamine and then by a polysaccharide such as cellulose. Indeed, in order to improve the compatibility of graphite oxide with organic matrix such as cellulose, the idea is to graft it onto polysaccharide chains. These results made it possible to demonstrate the partial exfoliation of the graphene sheets after functionalization and to obtain a percentage of grafting of about 35wt% for cellulose. The electrical conductivity of the corresponding nanocomposites has also been studied by dielectric measurements at various temperatures. The increase of the electrical conductivity after the functionalization of graphite oxide showed a solvo-thermo reduction simultaneously with the functionalization. Finally, the doping of this material by gold particles made it possible to obtain an electrical conductivity of 1.60 10^{-4} S m^{-1}. Concerning chitosan-based composite materials, the scientific approach was the same as cellulose substrate and we obtained a percentage of grafting of 20wt%. In addition, its catalytic activity for the conversion of 4-Nitrophenol to 4-Aminophenol was of high efficiency.



Keywords: Graphite oxide, Polysaccharides, Electric properties, Gold nanoparticles, Catalytic reduction.

Synthesis, structural and electrical study of a new strontium stannate substituted by Ge^{4+}

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$SrSn_{0.9}Ge_{0.1}O_3$ perovskite either massively or thin films were prepared by sol-gel method. Thin films were deposited by spin-coating and dip-coating on silicium substrate. Powder X-ray diffraction confirmed $SrSn_{0.9}Ge_{0.1}O_3$ crystallizes in the cubic system (space group Pm-3m), with lattice parameters a = 4.02576(4) Å. FTIR spectroscopy confirms the existence of vibration bands of existing groups in our material, in particular (SnO_6) and (GeO_6) and confirms the perovskite structure. The microstructural study of $SrSn_{0.9}Ge_{0.1}O_3$, prepared by the "sol-gel" method confirms the nanometric sizes of the crystallites, calculated from the profiles of X-ray diffraction lines. A measurement of the complex impedance at different temperatures in a frequency range, made it possible to draw the Nyquist diagram as well as that of permittivity and electrical dissipation. These measurements also confirm the dielectric nature of this material.

Key words: perovskite oxide, sol-gel, powder diffraction, physical properties.

Effect of nature and surface state of steel on structural and mechanical properties of galvanization coatings

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The aim of this research work is to study the effects of the nature and the surface roughness of steel substrate on structural and mechanical properties of intermetallic compounds of galvanization coatings obtained at different immersion time. After a best preparation of here surfaces by different roughness process, various steel of substrates were galvanized by immersion in a molten zinc bath maintained at 450°C During the galvanization process, the chemical reactions that take place between the steel and the liquid zinc give rise to the formation of different intermetallic. Thus, three phases of Gamma, Delta and Zeta are produced on the steel substrate. Theses metallic compounds have been coated then by a solid solution of iron in zinc Eta. These intermetallic compounds are hard and fragile and the product that is obtained is not suitable for working, since this would inevitably lead to cracking and detachment of the coating. The morphology and thickness of phases formed the coatings at different parameters took place with scanning optical microscope. Finally the hardness of coatings was measured with a Vickers hardness tester.

Key words: Steel, zinc, galvanization, iron

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Study of the nonlinearity effect on the optical properties of a one-dimensional photonic crystal

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The effect of nonlinearity on the optical properties of a 1D photonic crystal [1] of type $(HB)^n(BH)^m$ composed of linear and nonlinear materials has been studied. Linear and nonlinear transmission spectra are graphically illustrated using a numerical approach based on the transfer matrix method (TMM). The results show the appearance of a transmission peak in the photonic band gap, which means that the structure constitutes a monochromatic filter.

It is shown that the full width at half maximum (FWHM) of this peak depends on the number of layers of the studied structure and the refractive index of the nonlinear layers. The change in the refractive index (Kerr effect) leads to a dynamic displacement of the band gap, including the transmission peak. As a result, such a structure has the potential to be used to design optical filters and nonlinear optical devices.

Key words: Nonlinear 1D Photonic crystal, Transfer Matrix Method, Kerr effect.

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Effect of synthesized organic copolymers containing both carboxylate and hydroxyl groups on aqueous alumina dispersion

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Copolymers containing both carboxylate and hydroxyl groups noted PV2A have been synthesized in order to act simultaneously as dispersant and binder for spray drying alumina suspension. The quantity of the added copolymer was optimized to achieve adequate dispersion and stabilization of the suspension. Such investigation was done through a systematic analysis of the electrokinetic and rheological properties, from which the copolymer /alumina interactions during the powder dispersion can be evaluated. The addition of 1.2wt % of the PV2A copolymer in the formulation of an alumina suspension provides good stability, with a quasi-Newtonian rheological behavior and a minimum viscosity of 25 mPa.s.

Adsorption isotherm provided an electrosteric stabilization of alumina suspension, promoted by the adsorption of carboxylic groups onto the alumina surface and a loop-like conformation of hydroxyl groups.

The effect of polymeric chain length on the dispersion was studied using three copolymers $PV2A_L$, $PV2A_M$, $PV2A_H$ having respectively low, medium and high molecular weights estimated to 11,000, 19,000 and 47,000 Da. The strong attraction between dispersant and binding groups in the polymeric chains of PV2A prevents the competitive adsorption onto the alumina surface, usually obtained with commercial organic additives. As a result, the phenomenon of binder migration was prevented during the spray-drying, leading to a homogenous microstructure of atomized alumina powder.

Recycling of industrial tobacco waste to obtain bioinsecticide nanocomposite based on Nicotine to control *Tribolium castaneum* (Tenebrionidae) *

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Farmers lose high amounts of their grain crops due to insect infestations during storage. Although synthetic insecticides are efficiently used to reduce these losses, they have undesirable consequences for ecosystems. After application, these substances can be transferred into the ground water causing its contamination.

In order to obtain an eco-alternatives, the current study was designed to find a green process to elaborate a bioinsecticide nanocomposites films to manage against the devastating foodstuffs pest *Tribolium castaneum*. In this study, the chosen biomolecule is nicotine. To decrease the volatility of nicotine, this biomolecule was adsorbed on biocomposite films. First, nicotine was extracted from the waste generated by the factory of tobacco situated in Kairouan (Center Tunisia). This waste is a mixture of Virginia, Oriental and Burley tobacco varieties.

The biocomposite films were prepared by mixing clays (montmorillonite and Kaolinite), chitosan and cellulose acetate. The cellulose acetate is also a waste from the tobacco factory. Prepared composites were first characterized by XRD and infrared spectroscopy and then impregned by nicotine. The release of nicotine as function of temperature was studied by *in situ* IR DRIFT. Results shows that the type of clay has a great influence on the nicotine volatility and that the interaction between nicotine and cellulose acetate is stronger than between nicotine and chitosan.

The insecticidal activities tests indicated a good toxicity of films against *T.casteneuum* adults.

Therefore, the waste of tobacco can be recycled to obtain nanocomposites films in order to be used efficiently as a bioinsecticide to control *Tribolium castaneum* and probably other devastating pests of the foodstuffs.

Key words: Bioinsecticide, Industrial Tobacco Waste, Nicotine, *Tribolium castaneum*

Temperature sensor based on one-dimensional hybrid photonic crystals

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The temperature dependence in a one-dimensional dielectric photonic crystal with a dielectric-superconductor pair defect was theoretically investigated by simultaneously considering thermal expansion effect and thermal–optical effect. The use of hybrid photonic structures represents the originality of this work. First, we study the effect of the number of iterations in our systems. Then, we are interested to explain the effect of introducing a very temperature sensitive material in our hybrid multilayer structure, the material used is of superconductor type. The goal of this study is to optimize the performance of a temperature sensor.

Keywords : Photonic crystal, Transfer Matrix Method TMM, Temperature, Temperature sensor.

Effect of hydrothermal treatment on *Zyziphus lotus*'s integral valorisation

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The hydrothermal treatment of *Zyziphus lotus* was used as a pretreatment in this study, allowing for the total valorisation of this feedstock through the production of oligosaccharides, lignin, and cellulose nanofibers. First, the temperature of the hydrothermal treatment was optimized to maximize oligosaccharide production. The influence of the hydrothermal pretreatment on the efficacy of the subsequent biorefinery processes and the properties of the produced products was then investigated. The hydrothermal pretreatment not only boosted the organosolv delignification process, but it also influenced the polydispersity index and crystallinity of the produced lignins and cellulose nanofibers. Furthermore, this treatment would allow for the integral valorisation of the *Zyziphus lotus* via a biorefinery approach, which might be an example of the circular economy while also fitting the zero-waste concept.

Keywords: *Zyziphus lotus,* Oligosaccharides, lignin, cellulose nanofibers, integral biorefinery.

APPLICATION OF MOS$_4^{2-}$INTERCALATED MAGNETIC LAYERED DOUBLE HYDROXIDE FOR PRECONCENTRATION OF CADMIUM AND LEAD FROM WATER SAMPLES

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A MoS_4^{2-}–intercalated magnetic FeMgAl layered double hydroxide ($Fe_3O_4@MoS_4^{2-}$–FeMgAl LDH) nanocomposite was synthesised via hydrothermal assisted exfoliation. The material was applied as the adsorbent for extraction, preconcentration and removal of cadmium ions (Cd^{2+}) and lead ions (Pb^{2+}) from wastewater and river water. The structural properties and morphologies of the adsorbent were determined by transmission electron microscopy, scanning electron microscopy coupled with energy dispersive spectroscopy, Fourier transform infrared spectroscopy, zeta potential and X-ray diffraction. The parameters influencing the preconcentration and adsorptive removal process were optimised using the central composite design (CCD) method. The concentrations of Cd^{2+} and Pb^{2+}in the samples were determined using inductively coupled plasma optical emission spectrometry (ICP-OES). The preconcentration method developed in the study was ultrasound-assisted magnetic solid phase extraction (UA-MSPE). Under optimum conditions, linearity was 0.1-800 µg/L with the correlation of determination (R^2) of 0.9987.

Keywords: ultrasound-assisted magnetic solid phase extraction, layered double hydroxide, pre-concentration.

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Iron Chloride-catalyst as a convenient route to provide a selective, practical and green homo and cross-etherification reactions.

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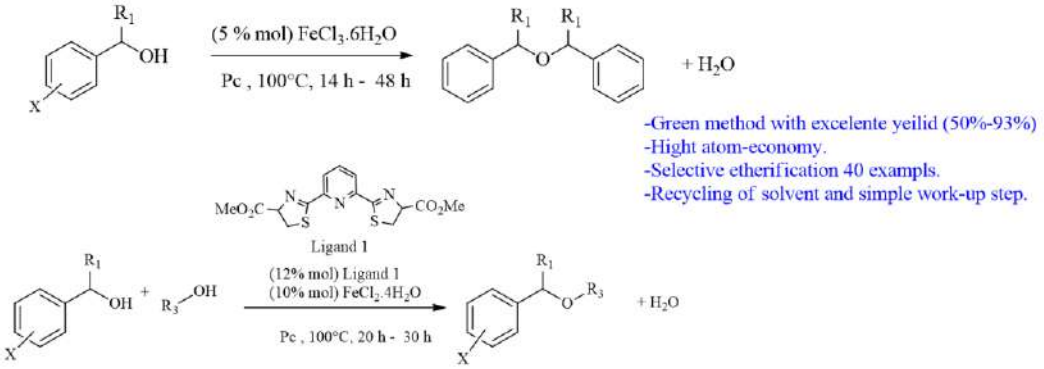
Iron chloride has been shown to be an efficacious catalyst for dehydrative O-alkylation reactions, furnishing facile, environmentally friendly, and easily scalable homo- and cross-etherification methods for the elaboration of useful symmetrical and unsymmetrical benzyl and aliphatic ethers in propylene carbonates at 100°C. Mechanistic studies revealed that Fe-bisthiazoline ligand offers a beneficial route for the selective etherification of two different alcohols. The catalytic method exhibits a broad substrate scope (**40 products**) while tolerating a range of heteroatom functional groups in forming ethers in moderate to excellent yields **50% - 93%**.



-Green method with excelente yeilid (50%-93%)
-Hight atom-economy.
-Selective etherification 40 exampls.
-Recycling of solvent and simple work-up step.

Key words: Catalysts / Ethers/ Iron chloride / Green / O-alkylation.

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Synthesis and catalytic applications of Bimetallic Ruthenium-arene complexes bearing fluorinated imidazolium-2-dithiocarboxylates zwitterions

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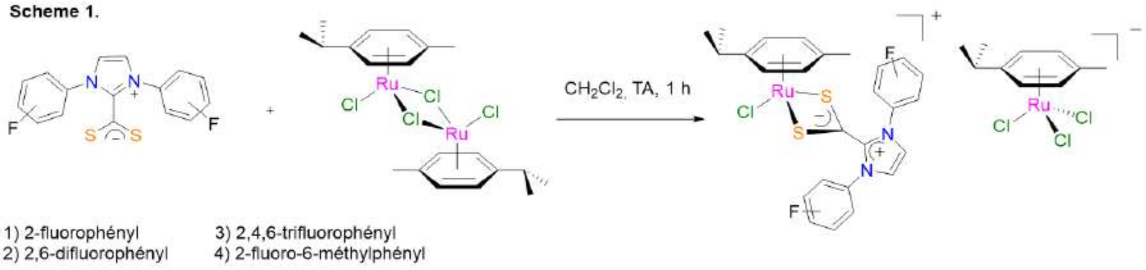
A series of fluorinated imidazolium-2-dithiocarboxylates zwitterions have been prepared according to the method described by Mazars and coworkers [1] and used as ligands for the synthesis of bimetallic Ruthenium-arene complexes (Scheme 2) [2]. These complexes were then evaluated for their catalytic activity in various reactions, such as the synthesis of enol esters from carboxylic acids and alkynes or the transfer hydrogenation of ketones.

Scheme 1.



Key words: Fluorinated imidazolium-2- .dithiocarboxylates zwitterions, Ruthenium-arene complexes, transfer Hydrogenation

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New Synthesis of Diaryl Tropane Derivatives by Palladium(II)-Catalyzed C(*sp*^{3})–H Activation

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Tropane alkaloids, derivatives of the *N*-methyl-8-azabicyclo[3.2.1]octane skeleton containing the famous cocaine, are relevant compounds in the field of therapeutic research particularly the arylated tropane class of derivatives (Figure 1A). For instance, compound **1a** was reported as a narcotic antagonist while **1b** was shown to lower circulating blood glucose levels by 60-80% and possesses an analgesic activity similar to codeine. Moreover, 2,3-aryltropanes (such **1c**), compounds that have been scarcely described to date, were found to be highly selective ligands for the dopamine transporter (DAT) at the nanomolar level.

As part of our ongoing interest in functionalization of tropane motifs, we sought to design a new C(sp^3)−H activation approach to synthesize unknown arylated tropanes in a site-selective manner. Herein (Figure 1B), we report the first pallado-catalyzed double C(sp^3)–H arylation of the tropane skeleton in positions 2 and 4 driven by the aminoquinoline directing group (DG) positioned in the C3 position.[4] The reaction is site-selective delivering 2,4-β-*cis*-diaryl tropanes. Preliminary biological evaluations showed that this series of compounds displays premising antiproliferative activities against colon cancer cell lines.

Key words: double C(sp^3)−H activation, cis-selectivity, antiproliferative activity.

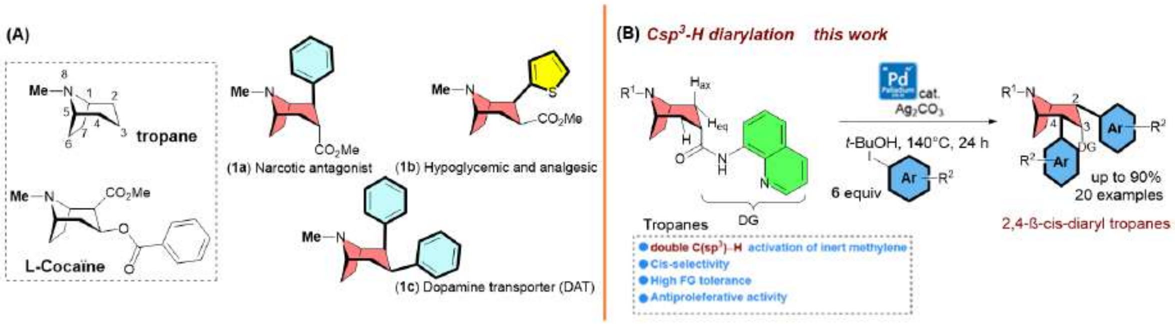

Figure 1

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[4] Mayssa Zayene *et al*. **2022**, *J. Org. Chem*. accepted.

Antioxidant Properties of phenolic compounds extracted from Olive mill wastewater using 2,2′-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) ABTS $^{\bullet+}$

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The olive oil industry is a very important industry that is centered basically in the Mediterranean region. However, the extraction of olive oil produces huge quantities of liquid effluents known as Olive Mill Wastewater (OMW) that are considered as a source of pollution due to their high concentration in organic matter. The recent studies were directed towards valorizing these effluents by extracting bioactive molecules known as phenolic compounds since it is proven that they are natural antioxidants. For this reason, our current study focuses on extracting phenolic compounds from Olive Mill wastewater using three extracting methods and study their antioxidant capacity.

The Olive Mill Wastewater (OMW) samples were collected from the Cap Bon, Tunisia after being stored for 3 months in evaporation baths. First the physicochemical characteristics of the samples were studied, which are composed mostly of 97.55% water, 2.45% solids, 0.69% total fat and 0.83% suspended solids. Then phenolic compounds were extracted using maceration and liquid-liquid extracting methods and to investigate the antioxidant capacity of the extracts ABTS •+ test was used. this test is based on the ability to scavenge the ABTS radical cation. It has shown that the polyphenols extracted via different solvents have an important antioxidant capacity. the lowest inhibition percentage is for ethyl acetate (90.78%) and the highest is for ethanol (93.98%) and the mixture of chloroform/methanol (93.88%). the IC50 values vary between 15,75 (mg ET/ L) for the methanolic extracts and 26.68 (mg ET/ L) for the ethyl acetate extracts.

Key words: Olive Mill Wastewater, physicochemical characteristics, phenolic compounds, antioxidant capacity

Chemical investigation and insecticidal effect of *Thapsia garganica* L. essential oil against *Tribolium castaneum*

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Recently, the use of essential oil obtained from aromatic plants has shown significant potential for insect pest management [1]. The present study was conducted to investigate for the first time the chemical composition and insecticidal activity of the essential oil isolated by hydrodistillation from the seeds of *Thapsia garganica* L., (Apiaceae family). Gas chromatography coupled to mass spectrometry (GC/MS) and flame ionization detection (GC-FID) were used for the qualitative analysis and quantification of the volatile constituents. 1,4-Dimethylazulene (51.3%) was identified as the main compound of the essential oil. Concerning the repellent effect, results revealed that SEO was strongly repellent towards *Tribolium castaneum* adults (PR = 100% after 2 h) and highly toxic reaching 93.3% mortality after 24 h of exposure. The median lethal dose (LD_{50}) of the topical application of the seed essential oil was 4.4%. These encouraging outcomes suggested that the essential oil of *T. garganica* could be considered a potent natural alternative to residual persistent and toxic insecticides.

Key words: *Thapsia garganica*, Essential oil, chemical composition, pest management.

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Synthesis of new chiral amino acid derivatives And study of their anti-inflammatory activity

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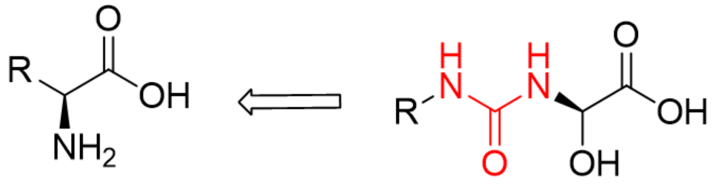
we have synthesized a series of chiral amino acid derivatives containing the urea units. *In silico* sudies, showed interesting anti-inflammatory activity. The selected compounds were subjected to the in vivo study for their anti-inflammatory activity. Then experimental results are in agreement with the theoretical study. All the prepared molecules were characterised with spectroscopic methods H^1 NMR, C^{13} NMR, and IR.



Amino acids

Amino acids derivatives

Anti-inflammatory activity

Key words: chirality molecule, Amino acids, Urea derivatives, Anti-inflammatory

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Effects of marine polysaccharides from Tunisian and Brittany seashore biodiversity on dermal fibroblast proliferation and matrix metalloproteinases secretion

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Since the end of the 20th century, a better understanding of connective tissue biochemistry has highlighted the physiological role of a class of polysaccharides, namely glycosaminoglycans (GAGs) that has led to the emergence of the concept of "bioactive polysaccharides". Some sulfated GAGs are involved in cell differentiation, cell adhesion, cell signalling as well as connective tissue structuring [1]. A lot of works or reports consider their use in tissue regeneration, tissue engineering, drug delivery and to design smart biomaterials or cosmetics [2] [3]. Unfortunately, these polysaccharides are hardly obtained from mammalian tissue and face technical or regulatory break due to sanitary risks. Thus, an advantageous alternative source of sulfated polysaccharides that has not been fully exploited yet come from the marine biodiversity. The aim of our work was to study the biological properties of polysaccharides extracted from marine organisms from Tunisian and Brittany seashores. We focused our study on impact of these polysaccharides on some interesting parameters involved in skin repair as dermal fibroblast proliferation and Gelatinase A (MMP-2) secretion. And our results showed that chondroitin sulfate (PHP) from sea cucumber and dermatan sulfate (DS) from fish skin could be good protectors of regenerative growth factors against proteolytic degradation. Furthermore, low molecular weight fucoidans (LMWF) obtained from brown algae can be regarded as regenerative tissue booster as they can promote growth factors signal and as fish DS prevent proteolytic tissue degradation.

Key words: Sulfated polysaccharides, Marine biodiversity, Dermal fibroblast, Biological properties.

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Synthesis, crystal structure, vibrational and optical properties of a new Bi(III) halide complex: $(C_9H_{13}N_2O_2)_2Bi_2Cl_8$

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A new Bi(III) halide complex, $(C_9H_{13}N_2O_2)_2Bi_2Cl_8$, was successfully grown by slow evaporation method. The structure of this hybrid compound was determined by single-crystal X-ray diffraction. This compound crystallizes in the monoclinic system $P2_1/n$ space group with the following lattice parameters: a = 10.2036(4), b = 9.8723(4), c = 14.5920(6) Å, β = 99.899(4)°, V = 1448.01(10) Å^3 and Z = 2. The crystal structure of this compound was solved by direct methods and refined to R = 0.038 (wR = 0.079), based on 4118 unique observed reflections. The crystal structure consists of a 1-(2-furoyl)piperazinium cation and discrete (0D) anion built up of edge-sharing bioctahedra which are linked by bifurcated N-H…Cl and N-H…O hydrogen bonds to build up the whole molecular packing. The optical properties of this compound were studied by UV-Vis, luminescence spectroscopy and by Time Dependent Density Functional Theory studies. The vibrational properties of this compound were investigated by Infrared and Raman spectroscopy and compared with the calculated ones. The nature and amount of contacts in the crystal packing were investigated by means of the Hirshfeld surfaces.

Keywords: Bismuthates, X-ray diffraction, Vibrational studies, DFT calculations, Luminescence

Mixing enthalpies of solid solutions (Cs_{1-x}, Tl_x) NO_3 at 298.15 K

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The determination of consistent thermodynamic properties is of paramount importance to both experimental and theoretical levels. In this context, the study of the consistency between the phase diagram and the thermodynamic properties of many systems is currently used.

Thermodynamic properties of the solid phases in $CsNO_3$+$TlNO_3$, for example, are useful in the study of this system which is characterized, in particular, by the existence of continuous solid solutions $\alpha(Cs_{1-x},Tl_x)NO_3$ stable in the temperature range T = (298 to 400) K [1]. So, we are interested, in this work, to determining, at 298.15 K, the mixing enthalpies of these solid phases. Direct measurements of these thermodynamic quantities are impossible. They can be deduced from the measurements, in the same solvent, of the solution enthalpies at high dilution of the solids α (Cs_{1-x},Tl_x) NO_3, $CsNO_3$ and $TlNO_3$. These measurements were performed using a C80 microcalorimeter.

A positive and asymmetric deviation from ideality is observed.

KEYWORDS: solid solutions, solution enthalpies, high dilution, C80 micro calorimeter, positive and asymmetric deviation.

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Combustion synthesis of nanosized Ag-doped Co_3O_4 as organic dyes degradation catalysts

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The development of nano-sized cobalt oxide powders such as Co_3O_4 have high potential for use as catalysts, magnetic materials, or electro-chromic devices, and this is due to their electronic and magnetic properties and their great capability as a photo-catalyst [1].

Among the various metals that could be incorporated in the spinel lattice, the use of silver ions as doping agent for Co_3O_4 was found to be beneficial for both photo-luminescent and photocatalytic organic dyes degradation [2].

In the present work, a series of Ag doped Co_3O_4 ($Ag_xCo_{3-x}O_4$, $0 \leq x \leq 3$) were prepared by the one step Solution Combustion Synthesis using glycine as fuel.

The obtained black powders were investigated by DRX, SEM-EDAX, FTIR and chemical analyses of oxygen non-stoichiometry and Co mean valency. The incorporation of Ag^+ ions favors the segregation of metallic silver and the surface enrichment of Co^{2+} cations. The catalytic performances of the Ag-modified Co_3O_4 were evaluated in the decomposition of methylene blue dyes. Our results showed that the most active catalyst is obtained for $AgCo_2O_4$ composition thanks to the co-presence of high Co^{2+} ion content and the segregation of metallic silver which promotes the electron mobility and radical formations that are responsible of methylene blue decomposition.

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Synthesis of hybrid perovskites by Sonochemistry: Effect of solvent

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Organic-inorganic hybrid materials are rapidly emerging as a new area of research of particular interest in materials science, including many fields of application such as optics, electronics, energy storage and conversion, catalysis, and sensors.

Within a few short years, hybrid perovskites have already shown enormous potential for fascinating basic and applied research [1]. Today, the energy issue receives the most attention on most of the world's environmental issues. In order to solve this problem, the renewable energy field had to integrate hybrid materials [2].

Indeed, most of the methods used for the synthesis of hybrid perovskites are complex and multi-step and require the use of multiple reagents. The sonochemistry method is not only a simple and reproducible method, but also it satisfies the criteria for green chemistry (chemistry without waste). Furthermore, sonochemistry is eligible in terms of cost and synthesis time.

However, it should be noted that studies relating to the synthesis of hybrid perovskites have used a variety of organic solvents in the synthesis. For this reason, we will concentrate on applying this method to hybrid perovskite ($MAPbCl_3$) synthesis by changing the chemical nature of the solvent and sonochemical synthesis conditions.

Key words: Hybrid perovskites, 3D, $MAPbCl_3$, solvent, sonochemistry.

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Decomposition mechanism of hydroxychloroquine in aqueous solution by gamma irradiation

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For removing pesticides and pharmaceutical products, the gamma irradiation technique is one of the advanced oxidative processes. Radiolytic degradation generates free radicals, which facilitate molecular lesion and break the chemical bonds. The use of hydroxychloroquine (HCQ), a pharmaceutical compound, was increased due to the Covid 19 pandemic situation. The aim of this study focused on gamma radiation-induced degradation of HCQ in aqueous solution. The degradation was monitored by High Performance Liquid Chromatography using an Eclipse XDB-C18 column and a mobile phase composed of 94% water (phosphate buffer) and 6% acetonitrile. The effect of different gamma radiation doses (0.05-3 kGy) was investigated. Chromatographic analysis shows that 1 kGy dose is effective to degrade completely HCQ at 20 ppm, following a first-pseudo kinetic order. LC-QToF-MS/MS identified the intermediate products and their kinetic constants were determined. A mechanism pathway was proposed for HCQ degradation under gamma irradiation in aqueous solution.

Keywords: Hydroxychloroquine; γ-irradiation; kinetic rate; LC-MS/MS; mechanism pathway.

A study of recycled low-density polyethylene membrane performance in vacuum membrane distillation unit powered by solar energy

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The lack of water resources present the biggest problem nowadays. Vacuum membrane distillation (VMD) presents an innovative process that must be adopted to cope with the lack of water with low energy consumption, since this process has the advantage of being easily coupled to an alternative energy source such as solar energy, or it has the problem of expensive membranes. In this context, the objective of this work is the modeling and simulation of VMD with recycled low-density polyethylene (R-LDPE) flat sheet hydrophobic membrane module unit coupled to solar energy. The developed model is solved by Matlab software. The obtained results of the simulation allow the studying of the permeate flux of the RLD-PE membrane in the function of the seawater feed temperature variations and the vacuum pressure. Compared to another membrane permeates, the obtained permeate, that reaches 1.6 kg/m².h, encourages the use of this type of membrane with is friendly to the environment and with low cost.

Key words: Vacuum membrane distillation, recycled low-density polyethylene, flat sheet membrane module, feed temperature, permeate flux.

Novel zeolite prepared using Tunisian raw clay: Study of C3H6 breakthrough dynamic adsorption onto zeolite material

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In this study, Tunisian raw clay (RC) was employed as a low-cost source of Si and Al in the synthesis of Faujasite zeolite (FAU syn) by means of the alkaline fusion method. Optical analysis was performed by means of a Scanning Electron Microscope and showed zeolitic crystals, with well-defined hexagonal morphology. The elemental analysis obtained via energy dispersive X-ray (EDX) proved the presence of principle elements of zeolitic structure (Al, Si, Na, O). The potential effect of bed height (10–18 cm) on the column performance was investigated. A model based on adsorbent pore diffusion, the langmuir isotherm without the axial dispersion was adapted to describe and predict column input. The model was implemented and solved numerically by Comsol Multiphysics software. The predicted breakthrough curve matched well the experimental data ($R^2=0.978$).). a few degrees discrepancy between the model and experimental data was attributed to the axial dispersion.

Keywords: adsorption, clay, comsol, modeling, zeolite

Ibuprofen retention using Biobased polymer From spent coffee grounds

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Over the past few decades, there has been a lot of interest in the use of biomaterials produced from lignocellulosic biomass in the treatment of water. These natural raw materials are attractive since they can be produced from renewable and nontoxic sources. Locally available materials, industrial byproducts, and even waste materials can be utilized as raw materials [1].

In this work biolignin was isolated from spent coffee grounds (SCG) and chemically modified using phenolation and acetylation. Different samples of lignin were used as adsorbent for Ibuprofen sodium salt from aqueous solution. Infrared Fourier-transform spectroscopy (FTIR), elemental analysis, solid-state 13C cross-polarization magic angle spinning (13C CP/MAS) NMR, and thermogravimetric analysis (TGA/DTA) were all utilized to examine the chemical composition and thermal stability of the isolated biomaterial. Various samples' surfaces were analyzed using field emission scanning electron microscopy (FESEM). The lignin's performance for adsorption of ibuprofen sodium salt was carried out. Also, theoretical modeling of isotherms investigation was realized.

Key words: .lignin, adsorption, spent coffee grounds, ibuprofen sodium salt.

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Design, modeling and simulation of a multi-concentrator solar water heater

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Given the promising prospects of the solar thermal in the residential sector, a new design of a solar water heater with a multi-concentrator collector has been studied. Each concentrator consists of three composite parabolic reflectors (CPC). This geometry has the effect of further minimizing thermal losses and concentrating the solar radiation captured on a focal plane of the absorber. A theoretical model describing its behavior is then developed. The solar water heater is then simulated under different conditions. For a collector geometric concentration factor C equal to 2.5, the temperature profile of the various components is similar to the solar flux curve. The highest absorber temperature is equal to 78 °C at 2 p.m., is reached 2 hours later compared to the maximum value of global solar flux. The maximal mass flow rate is reached at 1 p.m. and is about 0.012 kg / sec. The obtained results highlight the influence of the concentration on the various parameters which allows us to determine the optimal geometric characteristics of the collector. Finally, we carried out a comparative study of our system with other devices without concentration, which makes it possible to show the thermal and economic performances of the designed prototype. The results show that the multi-concentrator collector has a higher thermal efficiency than a tube collector for a standardized gain greater than 0.1 and much larger than the flat plate collector.

Key words: Solar Energy, Modeling, Multi-Concentrator, Parabolic Branch, Performance

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Heterostructured nanocomposite synthesized through ultrasonic-assisted method: Awards photocatalytic hydrogen production

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The evolution of hydrogen (H_2) from water under sunlight has been the target of promising methods for supplying renewable energy sources and decreasing the negative repercussions of global warming [1][2]. In this study, we fabricated $CdS/g\text{-}C_3N_4/ZnFe_2O_4$for hydrogen production from water by the visible light illumination. Firstly, the $CdS/g\text{-}C_3N_4/ZnFe_2O_4$ nanocomposite was synthesized via the ultrasonication procedure. Secondly, the crystal structure, morphology, chemical valence, and functional groups of all samples were examined by XRD, SEM, HRTEM, XPS, FTIR, UV–Vis, PL spectroscopy, etc. The electrochemical behaviors of all samples were measured via EIS, LSV, photocurrent, Tafel, etc. techniques. Finally, the hydrogen evolution rate of all samples was analyzed by gas chromatography and it was determined that the $CdS/g\text{-}C_3N_4/ZnFe_2O_4$ nanocomposite had the highest hydrogen production rate with 405 µmol g^{-1} under visible light.

Key words: $CdS/g\text{-}C_3N_4/ZnFe_2O_4$, photocatalytic hydrogen evolution, charge separation

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Synthesis of n-type Ag_2ZnSnS_4 thin films by thermally evaporated process for solar cell applications

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Special interest has been recently devoted to the quaternary material Ag_2ZnSnS_4 (AZTS) due to its remarkable electrical and optical properties. Our study proposes a new method for the synthesis of AZTS thin films by thermal vacuum evaporation on soda-lime glass (SLG) substrates by tuning their thickness. Structural characterization of the thin films, performed by X-ray diffraction and Raman spectroscopy, confirmed the presence of the AZTS stannite phase with the appearance of the Ag_8SnS_6 secondary phase. As the thickness increases, a transition from the amorphous to the crystalline state appears in the XRD spectra, along with an increase in intensity related to a refinement of the preferential peak (112), an increase in crystallite size, and a decrease in stress and dislocations. Compositional analysis confirms the stoichiometric composition of the films. Atomic force microscopy (AFM) and SEM images reveal a strong thickness dependence of the film surface structure. Moreover, the thickness affects significantly optical properties of the films. In particular, an increase of the absorption coefficients associated with a decrease of the direct gap energy and of the Urbach energy is observed with increasing thickness. The optical and dielectric constants have been studied and discussed in more detail based on the single oscillator model proposed by Wemple DiDomenico and other models. Finally, all samples display n-type conductivity according to the hot probe experiment. Such attractive characteristics can be useful to further improve the efficiency of thin film solar cells by adjusting the thin film thickness.

Key words: AZTS, Thermal evaporation, Structural properties, Optical constants, thickness.

Occurrences and origin of oil seeps and new marks of petroleum impregnations in Northwestern Tunisia: Implications from aliphatic biomarkers and statistical modelling

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Northwestern part is the tectonically impacted region in Tunisia, showing numerous hydrocarbon seeps. The aim of this study is to find a genetic connection between these oil seeps and the potential source rocks in the region. Here we report the organic geochemical data of eighteen oil seeps samples and four source rocks (M'Cherga, Fahdene, Bahloul, and BouDabbous) using aliphatic biomarkers evaluated by GC-MS. Terpanes, hopanes, and steranes biomarkers were identified and statistical analysis was performed to establish oil-oil and oil-source rock correlations. The studied source rocks are derived from a marine environment of deposition, under suboxic conditons, with some traces of continental input for M'Cherga Formation. These source rocks are mature and have entered the oil window, according to C27 18–22,29,30-trisnorneohopane (Ts) and C27 17–22,29,30-trisnorhopane (Tm) biomarkers. About oil seeps, geochemical data suggest that the majority of samples were deposited in an open marine environment, with the exception of four samples that had some continental marks. These latest oil seeps samples have a distinctive lithology (marl) that sets them apart from the rest (carbonate). Statistical study of oil-oil and oil-source rock correlations reveals the existence of two classes of oil seeps. The first included samples that had a positive correlation with BouDabbous black shaleshaving a marine origin and a carbonate lithology. The second is due to M'Cherga source rock and consists of oil seeps with terrestrial traces and a marl trend lithology. The studied oil seeps have no relationship with the Fahdene and Bahloul source rocks. Besides the presence of two generations of hydrocarbon spills in northwestern Tunisia (Lower Cretaceous/ Ypresian), there are two types of hydrocarbon spills based on their relationship to tectonic deformations (oil seeps) and outcropping mature source rocks (oil impregnations).

Key words: Oil seep, Impregnation, Source rock, Biomarker, Statistic, Northwestern Tunisia.

Performance and exhaust emissions of an Internal Combustion IC engine operated with Olive Pomace pyrolysis oil

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This study investigates the use of Olive Pomace (OP) pyrolysis oil as a renewable fuel in internal combustion engines. OP pyrolysis oil was mixed with pure diesel (designated B0). The mixture used, B10 containing 10% by volume of biofuel, was tested. This article focuses on the experimental study of the performance, gaseous and particulate emission characteristics of a diesel engine using OP pyrolysis oil as a partial replacement of conventional diesel fuel. All experiments were carried out with a constant engine speed (1500 rpm). Three different engine loads were tested. Using B10 at a high engine load resulted in a lower Particulates and CO_2 emission levels, respectively by 13.2 and 3.4% compared to that of pure diesel. In addition, the thermal efficiency obtained with B10 was higher than that of diesel with a maximum value of 34.3 % obtained at 3.8 Kw. The obtained results was compared with literature[1], [2][3], [4]

Key words: Biofuel-Diesel Blend, Emission, Internal Combustion Engine, Olive Pomace

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Experimental investigation of Date palm wastes by pyrolysis: Date Palm Leaves and Date Palm Leaf stems

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Abstract- Date Palm Leaves DPL and Date Palm Leaf Stems DPLS are widely available biomasses in Tunisia. Their thermo-chemical valorization by pyrolysis is very interesting due to their chemical characteristics, abundance and applications [1, 2]. In fact, pyrolysis is a thermo-chemical process which allows the production of oils, gases and coals under defined operating conditions. In this study, the pyrolysis of these date palm residues in a fixed bed reactor under inert atmosphere was investigated. Date palm residues were heated from room temperature to 500 °C, with 10 °C/min as a heating rate. The physiochemical characteristics of the feedstock were determined, discussed and compared. Elemental analysis showed that DPL contained higher amounts of Carbon (46.57 %) and Hydrogen (5.66 %), lower amount of Oxygen (46.76 %) and therefore higher High Calorific Value HCV (17.60 MJ/kg) comparing to DPLS. Under the same operational conditions, DPLS produced higher bio-oil yield (29.68 wt%), lower bio-char (40.28 wt%) and syngas (30.04 wt%) yields comparing to DPL. The gaseous products were analyzed using a micro-GC analyzer. Syngas chemical composition was determined and discussed. The obtained results were compared with other published works in the literature [1, 2, 3, 4, 5].

Keywords: Date Palm Leaves, Date Palm Leaf Stems, pyrolysis, syngas.

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Synthesis and molecular docking study of new sesquiterpene coumarin arylidene conjugates from the natural coladonin

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Some plants containing sesquiterpene coumarins are used in the form crude drugs for traditional medication such as *Ferula* species. Sesquiterpene coumarins, naturally present in many plants, possess anticoagulant, antimicrobial, antioxidant, anti-inflammatory, anti-allergic and anticancer properties [1]. *Ferula tunetana*, an endemic Tunisian plant, belonging to the Apiaceae family, presents interesting phytochemical futures, as the occurrence of sesquiterpene coumarins such as coladonin [2]. This secondary metabolite was cited to be an acetylcholinesterase inhibitor, antibacterial and cytotocix against HCT-116 and HT-29 [2, 3]. In view of the broad biological importance of coladonin, we proposed to isolate it from the roots of *F. tunetana* and to investigate the behavior of its oxidized derivative towards a series of aryl aldehyde. All products were identified by spectroscopic (1D and 2D NMR) and spectrometric (ESI-HRMS) methods. The anti-α-amylase activity of all the synthesized products was predicted by means of molecular docking and the structure-activity relationship was also discussed.

Key words: *F. tunetana*, coladonin, arylidenes, anti-α-amylase, molecular docking.

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Chemical variability and antioxidant activities of spontaneous and cultivated *Rosmarinus officinalis* essential oils according to the geographical origin of their exploited organs

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The present study described the variation of the chemical composition of different organs essential oils from cultivated and spontaneous *Rosmarinus officinalis* collected from some regions of the south of Tunisia as well as the evaluation of their antioxidant activities. These essential oils were isolated by hydrodistillation from different organs (stems, leaves and flowers) of *R. officinalis* collected at the flowering and the vegetative phases and analyzed by gas chromatography (GC) and gas chromatography-mass spectrometry (GC–MS). Twenty-nine compounds were identified in these essential oils representing from 88.3 to 99.3% of the total essential oil in which five chemotypes were assigned to different organs essential oils of rosemary collected from some locations of Tunisia (camphor, camphor/borneol/α-terpineol/α-eudesmol, camphor/borneol/α-terpineol, camphor/borneol/bornyl acetate/α-eudesmol and camphor/borneol/α-terpineol/caryophyllene). Furthermore, the antioxidant activities of all essential oils samples were evaluated using the DPPH assay and the reducing power test. Thereby, it is interesting to emphasize that all studied essential oils presented very important antiradical activity (IC50=0.093-0.623 mg/ml) and reducing power (EC50 = 0.121-0.523 mg/ml). Indeed, our results showed clearly that the flowers essential oil of Majoura city exhibited the highest antiradical activity whereas the leaves essential oil of Majoura showed the highest reducing power at the vegetative phase. These results suggest that the chemical composition of the studied essential oils of *R. officinalis* is strongly correlated to their antioxidant activities as well as these essential oils have potential to be used as a natural antioxidant agent.

Keywords: Antioxidant activity, Chemical composition, Essential oils, Geographical origin, *Rosmarinus officinalis.*

Extraction, physicochemical characterization and biological activities of chondroitin sulfate

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Chondroitin sulfates (CS) have attracted considerable interest in recently years due to their potential therapeutic applications and structural heterogeneities [1]. Indeed, the CS from avian origin *(Gallus gallus, Meleagris gallopavo)* was isolated, characterized and essayed for antioxidant activity, anti-inflammatory activity and anti-nociceptive activity. Chondroitin sulfate was extracted from the species by digestion with papain followed by precipitation with cetylpyridinium chloride and ethanol and was subjected to electrophoresis on cellulose acetate, then the structure was characterized by FT-IR and physicochemical procedures, Molecular weight measurements were performed by SEC-MALLS. The antioxidant activity was studied by three tests (DPPH, ABTS and FRAP). Then, the *in vivo* anti-inflammatory activity was evaluated by the paw edema test in rats and finally test the anti-nociceptive activity in rats using the Von Frey test. The results showed that the chemical structure of this CS is also characterized by a remarkable negative charge density due to the abundance of sulfate groups and by a weight average molar mass (Mw). The results of the study of the biological activities of the CS show that this polysaccharide in the two species is endowed with a remarkable antioxidant, anti-inflammatory, anti-nociceptive activity. Extracts show different anti-radical activities depending on their origin. Thus, they constitute an antioxidant molecule and can have valuable anti-inflammatory properties in the field of osteoarthritis pathology.

Keywords: Chondroitin sulfate, *Gallus gallus, Meleagris gallopavo,* antioxidant activity, anti-inflammatory activity *in vivo*, anti-nociceptive activity

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UPLC-ESI-MS/MS polyphenolic profile and antioxidant activities of Pistachio female leaves extracts obtained by microwave assisted extraction

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Pistacia vera L. is well known for its beneficial health properties, which are mainly related to polyphenols that have accumulated in all parts of the plant. Pistachio production in Tunisia has generated a large amount of potentially valuable waste that could be used as a source of bioactive compounds. The present work aims at a chemical characterization of female leaves of *Pistacia vera* L. leaves were used to extract the secondary metabolites using an unconventional method called microwave assisted extraction. Microwave-assisted extraction is a rapid and effective green extraction method for isolating plant polyphenols. The polyphenolic profile was evaluated by UPLC/ESI-MS-MS and the antioxidant capacity was measured by DPPH and FRAP assays.

The polyphenolic profile of female leaves extracts included different compounds, with phenolic acids, flavonoids and its derivates (quercetin, myricetin and apigenin). Antioxidant assays showed higher antioxidant capacity for *Pistacia vera* L. leaf extracts.

Thus, female leaves of pistachio tree are a rich source of phenolic compounds and have strong antioxidant capacity, so their extracts obtained by microwave-assisted extraction method could be used in different applications such as medicine, cosmetics and food industries.

Key words: microwave assisted extraction, phenolic compounds, UPLC/ESI-MS-MS, antioxidant activity.

Structural studies and electrical and optical properties of $LaSrSnInRuO_9$ simple perovskite prepared by the mechano synthesis route.

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The double substitution of the B site, simultaneously, with the single substitution of the A site in the single perovskite "$SrSnO_3$" allowed the synthesis of a new single perovskite $LaSrSnInRuO_3$ by the solid-solid process. The crystal structure was confirmed by X-ray powder diffraction using the Rietveld refinement method and vibrational analysis by infrared absorption spectroscopy (IR). The band gap value of 1.37 eV, determined by UV-visible spectroscopy indicates a rather conductive behavior. Microstructural evaluation of the prepared compound, by Scherrer formula and Williamson-Hall method, affirms the nanometer sizes of the crystallites, calculated from the X-ray diffraction line profiles and provides the value of the macrostrain. The SEM reveals the morphology and size distribution of the obtained $SrSnO_3$ nanoparticles, and also justifies the nanometric size as well as the material formula.

Keywords: Stannate perovskite, Retvield analysis, UV-visible

Synthesis, structural studies, conduction properties of double perovskites based on calcium stannate $SnCaO_3$ substituted with rare earths and transition metals: CaNd2Fe2SnO9, NdCaFeSnO6, Ca1±x Nd1±xFeSnO6 and CaNdFe1±x Sn1±x O6 with (0.25< x<0.75)

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The perovskite structure is widely studied since several decades and a myriad of materials presenting this structure are used in numerous applications. These materials can in particular be used as capacitors, anodes for fuel cells, catalysts, mantellic perovskite analogues (Bridgemanite), photovoltaic cells or even as matrix for nuclear waste storage. The perovskite structure can be described as simple (ABO3) or complex (A'A"BO6, AB'B"O6, A'A"B'B"O6, …) depending on the chemical composition and the atomic arrangement of elements in the structure. The addition of trivalent ion Nd3+ in the A site and iron in the B site in the simple perovskites Ca2+Sn4+O3 induces structural modifications and problems of charge compensation. The crystallochemical study of these substituted perovskites is necessary to understand the physical properties of these materials.

Keywords : DoublePerovskite; XRD; Rietveld refinement; Gap energy; IV measurement.

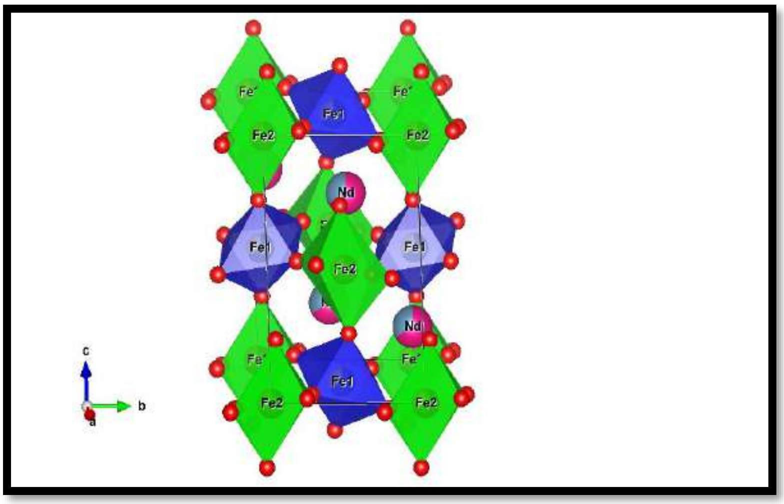

Figure: P21/c structure of CaNd2Fe2SnO9 and CaNdFeSnO6

Natural cellulosic fiber from Alfa (Stipa Tenacissima): Extraction and characterization

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Modification of natural polymers as the cellulose and its derivatives are considered as a very useful way to enhance their properties and to extend the field of their applications.The aim of this work is to extract cellulose nanofibrils from Alfa (Stipa tenacissima) after several treatments including purification, delignification\bleaching by chlorite and alkaline extraction of hemicelluloses.The resulting CNs was characterized using the X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR) and Scanning electron microscopy (SEM).

Key words: Polymers - Hemicelluloses - Cellulose – Nanofibrils

Investigation of optical, dielectric and conductivity studies of new $Sr_2Sn_{1.33}In_{0.33}Ni_{0.33}O_{6-\delta}$ double perovskite

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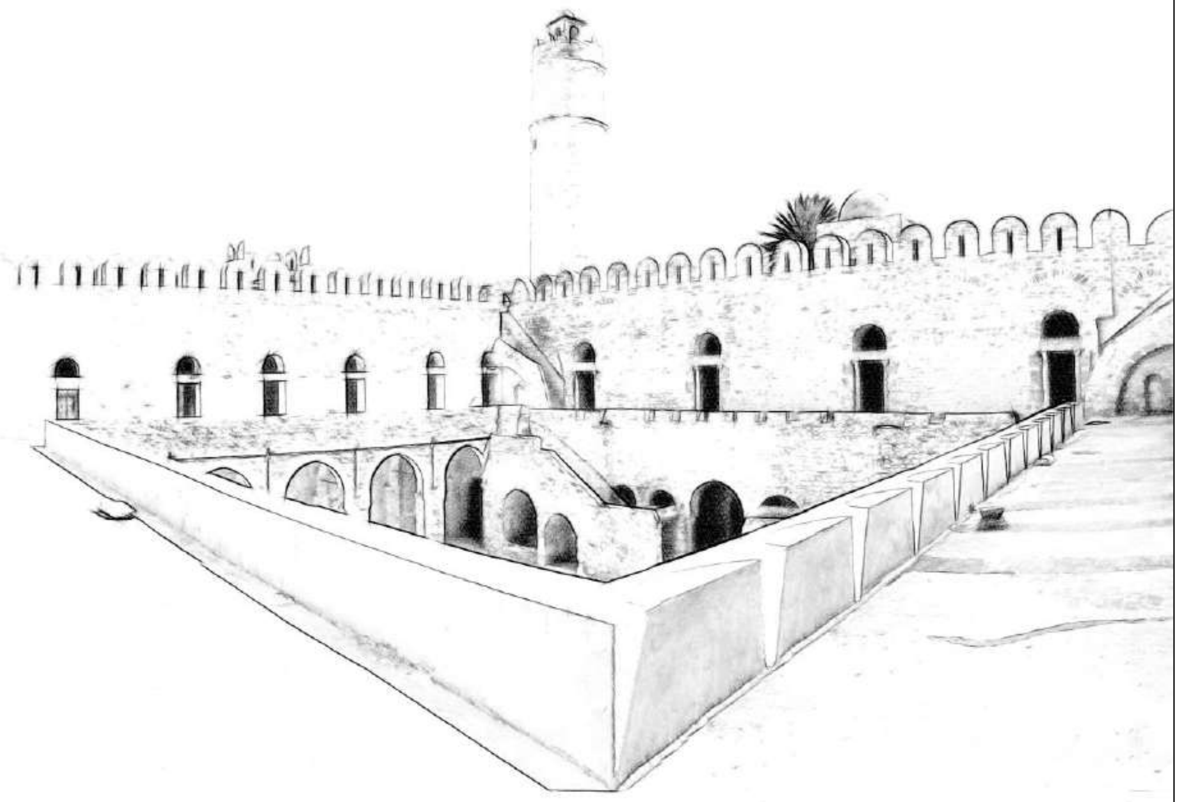
$Sr_2Sn_{1.33}In_{0.33}Ni_{0.33}O_{6-\delta}$ double perovskite oxide is prepared by solid state reaction. The synthesized sample is subjected to structural, optical, and electrical properties. Rietveld refinement of XRD data shows monoclinic phase under $P2_1/c$ space group. The structure is best described as a √2ap x √2ap x 2ap distorted perovskite with an arrangement of B cations that produces distinct (tin/Nickel)-oxygen and (tin/indium)-oxygen layers. FTIR spectroscopy studies show the presence of vibrations of B/B'–O around 487cm^{-1}. UV-Vis study of the sample illustrates a wide bandgap semiconducting nature of sample of 3.6 eV.

The dielectric analysis and electrical conductivity of the sample are carried out at different temperatures and frequencies using the complex impedance spectroscopy technique. The Nyquist plots (- Z'' vs. Z') revealed the presence of the contribution of the grains and the grain boundaries in the conduction mechanism. The temperature dependence of the bulk conductivity was found to obey the Arrhenius law with activation energie E_a = 1.93 eV

Keywords: Stannate perovskite, Retvield analysis, UV-visible, semiconductor, Complex Impedance spectroscopy



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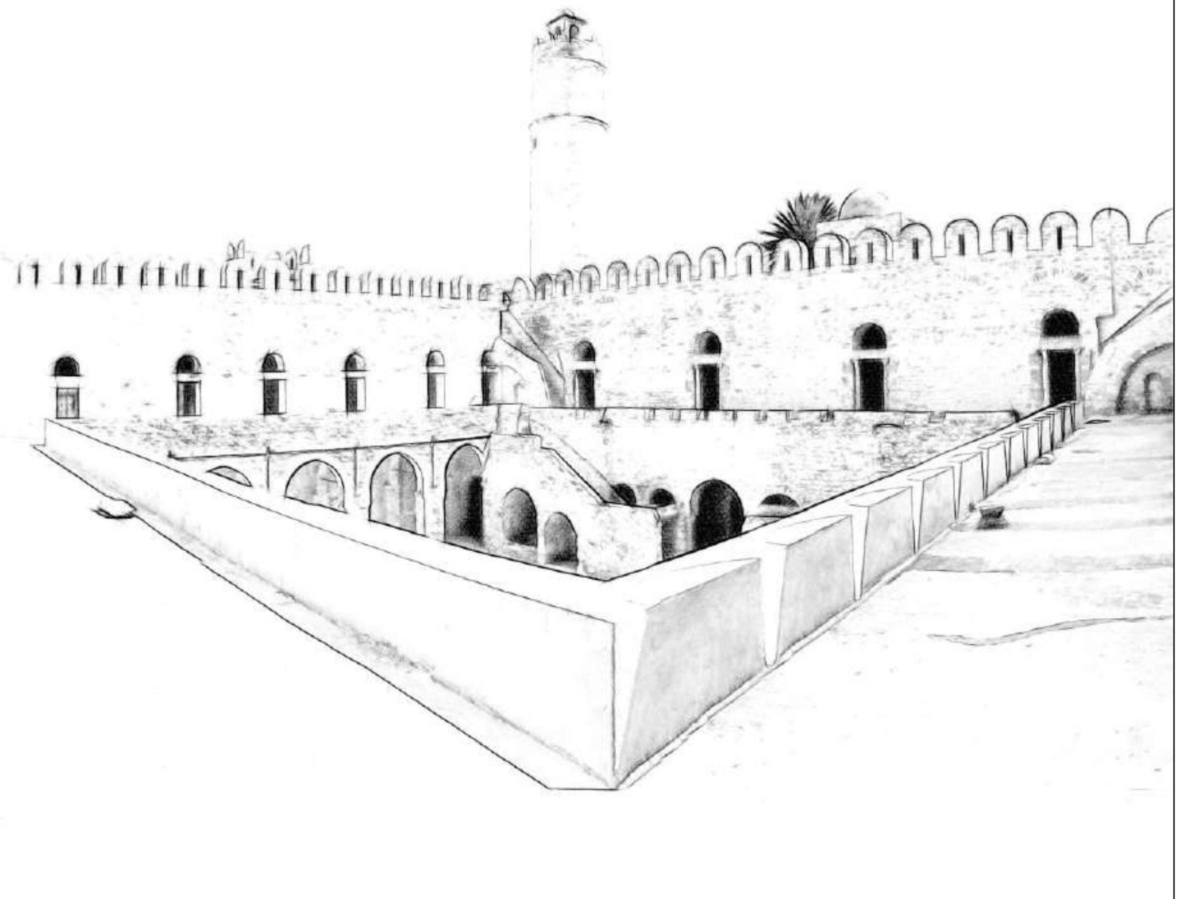

Abstracts of Poster Communications

Bisphosphonylallenes as suitable scaffolds for unprecedented 4,5-diphosphonyldihydropyridazines and 3,4-diphosphonylpyrroles displaying anti-melanoma activity

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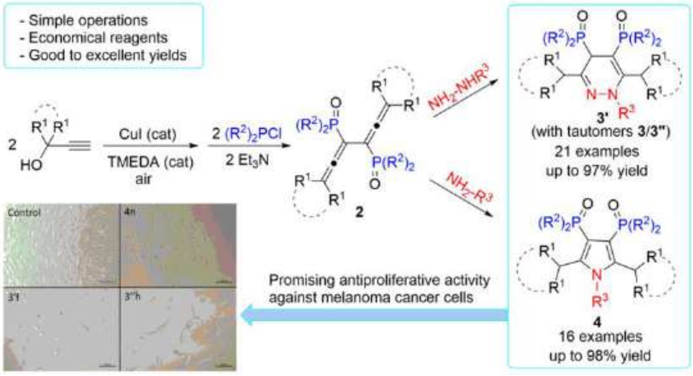
Allenyl-phosphonates and -phosphine oxides, an important subclass of allenes, are recognized as powerful building blocks for the synthesis of a wide variety of molecules of commercial significance. Over the past few years, allenyl-phosphonates and -phosphine oxides have been involved in diverse organic transformations. In particular, their heterocyclization reactions have emerged as powerful tools for the construction of a wide range of valuable phosphorylated heterocycles.[1] However, bisallenyl-phosphonates and -phosphine oxides were much less studied and their reactivity remains underexplored, despite their unique structure which suggests the possibility of many heterocyclization reactions that could lead to novel diphosphonylated heterocycles with good therapeutic or metal-complexing potential. With this in mind and in the continuation of our studies on the synthesis and reactivity of bisphosphonylallenes,[2] we now report an efficient and simple approach to unprecedented 4,5-diphosphonyldihydropyridazines and 3,4-diphosphonylpyrroles, through the condensation of bisphosphonylallenes with hydrazines and primary amines, respectively (Scheme 1). The salient features of these syntheses include high yields, simple operations, mild and catalyst-free conditions, and broad substrate scope, which make these protocols more amenable for high throughput library synthesis. The synthesized compounds were screened for their antiproliferative activity against melanoma cancer cells, and they showed promising growth inhibition.



Scheme 1. Synthesis of 4,5-diphosphonyldihydropyridazines and 3,4-diphosphonylpyrroles

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Physico-chemical characterization of an Algerian biomass, application in the adsorption of an organic pollutant

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The objective of this work is to study the retention of methylene blue (MB) by biomass. The effect of certain physico-chemical parameters on the adsorption of MB is studied. This study shows that the increase in the initial concentration of MB leads to an increase in the adsorbed quantity. The adsorption efficiency of MB decreases with increasing biomass mass. The adsorption kinetics shows that the adsorption is rapid and the maximum amount is reached after 120 min of contact. It is noted that the pH has no great influence on the adsorption. The isotherms are best modeled by the Langmuir model. The adsorption kinetics follows the pseudo-second order model. The thermodynamic study of adsorption shows that the adsorption is spontaneous and exothermic.

Keywords: dyes, adsorption, biomass, methylene blue, Langmuir.

Multi-Substituted Imidazoles: Green Optimized One-pot Synthesis Via Recycled Magnetic Functionalized Nanocellulose Catalyst and Their Use as Chromogenic and Fluorogenic Probes for Metal Cation's Detection

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In this contribution, we report the design of magnetic functionalized Nanocellulose by an in-Situ approach. The fabricated polymer matrix was utilized as an efficient heterogeneous catalyst for one-pot multi-component synthesis of fluorescent multi-substituted imidazoles under green optimized conditions. The eco-friendly protocol afforded, short reaction times, excellent yields and catalyst easy recycling through magnetic recovery. The geometric optimization, MEP and FMOs have also been carried out at B3LYP-D3/6–311++G (d, p) level of Density Functional Theory simulations in ethanol to elucidate the substituent's effect on molecule's planarity, surface studies, their electronic structure as well as their intermolecular charge transfer. Furthermore, the synthesized multi-substituted Imidazole derivatives exhibited remarkable fluorescent properties explored in cation metal's chromogenic and fluorogenic detection.

Keywords: Magnetic Functionalized Nanocellulose, Heterogeneous Catalysis, Optimized Protocol, Fluorescent Substituted Imidazoles, Chromo-Fluorogenic Detection

Voltammetric study of hydroxychloroquine oxidation in aqueous media

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Hydroxychloroquine (HCQ) is a medical active ingredient marketed under the name Plaquenil in Tunisia. It is prescribed for certain types of malaria and for covid-19. High doses of this drug can cause alopecia and aplastic anemia because it can affect immune function. Different techniques can be applied to the detection of HCQ in various samples, but they are generally complicated and expensive. Therefore, there is still a need for other methods of determination of this drug. Cyclic voltammetry (CV) and square wave voltammetry (SWV), two fast and environmentally friendly electrochemical methods, can be used for analysis of HCQ with a good degree of sensitivity.

The present work deals with the study of the performance of boron-doped diamond (BDD), glassy carbon (GCE) electrodes for the analysis of aqueous solutions containing HCQ. The effect of different parameters such as pH, drug concentration, potential seep rate (for CV) and frequency (for SWV) was studied. The CV study of aqueous HCQ solutions revealed the presence of a single irreversible oxidation peak related to two electrons transfer for both working electrodes. In addition, charge transfer coefficient α is calculated. It is equal to 0.385 and 0.468 for the BDD and GCE respectively; this result can be in agreement with the irreversible peak. Furthermore, after optimization of experimental parameters for SWV, limit of detection (LOD) and limit of quantification (LOQ) was investigated. They are respectively equal to 5.96 and 19.86 $\mu mol.L^{-1}$ for GCE and 1.31 and 4.36 $\mu mol.L^{-1}$ for the BDD electrode. In this latter case, values of LOD and LOQ are low enough for specific analyses comparable to other analytical techniques.

Keywords: Hydroxychloroquine; Electrochemical analysis; Boron doped diamond electrode; Glassy carbon electrode; Limit of detection; Limit of quantification

Theoretical Study of The Pentavalent Halosiliconate: Structure and Charge Delocalization

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This study was performed to detected the pentavalent silicon center in the structure of the pentavalent-halosiliconate R-O-Si$(CH_3)_3X^-$ and the halotrimethylsilyloxyfurane structures (X-TMSOF), (X = F^-; Cl^-; Br^-) and (R = CH_3-; CH_2-CH_3; -$CH(CH_3)_2$; -CH=CH_2; C_6H_5-). DFT calculations at the B3LYP/6-31G(d) level were caried out to understand their structures and their charge delocalization. These intermediates were obtained by attacking the silicon center in trimethyl-alkoxysilanes and trimethyl-silyloxyfurane with halogen ions X^-. The results obtained show that the attack by F^- generates a more stable structures because of the strength Si-F bond. In the case of Br^- and Cl^- the structure of intermediates appears as an interaction between the ions and the silicon center. NBO analysis shows that one of the lone pairs of F^- takes part in Si-F bond formation. However, the lone pairs of Br^- and Cl^- did not contribute to generate a real bonding.

Key words: DFT, pentavalent halosiliconates, Si-F bond, NBO, charge delocalization.

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Hexa[4-methylimidazolium] decavanadate trihydrate : Synthesis, structure, physico-chemical characterization and anticancer activity against human glioblastoma

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Decavanadates are a subgroup of polyoxovanadates with interesting pharmacological actions that have been widely studied both in vitro and in vivo as a treatment for several global health problems such as diabetes, cancer, and Alzheimer's disease. In the present study, we have synthesized an hexa[4-methylimidazolium] decavanadate trihydrate, $(C_4H_7N_2)_6V_{10}O_{28}\cdot3H_2O$ for an eventual therapeutic application. The structure of this compound has been characterized by: crystal X-ray diffraction, SEM-EDX, IR and UV spectroscopies. Single-crystal analysis indicates that the formula unit is composed of one decavanadate $[V_{10}O_{28}]^{6-}$ anion, six 4-methylimidazolium $[C_4H_7N_2]^+$ cations and three water molecules. The cohesion is provided by N-H···O, O-H···O hydrogen bonds, and van der Waals interactions leads to a three-dimensional structure. The Hirshfeld surface (HS) and their relative two-dimensional fingerprint plots (2D-FP) reveal that the structure is dominated by O…H/H…O and H…H contacts. Interestingly, when tested on U87 human brain cancer cells, the $(C_4H_7N_2)_6V_{10}O_{28}\cdot3H_2O$ compound inhibits its proliferation and migration at a micromolar range with an IC_{50} values of 0.53 µM.

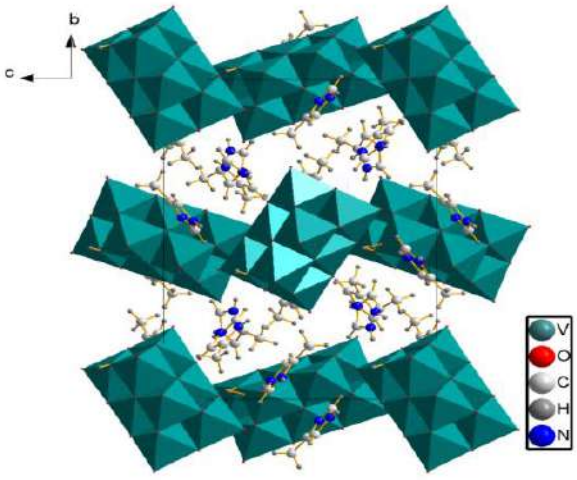

Figure 1. Projection of $(C_4H_7N_2)_6V_{10}O_{28}\cdot3H_2O$ compound along the a-axis

Keywords: Decavanadate, Crystal structure, characterizations, Hirshfeld surface, Glioblastoma, Cancer inhibitor

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Chemical composition and antiparasatic efficacy of *Ocimum basilicum* essential oil and its major constituents estragole and linalool

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The present study evaluated the acaricidal and anthelmintic action of *Ocimum basilicum* essential oil and its main components against ticks and helminth parasites as well as to relate these activities to acetylcholinesterase in-hibition. The in vitro acaricidal activity against Hyalomma scupense was evaluated by Adult Immersion Test (AIT) and Larval Packet Test (LPT), while the *in vivo* nematocidal potential was assessed in laboratory mice infected with *Heligmosomoides polygyrus* using fecal egg count reduction (FECR) and total worm count reduction (TWCR). Chemical analyzes were performed by gas chromatography coupled to mass spectrometry (GC-MS). Estragole (80.87%) and linalool (16.12%) were the major compounds detected in O. basilicum essential oil. In the AIT assay for H. scupense tick, LC_{50} of estragole, *O. basilicum* oil and linalool were 0.73, 0.81 and 0.97 mg/mL, respectively. In LPT, estragole, linalool and essential oil showed LC of 0.22, 1.11 and 1.19 mg/mL, respectively. Against *He. polygyrus*, the highest activity was observed with estragole administered at 100 mg/kg body weight (bwt), which resulted in a FECR of 90.86% and a TWCR of 82.91%. The O. basilicum essential oil, estragole and linalool inhibited the enzyme acetylcholinesterase (AChE) extracted from both parasites species. Estragole was found the most active AChE inhibitor with IC_{50} of 0.176 mg/mL for *H. scupense* and IC_{50} of 0.138 mg/mL for *He. polygyrus* larvae. The results of the present study pointed out the importance of the traditional use of *O. basilicum* as an eco-friendly alternative against endo and ectoparasites. In vivo trials should also be conducted to confirm the above- mentioned activities and to assure the safe use of natural plants.

Key words: *H. scupense*, *Ocimum basilicum*, Linalool, Acaricidal effect, Estragole, GC-MS

Nucleophilic Reactivity of 1, 3, 5-trinitrobenzene

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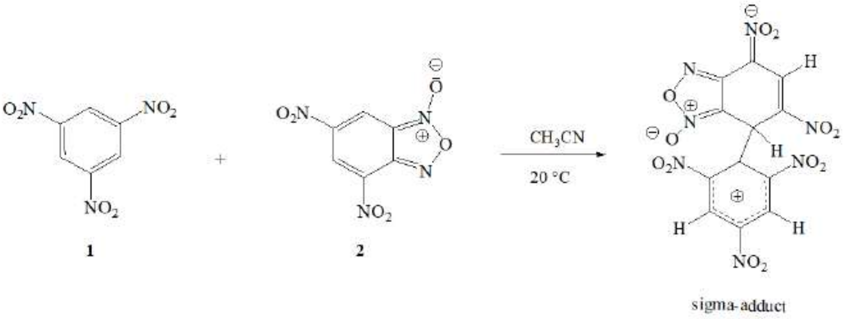
The kinetics of the reactions of 1, 3, 5-trinitrobenzene **1** with three superelectrophiles (4,6-dinitrobenzofuroxan **2**, 6-cyano-4-nitrobenzofuroxan **3** and benzhydrylium ions (mfa)$_2$CH$^+$ **4**) have been studied by UV-vis spectroscopy in acetonitrile solution at 20 °C. The reactions proceed via nucleophilic attack of the trinitrobenzene at the superelectrophiles **2-4** to give σ-adducts.

An analysis of the second-order rate constants, k, in terms of Mayr's equation [1] reveals that the compounds **2-4** can be used as reference superelectrophiles for the determination of the nucleophilicity parameters N and s_N of 1, 3, 5-trinitrobenzene.

This result is a clear reflection that the trinitrobenzene can exhibit nucleophilic reactivity towards superelectrophiles. We note that the trinitrobenzene is considered to date as the reference electrophile for S_NAr and σ-complexation processes (E = -13.19). [2]



Reaction of 1, 3, 5-trinitrobenzene **1** with the superélectrophile 4,6-dinitrobenzofuroxan **2**

Key words: Kinetics / Superelectrophiles / Nucleophilicity / Electrophilicity / σ-adduct / Equation of Mayr.

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Physico-chemical characterization and valuation of the carbonate rock of the Kefeddour formation in the Metlaoui region

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The physico-chemical study and mechanical characteristics of dolomitic formation in Oum Elkecheb (Gafsa basin) shows an important valuation.

Field observations show that the lithology of this sector is formed by an alternation of competent series such as limestones, gypsum, and dolomite and tender series such as clays, marls and phosphates.

A geochemical study shows that these rocks are distinguished by a variable proportions of minerals dominated by calcite, with the chemical formula CaCo3 and dolomite, (Ca, Mg) $(CO_3)_2$; with changes in lithology at the lower dolomitic series related to the diagenesis.

The dolomite of Oum Elkhecheb can be valued as white dolomite thanks to the important value of Caco and Mgo, this later is an white cement addition

Keywords : deposit, dolomitic formation, Oum Elkecheb, Gafsa basin, geochemical, dolomitic limestone.

Structural, electronic and magnetic properties of NiO/Fe: First Principle Investigation

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Structural, electronic and magnetic properties of NiO/Fe in the cubic structure have been investigated using the full-potential augmented plane-wave (FP-LAPW) method within the density functional theory (DFT). The exchange-correlation potential is treated by the two approximations, the generalized gradient approximation (GGA-08) and the orbital independent modified Becke–Johanson (mBj) potential coupled with GGA (mBj-GGA). Based on the energy optimization, the equilibrium lattice constants (a, c and μ) and bulk modulus B are found to be in a good agreement with experimental and theoretical values. In addition, the electronic properties (band structure, density of state and charge density) and magnetic properties (total and partial magnetic moments, exchange constant and spin polarization in Fermi level) have been also studied. Indeed, the obtained values of gap by *GGA-mBJ* for NiO/Fe compounds are given a good agreement with author experimental results.

Keyword: NiO/Fe; FP-LAPW; magnetic properties; Band-gap; DFT.

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Application of magnetic almond shell biochar as a new sorbent for magnetic solid-phase extraction of NSAIDs from aqueous solution

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In the past few years, the focus paid on sample pretreatment within green analytical chemistry links to its essential role not only in being the limiting step of the entire analytical method but to its role in overcoming analytical chemistry challenges [1]. Biochar (BC) derived from agro-wastes has attracted much attention due to its excellent adsorption capacities, ability for functionalization, low cost, and the possibility of renewability [2]. This work studies the potential of BC, as sorbent in microextraction for the determination of nonsteroidal anti-inflammatory drugs (NSAIDs) from aqueous solution. Magnetic almonds shell biochar (MASBC) was synthetized and characterized by TEM/EDX, FTIR and XRD. An experimental design was applied for the optimization of magnetic solid phase extraction process. A two-level full factorial design was used for optimizing experimental conditions such as extraction time, sample volume, eluent volume and adsorbent mass. The MASBC exhibited high relative recovery and can be reused five times without any decrease in adsorption capacity. The results demonstrate the potential use of biochar as new adsorbent in magnetic solid-phase extraction devices for the removal of NSAIDs in aqueous solution.

Key words: Biochar, magnetic solid phase extraction, NSAIDs, chemometrics, HPLC-UV.

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Phosphonothioamidates as ligands in coordination chemistry

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The phosphonothioamidates $(RO)_2P(=O)C(=S)N(H)R^1$ **L** (R =Me, R^1=Ph **L1**; R = Cy **L2**; R^1 =Et, R^1= Cy **L3**; R = Bz **L4**) have been prepared by nucleophilic addition of $K[(EtO)_2P(=O)]$ to R-N=C=S and crystallographically analyzed. These compounds **L2-4** are associated pairwise through strong intermolecular N-H···O bonding giving rise to 10-membered supramolecular macrocycles. Complexation of **L** on CuI in MeCN solution in MeCN solution affords a new polymer $[(CuI)_3$**L1**$]_n$ **CP1** and three novel complexes of type $[Cu(\mu_2\text{-}I)2Cu\{$**L2**$\}_3]$ **C1** and$[\{Cu(\mu_2\text{-}I)_2Cu\}(\}(\eta^1\text{-}$**L**$)_2]$ (**C2**,L=**L3**; **C3**,L=**L4**). The molecular structures of **CP1** and **C1-3** have been elucidated by X-ray diffraction studies, which show that the complexation of **L** on CuI occurs via the thiocarbonyl function. The dinuclear complexes $[\{XHg(\mu_2\text{-}X)_2HgX\}(\eta^1\text{-}$**L**$)_2]$ (X = Br, **C4** L = **L3** ; L = **L4**, X = Br **C5**; X = Br **C6**) were formed by stoichiometric addition of **L** to HgX_2. The molecular structures of **C5** and **C6** have been elucidated by X-ray diffraction studies, which show that individual complexes are connected through intermolecular N-H···O bonding generating a supramolecular 1D ribbon. Treatment of **L3** with two equivalents of $HgBr_2$ produces the tetranuclear compound $[Hg_4Br_8(\kappa^1\text{-}$**L3**$)_2]$ **C7**, whose unusual bromide-bridged architecture has been elucidated by X-ray crystallography.[1]

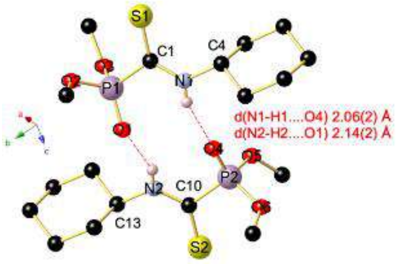

Figure. Molecular structure of **L2**.

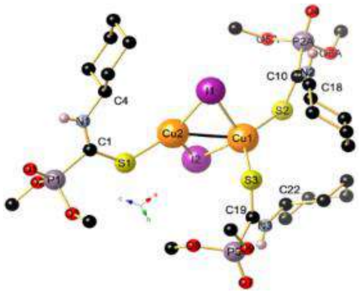

Figure. Molecular structure of **C1**.

KEYWORDS: Phosphonothioamidates; CuI; HgX_2; complexation; crystal structure; complexes;polymer; intermolecular N-H···O bonding; supramolecular 2D ribbon.

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Synthesis, Structural and Physico-chemical Characterization of a novel copper cyclohexaphosphate

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Transition-metal phosphates (TMP) have received significant attention over the last decades owing to the structural diversity of these compounds associated with their potential applications in areas such as catalysts, optics, electronics, and magnetic [1]. The work described herein reports the synthesis and characterization of a novel (TMP) based on cyclohexaphosphate anions. $(C_6H_{16}N_2)_2[CuP_6O_{18}]$ is prepared in aqueous solution and characterized by X-ray diffraction (XRD), UV-vis diffuse reflectance, fluorescence and differential thermal analysis (DTA). The presence of functional group vibrations is ascertained through FTIR study. Single-crystal X-ray diffraction analysis reveals that this novel compound crystallizes in the triclinic system, with the space group $P\bar{1}$. In the crystal structure, the phosphate anion acts as a bridge, linking adjacent copper cations as to form an anionic coordination polymer $[CuP_6O_{18}]_n^{4n-}$, extending along [100] direction. The double protonated trans-2,5-dimethylpiperazine cations ensure the interconnection between polymers and thus giving rise to three dimensional supramolecular networks. The molecular Hirshfeld surface indicates that the crystal packing is stabilized by H-bonds interactions to generate a 3D supramolecular framework. Furthermore, the optical constants such as band gap energy, refractive index and dielectric constant of the compound were determined.

Keywords: Organic-inorganic hybrid; Transition metal; X-ray diffraction; Hirshfeld surface; Optical properties.

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DIASTEREOSELECTIVE SYNTHESIS OF 3-AMINOPYRROLIDIN-2-ONES 4-CARBOXYLATES

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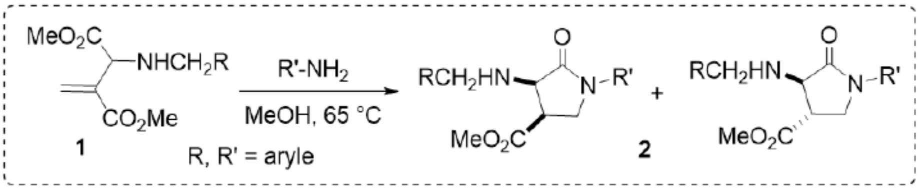
Nitrogen-containing heterocyclic products are prevalent in a multitude of natural and unnatural products.[1] 3-Aminopyrrolidines are a subset of this molecular class that have been used widely as chiral ligands [2] and as common building blocks in the preparation of bioactive compounds.[3,4] The aim of this communication is to present and discuss a convenient alternative for the diastereoselective conjugate addition of primary amines to dimethyl 2-(arylamino)-3-methylenesuccinate **1**[5] has been used as the key step in a simple and efficient protocol for the preparation of 3,4-disubstituted aminopyrrolidin-2-ones **2** in medium to good yields. In this approach, the construction of the heterocyclic ring **2** was based on an efficient coupling of one equivalent of primary amines with the allylamine **1** in methanol at 65 °C, involving two-step sequence: conjugate addition followed by heterocyclization to provide both *anti*- and *syn*-3-aminopyrrolidin-2-ones 4-carobxylates **2**.



Key words: 3-Aminopyrrolidin-2-ones 4-carboxylates, allylamine, diastereoselective synthesis.

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Synthesis, crystal structure, physico-chemical caracterization and theoretical studies of morpholine diaquadioxalatochromate(III) tetrahydrate, $(C_4H_{10}NO)[Cr(C_2O_4)_2(H_2O)_2].4H_2O$

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A new morpholine diaquadioxalatochromate(III) tetrahydrate $(C_4H_{10}NO)[Cr(C_2O_4)_2(H_2O)_2].4H_2O$ was synthesized using slow evaporation method at room temperature. This complex has been caracterized through powder and single-crystal X-ray diffraction, FT-IR and UV-Vis spectroscopy, Field Emission Scanning Electron Microscopes (FE-SEM), Followed by TGA-DTA analysis. The single crystal X-ray proves that it crystallizes in the noncentrosymmetric space group $Cmc2_1$. The crystal structure consists of $[Cr(C_2O_4)_2.(H_2O)_2]^-$ octahedral anions, morpholine $(C_4H_{10}NO)^+$ cations, which are linked together through uncoordinated water molecules via O/N-H…O hydrogen bondes. The powder XRD data affirms the purity of the synthesized phase, while the composition of our phase was confirmed by FE-SEM. The thermal analysis (TGA-DTA) showed that our complex possesses considerable stability. In addition, the density functional theory DFT calculation was performed via the hybrid B3LYP **[1, 2]** at 6-311++G(d,p) basis.

Keywords : morpholine diaquadioxalatochromate(III) tetrahydrate, crystal structure, XRD, spectroscopic study, FESEM, DFT calculations.

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Anti-corrosion behaviour of carbon steel by expired pharmaceutical product in acid medium

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Corrosion studies are a subject of interest to interdisciplinary research communities, combining areas of materials science, chemical engineering, physics, environmental, metallurgy and civil engineering. Hence, these negative effects can be minimized or eliminated using diverse techniques to protect the surface of the metal from the aggressive environments. An expired pharmaceutical product was studied as save drug to prevent carbon steel corrosion in acidic environments by using weight loss. The influence of the concentration of inhibitor, immersion time, temperature, activation energy, enthalpy and entropy has been reported. The inhibition of carbon steel corrosion can be attributed to the adsorption ability of drug molecules onto the reactive sites of the metal surface. It was also found that the adsorption as well as the inhibition process obeyed Langmuir's adsorption isotherm. The thermodynamic parameters show that adsorption reaction on the carbon steel surface is spontaneous and exothermic. In order to elucidate the mechanism of protective layer formation, the free energy of adsorption value was calculated. This indicates that the inhibitor acts by both adsorption (physical and chemical) on the steel surface.

Key words: Corrosion, pharmaceutical product, inhibition, thermodynamic parameters

Selective syntheses of novel β-lactams and azetidines by ring expansion of carboxylic aziridines

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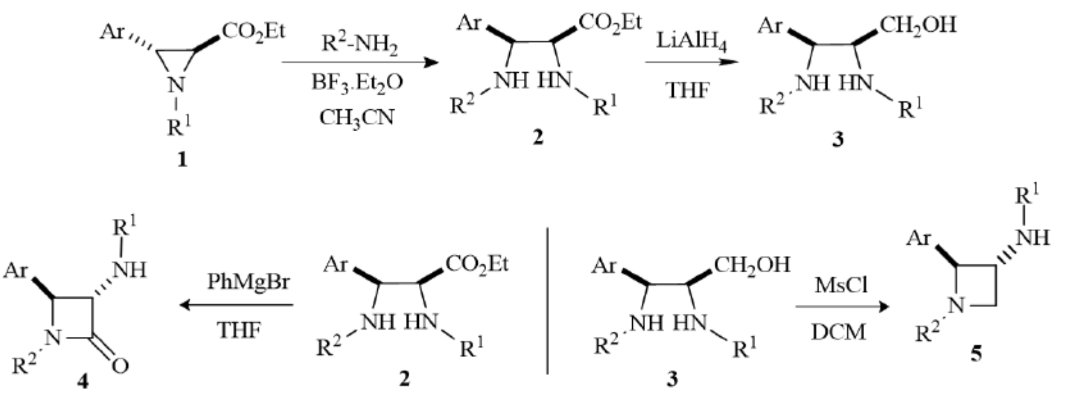
Aziridines [1] represent an important class of substrates that can be useful for developing new methodologies, providing access to interesting nitrogen heterocycles. In this context, we have initiated the reaction of the aziridine rings opening **1** with primary amines in order to prepare diamine esters **2**. Reduction of the ester function of **2** provided the diamine alcohols **3**. Depending on the operating conditions, these diamines **3** give rise to new β-lactams **4** and azetidines **5** using two different synthetic routes. These motifs are present in many natural or biologically active molecules [2-4].



Keywords: Aziridines, nitrogen heterocycles, diamine, β-lactams, azetidines.

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Comparison between Experimental and Theoretical Scales of Electrophilicity of 7-L-4-nitrobenzofurazans

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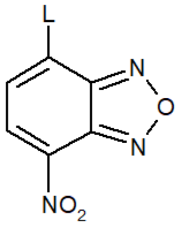
The kinetics of the reactions of 7-L-4-nitrobenzofurazans **1a-d** (L = Cl, C_6H_5O, CH_3O and Im^+) with various nitroalkyl anions have been investigated photometrically in water solution at 20 °C. The derived second-order rate constants (k) have been used to determine the electrophilicity parameters (*E*) for these series of electrophiles **1a-d**, as defined by the linear free energy relationship (Eq. (1)). The structure–reactivity relationships have been discussed.

In this work, we also compare the experimental model of electrophilicity proposed by Mayr with the definition of electrophilicity proposed by Parr, based on reactivity indexes (Eq. (2)) for these series of 4-L-7-nitrobenzofurazans **1a-d**.

$$\log k_1 \,(20\,°C) = s\,(E + N) \qquad (1)$$

$$\omega = \mu^2 / 2\eta \qquad (2)$$



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L = Cl, C_6H_5O, CH_3O and Im^+

Keywords: Kinetics / 4-L-7-nitrobenzofurazans / Equation of Mayr / Parr's Approach.

Preparation and characterization of TiO_2-$Co_{0.5}Mn_{0.5}Fe_2O_4$/Graphene oxide nanocomposite for the degradation of methylene bleu dye

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In this work, a nanocomposite (CMFT/GO) based on ferrite, TiO_2 nanoparticles and graphene oxide (GO) was successfully synthesized for application in the photocatalytic degradation of methylene bleu dye (MB). TiO_2 was first incorporated into GO to form the TiO_2/GO composite, followed by the addition of ferrite. The different stages of preparation of those composites were characterized by :X-ray diffraction (XRD), infrared spectroscopy (FTIR) and Raman spectroscopy. The results of these analyses confirm the success of the synthesis and formation of GO, ferrite CMF and the composite CMFT/GO. Degradation of MB through the process of heterogeneous photocatalysis by the CMFT/GO composite shows a high efficiency and the best degradation is obtained with the CMFT/GO composite (10%), The results of the compound indicate its wider potential for use.

Keywords: TiO_2, graphene oxide, ferrite, photocatalysis, pollutant, XRD.

Development of a new method for the simultaneous determination of zoledronic acid and its impurities by high performance liquid chromatography

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The aim of this study was to develop a new method for the determination of zoledronic acid and its impurities imidazole-1-yl acetic acid and imidazole by high performance liquid chromatography (HPLC). Separation was carried out using an X bridge C18 column (5µm, 250×4.6 mm) and a mixture of water and methanol (80:20, v/v) containing 7 mM of tetrabutylammonium sulfate adjusted to pH 7 as a mobile phase at a flow rate of 1 mL min^{-1} and monitored at 215 nm. The method was validated to fulfill the International Conference on Harmonisation (ICH) requirements and this validation included specificity, linearity, accuracy and precision. Good linear relationships were obtained ($r \geq 0.99$) for zoledronic acid and its impurities over their respective concentration ranges. Intra- and inter-day precision were less than 2% and recoveries were ranged from 98 to 102 %. The suggested analytical method can be used for quality control of pharmaceutical products containing zoledronic acid.

Key words: Pharmaceuticals, zoledronic acid, impurities, HPLC

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Synthesis of a new tripeptide structure with a phosphinic acid moiety.

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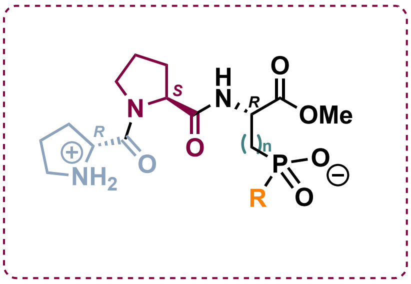
Enantioselective organocatalysis has bloomed extensively[1], in the last decade, with the introduction of a variety of metal-free and more practical catalysts for the construction of enantiopure organic structures, from a small collection of chemically unique reactions to a thriving area of general concepts and widely applicable reactions[2]. Recently, many efforts are directed towards the development of the perfect design of a catalytic system in correlation with the need to optimize the efficiency of resource usage, and to fulfill the principles of green chemistry[3]. Within this concept, peptides have enjoyed ever increasing interest as a metal free catalyst for many enantioselective transformations[4]. Inspired by this field, we envisioned a simple and an attractive approach for the formation of a new generation of bifunctional tripeptides as organocatalysts combining both aminocatalysis and an activation with a phosphinic acid moiety for the asymmetric Michael Addition.



**With the financial support of the Hubert Curien "Utique" partnership (N° 46347XD) of the French Ministry of Europe and Foreign Affairs and the Tunisian Ministry of Higher Education and Scientific Research (21G1207).

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Synthesis of O-P heterocycles from Phosphinic acid under microwave irradiations

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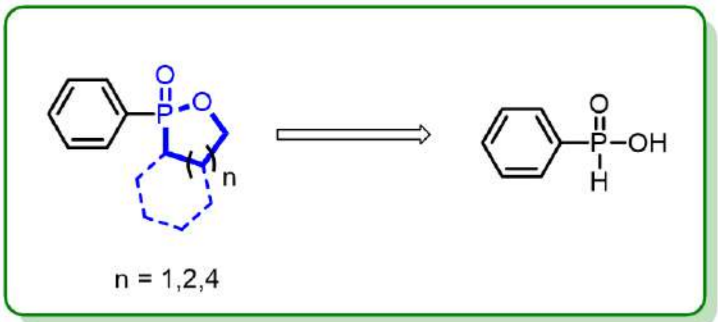
In this communication, we report on the first issues towards [5]-, [6]- and [8]-cyclic annelated phosphinates[1,2] from commercially available phenylphosphinic acid. Our approach is based on the reaction of this starting material with biselectrophiles. In this context, one pot-two steps processes allowed forming 1,2-oxaphosphirane and 1,2-oxaphosphacane. In addition, the two-steps sequence involving the installation of functional groups at the phosphinate moiety prior to the formation of the C-P bond has been shown to give 1,2-oxaphospholane.



Keywords: O-P heterocycle, free catalyst.

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Functionalization of graphene-like BC_6N with nitrenes using [1+2]-cycloaddition reaction - A DFT investigation

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Several experimental and theoretical investigations examined the chemical and physical functionalization of pristine graphene to open its zero bandgap to transform it into semi-conducting materials, which will make it useful for sensing and elaboration of electronic device [1-2]. In this work, we examined the thermodynamics and electronic structure of the functionalization of BC_6N graphene-like substrate, recently prepared in a wet-lab [3] and received increasing interest from the theorectical scientists [4]. Methylnitrene, generated from the decomposition of methylazide, adsorbs preferably on the top position perpendicular the nitrogen atom or on the bridge position over the BN bond. The most stable three-membered ring obtained [1+2]-cycloaddition is the one formed by the reaction with the BN bond ($\Delta E_{rxn} = -2.65$ eV), which is more stable than the one from the CN bond ($\Delta E_{rxn} = -2.22$ eV) and the CC bond ($\Delta E_{rxn} = -2.10$ eV). The chemical reaction also induces changes in the DOS and band structure of the pristine materials. Investigations are under way to devise sensors for small organic and inorganic gaseous molecules.

Keywords: DFT; Functionalization; Graphene-like; BC6N; Nitrene; Thermodynamics; DOS

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Synthesis, characterization and TD-DFT calculations of a new distyrylbenzene derivative for OLEDs application

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New soluble, fluorescent and conjugated small molecule M-DSB was synthesized via Williamson reaction for OLED application. In this study, the structural properties of the new distyrylbenzene displaying three different stereoisomers: E-E, Z-Z and Z-E were investigated through density functional theory (DFT) optimization. Detailed DFT and TD-DFT analysis of M-DSB provided insight into the structure-property relationship and revealed good agreement with experimental data. The material exhibits nearly the same absorption spectrum in dilute solution and in the solid state, with a maximum wavelength at 363 nm and an Eg value of 2.99 eV. Compared to experimental UV-visible spectra, the TD-DFT simulation shows the presence of a mixture of cis and trans diastereomers of M-DSB. A broad, red-shifted PL spectrum was obtained in the solid state with blue emission compared to the solution which shows purplish blue emission with relatively narrow emission. The HOMO/LUMO energy levels were calculated by cyclic voltammetry measurements and indicate a p-type semiconductor material. DFT calculation of the molecular orbital distribution shows a break in π-electron conjugation, maintaining the individuality of each fragment which induces an increase in the gap energy. The temperature and frequency dependence of the conductivity shows an activation energy value of about 0.89 eV. Impedance spectroscopy of the ITO/M-DSB/Al device indicates a typical behavior of a single relaxation process and confirms that by increasing the temperature, the electrical response becomes faster, and the mobility of the charge carriers is enhanced.

Keywords: Cis/trans isomerization; Distrylbenzene; Fluorescence; TD-DFT calculation; OLEDs; impedance spectroscopy

Flavonoid glycosides from the flowers of the endemic Tunisian plant *Ferula tunetana* Pomel ex Batt.: Isolation, structure determination and prediction of the anti-*α*-amylase effect

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The genus *Ferula* is widely used in traditional medicine. Several biological activities have been reported for different species of this genus: antifungal, antitumor, antispasmodic, antidiabetic, anti-inflammatory and antiviral properties [1]. These data led us to choose *Ferula tunetana*, an endemic Tunisian plant to investigate the ethyl acetate extract of its flowers using preparative HPLC affording six flavonoid glycosides *viz.* kaempferol-3-*O*-*α*-L-rhamnopyranoside **(1)**, quercetin-3-*O*-*α*-L-rhamnopyranoside **(2)**, kaempferol-3-*O*-*α*-L-(3″-(*E*)-p-coumaroyl)-rhamnopyranoside **(3)**, 3″-(*E*)-*p*-coumaroylquercitrin **(4)**, kaempferol-3-*O*-*α*-L-(2″,3″-di-(*E*)-p-coumaroyl)-rhamnopyranoside **(5)** and quercetin-3-*O*-*α*-L-(2″,3″-di-*O*-(*E*)-coumaroyl)-rhamnopyranoside **(6)** (Figure 1). Their structures were established by NMR (1D and 2D) and ESI-HRMS. The molecular docking was used to predict the anti-*α*-amylase activity of isolated compounds.

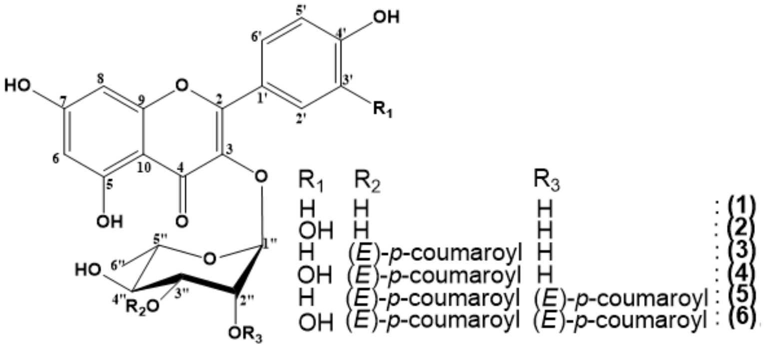

Figure 1. Structures of the isolated flavonoid glycosides from *F. tunetana*.

Key words: *F. tunetana*, flavonoid glycoside, anti-*α*-amylase, molecular docking

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Synthesis and study of properties of new mesogenic dimers

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In recent years, liquid molecules with curved cores have attracted the attention of several research groups because of their rich polymorphism. Indeed, they represent the state of matter characterized by the unique combination of order and molecular mobility. It is a thermodynamic state that has been accepted as the 4th state of matter after solid, liquid and gas[1].

The introduction of several fluorine atoms into these molecular structures presents an interesting strategy to control the properties of liquid crystals such as high viscosity, high density, high chemical stability, a surface tension base a low dielectric constant and a low refractive index[2].

With this in mind, we looked at the synthesis of new mesogenic dimers (Figure 1) known as "curved" according to Figure 1 below, because the preparation of these chemical entities was carried out by various reactions catalyzed by transition metals (palladium, copper, etc.). The achievement of these new mesogenic dimers is intrinsically associated with the development of methodologies for their functionalization in order to study the influence of these changes on the properties of these new compounds.

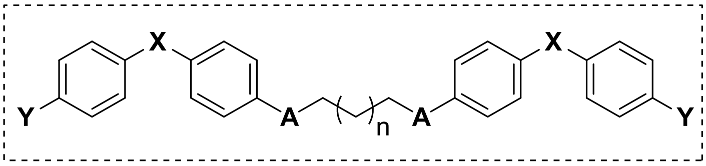

Figure 1: Access to new curved mesogenic dimmers

Key words: liquid: crystal, mesogen, thiolene, cross coupling.

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A SIMPLE STRATEGY TOWARD THE SYNTHESIS OF CYCLOPROPANE MOIETY

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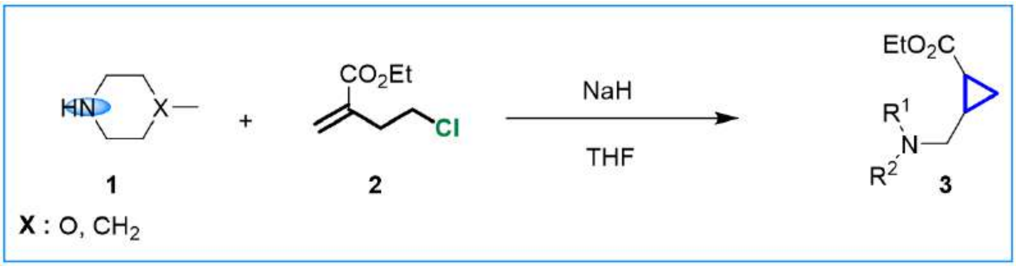
The combination of a homoallylic living group with secondary amines such as piperazine and morpholine generates several interesting pharmaceutical properties within the corresponding molecule. We describe a method for the synthesis of cyclopropane by reacting secondary amines **1** with chlorinated derivatives **2** through Michael addition followed by intramolecular substitution lead to the desired product in moderate to good yield.[1]



Scheme: Aza Michael addition of secondary amines to homoallylic living group

Key words: Homo allylic living group (chlorinated)**,** Aza Michael, Cyclopropanes

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OPTIMIZATION OF THE RESUE OF DEMOLITION WASTE BY EXPERIMENTAL DESIGN METHODOLGY

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Building construction and demolition waste [1] constitutes one of the largest waste deposits in the world. Major actions for valorzation must be implemented. In this context, the recycling of demolition waste represents a considerable challenge in the building sector.

On the other hand, Tunisia has recorded in recent years a strong urbanization which results in an excessive increase in construction sites and therefore in the number of anarchic dumps and large quantities of demolition waste, resulting in increased pressure on ecosystems and excessive exploitation of natural resources. This is why it is imperative to reduce the consumption of materials, and to use natural resources efficiently through waste recycling. As a result, the recovery of demolition waste, their exploitation and their reintegration into a new life cycle requires detailed studies of the properties of this waste.

In this context, this work focuses on other possible applications of these types of waste through their integration as an additive to cement [2]. Six types of demolition waste are then selected, namely concrete, brick, tiles, plaster, earthenware and marble, with different proportions.

This work concerns the use of experimental design methodology to optimize the effect of addition of those different demolition wastes on mechanical and chemical properties for new developed cement.

Key words: demolition waste, recycling, additive, cement

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Study of essential oils composition in a variety of aromatic plants sampled from “Jebel Serj” region located in the northwest of Tunisia

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The Mountain of Jebel Serej located in the Governorate of Siliana in the northwest region of Tunisia is locally known of its high diversity of medicinal and aromatic plants. The present study endeavors to highlight the variability in essential oils composition of its variety of aromatic plants belonging to several botanical families. The list of selected plants, that were sampled includes Carum carvi (Caraway), Salvia Rosmarinus (Rosemary), Artemisia Herba-alba (Wormwood), Pelargonium Odoratissimum (Pelargonium), seeds of Foeniculum vulgare (Fennel), Eucalyptus Gomphocephala (Eucalyptus), Alluim Sativum (Garlic), Pinus Pinaceae (Pine), leaves of citrus limon (limon) and Artemisia absinthium (Absinthe wormwood).

Essential oils were extracted then investigated by GC–(EI)-MS technique. Identification of individual components were based on their mass spectra that were matched with commercial NIST Database.

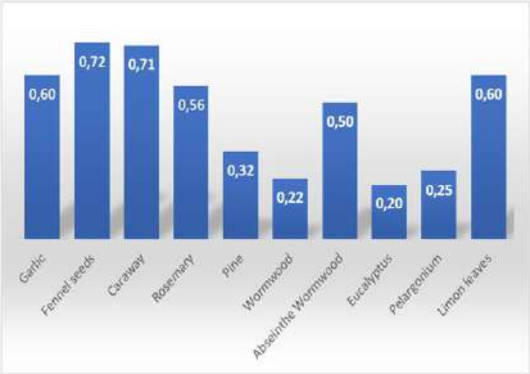

Fig.1: Extraction yields of EO (%)

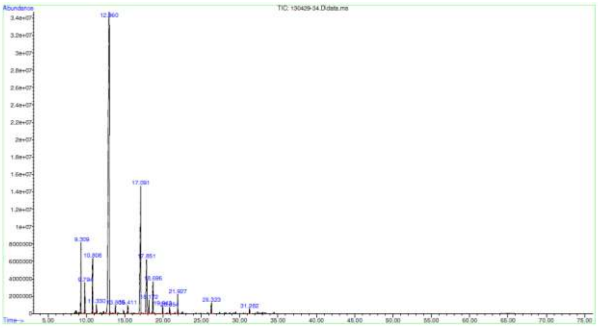

Fig. 2: Volatile components from Rosemary extract

Key words: Gas Chromatography, Essential oil composition, aromatic plants

Development of a new method for the simultaneous determination of selexipag and its impurities by high performance liquid chromatography

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A simple and rapid high-performance liquid chromatographic method for the determination of selexipag and its impurities was developed. The separation was achieved on a Phenomenex Kinetex® C_{18} column (5 µm, 250 × 4.6 mm). The mobile phase was composed of acetonitrile and phosphate buffer (pH 4; 10 mM) (60:40, v/v), at a flow rate of 1 mL min $^{-1}$ and UV detection at 270 nm. The method was found to be linear ($r \geq 0.999$), accurate and precise. Suitability of the method for the quantitative determination of the drugs was proven by validation in accordance with the requirements laid down by the International Conference on Harmonization (ICH) Q2 (R1) guideline. As the method could effectively separate the drug from the related substances, it can be employed as a stability-indicating one. The proposed method shows high efficiency, allowing the simultaneous determination of selexipag and its impurities.

Keywords: Selexipag, impurities, HPLC, Pharmaceuticals

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Development of a new method for the simultaneous determination of seven sartans by high performance liquid chromatography

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A rapid, accurate and sensitive new reverse-phase high-performance liquid chromatography (RP-HPLC) was developed for the quantitative determination of seven sartans: losartan, candesartan, eprosartan, olmesartan, telmisartan, valsartan and irbesartan. The chromatographic separation was performed using a Nucleodur® C18 (250 mm×4,6 mm, 5 µm) column. Separation was achieved using a mobile phase consisting of a mixture of methanol and phosphate buffer (7.35 mM) at pH 6 (47:53 (v/v)) at a flow rate of 1 mL min^{-1} and UV detection at 230 nm. The optimized method was then validated according to the ICH guideline Q2 (R1). Peak homogeneity was expressed in terms of peak purity values and was obtained directly from spectral analysis report obtained using the instrument software. The statistical evaluation of the method was examined by performing intra-day and inter-day precision assays and was found to be satisfactory with high accuracy and precision. Our method is linear over the concentration range of 37.5 to 87.5 µg mL^{-1}. The validated RP-HPLC method was successfully applied to the direct determination of the selected compounds in drug products. It can be applied for quality control of bulk substance as well as of pharmaceutical products.

Key words: Pharmaceuticals, Sartans, HPLC, Validation

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Optimization of catalysts and valorization of carbon dioxide in the production of dimethyl carbonate

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Carbon dioxide (CO_2), one of the greenhouse gases which accumulate in the atmosphere, is a major contributor toward severe climate change and global warming problems. The valorization of CO_2 into added-value products such as dimethyl carbonate (DMC) appears as a promising strategy for reducing CO_2 emissions. DMC as an environment-friendly building block has attracted much attention as methylating and carbonylating agents, fuel additives, as well as polar solvents. The direct synthesis of DMC from methanol (CH_3OH) and CO_2 is a promising alternative due to high atom efficiency, low toxicity, and the use of readily-available feedstock. The present work is aimed to produce DMC by coupling of CH3OH and CO_2 with 2-cyanopyridine over CeO_2-ZrO_2 catalysts prepared by co-precipitation method. 2-cyano pyridine has been used as dehydrating agent to remove water, shift the thermodynamic equilibrium and facilitate higher DMC formation. The catalysts were characterized by X-ray diffraction, Brunauer−Emmett−Teller method and NH_3/CO_2 temperature-programmed desorption. The catalytic activities were correlated with the basic and acidic properties of ceria catalysts for the synthesis of DMC in a batch reactor. The larger acidic and basic sites facilitated the DMC formation due to activation of methanol to methoxyl species and further reaction with CO_2.

Key words: Dioxide carbon, DMC, CeO_2-ZrO_2, surface structure.

Effects of hydrogen/halogen -edge termination on the structural, electronic and optical properties of SiNRs: ab-initio Simulation

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The effects of (hydrogen /halogen)–edge termination on the structural, electronic, and optical properties of planar SiNRs with either zigzag (ZSiNRs) and armchair (ASiNRs) edges are investigated by means of DFT calculations. The obtained results show that X-edge termination is a new approach to tune and open the band gap in planar SiNRs, and exhibiting a metallic character. The density of states (DOS) analysis reveals a strong hybridization between halogen-*p* and edges Si-*p* states, which is not the case of H-*s* and edges Si-*p* states. The calculated charge density contours manifest the ionic nature of Si–X (X = H, F, Cl, Br, and I) bonds. However, the Si–Si bonds display a typical covalent bonding feature. The investigation of the optical properties for both polarizations indicates that 7-ASiNR-X and 5-ZSiNR-X exhibit strong optical anisotropy in infrared (IR), visible (VIS), and ultraviolet (UV) regions under both polarizations, making them promising candidates for optoelectronics and optical nanodevices such as polarization-sensitive photodetectors. Besides, for perfect planar ASiNR and ZSiNR, the strong absorbance peak of $\varepsilon_2^{yy}(\omega)$ has been found to occur at 0.32 (0.36) eV, respectively, suggesting that these compounds may be candidates for IR optoelectronic devices. The most dominant absorption peaks centered at 5.17 and 4.5 eV for ASiNR-H and ZSiNR-H systems, respectively, indicate a high absorbance in the UV range, making them prospective nanomaterials for photovoltaic devices.

Keyword: NiO/Fe; FP-LAPW; magnetic properties; Band-gap; DFT.

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Effect of Erbium doping on structural, physical and photoluminescence properties of $CuTe_2O_5$, x%Er_2O_3
(x=2, 5 and 7%)

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The crystal structure of $CuTe_2O_5$,x%Er_2O_3 (x=2, 5 and 7%) was determined from X-ray powder diffraction data using Rietveld refinements. The new structure was solved in monoclinic system through the $P2_1/c$ space group with parameters equal to a=6.868Å, b=9.316Å and c=7.601Å.

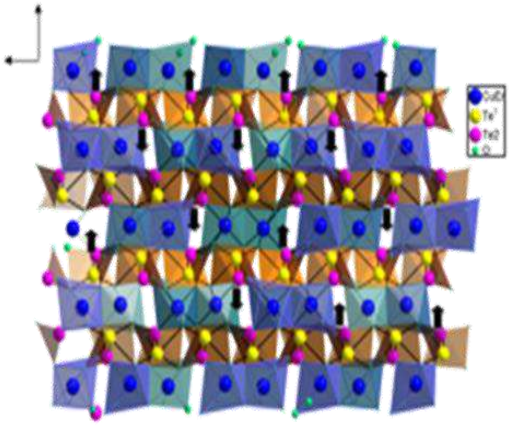
The structure can be described as a three dimensional network made of layers parallel to the (010) which contain two kinds of polyhedra TeO_4 and TeO_5 connected through a corner. These sheets are interconnected by Cu_2O_{10} dimers.

A deep spectroscopic study was carried out using the Infrared and Raman techniques in order to prove the presence of different polyhedron CuO_6, Te(1)O_5, and Te(2)O_4E.

The dielectric data were analyzed using complex permittivity (ε'), (ε'') and tan (δ) for the sample at various temperatures.

The study of the permittivity proves that this compound has a very low permittivity of the order of 100 from which it can be considered that this dielectric is of type I and can be use as a capacitor used in microwave field.

The $CuTe_2O_5$,2%Er_2O_3 exhibited strong red-green emissions due to homogeneously occupied Er^{3+} ions in the host lattice which is confirmed by Photoluminescence which offers this compound to be used on LED's fabrication.



Projection on the bc plane of the chaine of polyhedra

Contribution to the integration of plastics regrished in the manufacture of automotive parts

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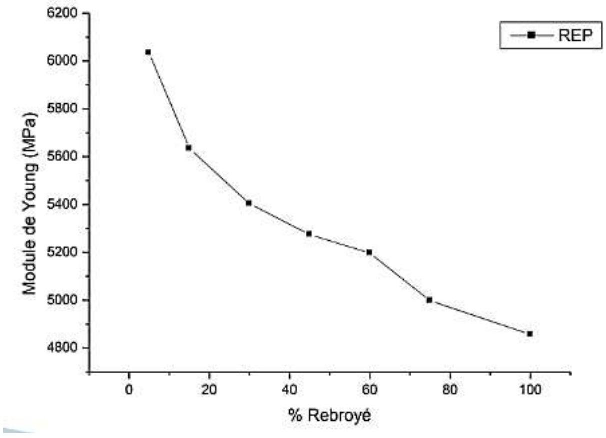
Laboratory of useful material Valuation, National center for research in material sciences

Nowadays, and due to the global plastic materials and technical polymers deficiency, the use of regrinded materials is more an more requested. In this contexct many automotive company started to intergrate recycled polymers into their injection process. But, in order to garantee the same mechanical and physical properties of delivered products as the produced parts without regrind, many investigation on regrind proportions and working conditions must be done. Therefore, and with the assistance of Mista Tunisia, a company specialized in the production of automotive parts with plastic injection, we introduced different percentages of regrind to PBT and PBT 15% of glass fiber (GF). We investigated the effect of material temperature, tool temperature, humidity percentage and % of regrind on standard speciment. The prepared sampels were used to determine mechanical properties such as Young modulus, fracture stress and fracture strain and also thermal properties such as the fusion temperature, the glass transition temperature and also degradation temperature. Results showed that we can maintain the same injection conditions like for serial production without any effect on final product if we add no more than 15% of regrinded polymers for PBT. But for PBT 15% GF, it was recommended to not to go further than 10% of regrind.



Keewords : regrind, PBT, young modulus, automotive.

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A New Co(II) Metal Complex Template with 4-dimethylaminopyridine Organic Cation: Synthesis, Phase transition, electrical study and dielectric behavior

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Great attention has been paid to the design and synthesis of novel organic-inorganic compounds in recent decades. These compounds attract considerable interest because of their structural variety and interesting properties. In this work, a Co(II)-based organic-inorganic hybrid compound dimethylaminpyridine tetrachlorocobaltate $(C_7H_{11}N_2)_2CoCl_4$ prepared by slow evaporation method at room temperature has been successfully synthesized. The X-ray diffraction results indicate that the hybrid material has a triclinic structure with a $P\bar{1}$ space group.

A phase transition was discovered by thermal analysis at 390 K, and comprehensive dielectric research was reported, showing a good agreement with thermal data.

Impedance spectroscopy measurements were used to study the electrical and dielectric characteristics over a wide range of frequencies and temperatures, 40 Hz–10 MHz and 313–483 K, respectively. The Nyquist plot (Z" versus Z') from the complex impedance spectrum revealed semicircular arcs described by a Cole-Cole model. Using Z-view software, an electrical circuit consisting of a link of grain and grain boundary elements is employed. The real and imaginary parts of dielectric permittivity, as well as tg(δ) of $(C_7H_{11}N_2)_2CoCl_4$ at different frequencies, reveal a distribution of relaxation times. The presence of grain and grain boundaries is confirmed by the modulus investigations. Electric and dielectric analyses highlight the good protonic conduction of this material.

These findings will offer useful clues for investigating the electrical characteristics of Organic-Inorganic hybrid materials.

Keywords: Organic-Inorganic, Phase transitions, Complex impedance, Protonic conduction, dielectric analysis.

Synthesis of Functionalized Six and seven-Membered-Ring carbohelicenes: Effect of Cyano Group

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Helicenes are unique helical chromophores possessing advanced and well-controlled spectral and chemical properties owing to their diverse functionalization and defined structures. Functionalization, of a helicene, may have either the purpose of modifying the electronic properties of the parent helicene, e.g., by adding electron-withdrawing groups, or the scope of providing the helicene with a “handle”, which can be reacted to bind the molecule to a metal surface, or again to allow for complexation of the helicene with metal ions.

In this context, the purpose of this study is to screen our continuing efforts on the synthesis of new functionalized helical scaffolds. The synthetic approach followed in this work is founded on the use of 4-Bromophenylacetonitrile as a convenient building block to provide the appropriate 1,2-diarylethene via Knoevenagel condensation. Helicenes precursors were then properly transformed into the functionalized helicene under UV irradiation. Upon success of this this goal, it was interesting to investigate experimental chiroptical, photophysical and electrochemical behaviors of such derivatives. Moreover, the cyano group grafted on the poly aromatic structure serve for increasing the solubility of the helicene in organic solvents, may improve its photophysical properties and may convert the helix skeleton into variously substituted large derivatives through different couplings.

Keywords: Helicene, Photooxidation, photophysical properties

X-Ray PhotoelectronSpectroscopy Analysis of the Juniperus Communis Leaves Extracts on Tin Bronze Corrosion

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Most of the organic compounds reported in the literature as effective corrosion inhibitors are toxic to humans and environments. Hence, several research teams tested plant extracts as eco-friendly inhibitors. However, the effects of such mixtures on tin bronze corrosion were not exhaustively studied. This work aims the investigation of the effects of a *Juniperus communis* leaves (JC) methanolic extract on the interfacial behaviour of a Cu10Sn modern bronze analogous to a punic material. Polarization curves and X-Ray Photoelectron Spectroscopy (XPS) were used in order to understand the alloy corrosion behaviour in aqueous 0.5M chloride medium without and with the extract addition.

The I-E curves obtained when the bronze was immersed in the corrosive medium showed that the anodic current decreased in the entire potential domain explored whereas the cathodic curve shape was almost unchanged when the JC extract added. When analysing the electrochemical parameters obtained in the Tafel field it was concluded that the extract affected both anodic and cathodic reactions. However, the inhibition efficiency was lower than 70%.XPS semi quantitative characterisation revealed that the cationic composition at the material surface when submitted to the aggressive medium was 97.9%, 1.8% and 0.3% respectively for Cu(I), Sn(II) and Sn(IV). Furthermore, the bronze surface composition was 7.2%, 24.9% and 67.9% respectively for Sn(II), Cu(I) and Cu(II) when the JC extract was added. The decuprification factor f_{Cu} was -1 and 0.23 respectively without and with the plant addition. The JC methanolic extract was concluded inhibiting tin oxidation and promoting Cu(I) tranformation

Keywords: Synthetic bronze, Corrosion, Copper–tin alloy, Juniperus Communis, X-ray photoelectron spectrometry.

Extraction and characterization of polysaccharides from Tunisian lemon peels: Elaboration of food packaging films

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Researches for the development of materials with less environmental has been more frequent. Pectin is a naturally occurring polysaccharide found in plants and the peel of some fruits. It is non-toxic, biocompatible, and inexpensive, and it is a byproduct of the fruit juice industry [1]. In this work, pectin was obtained by High pressure processing from lemon (*Citrus Limon*) peel. The experimental yield and uronic acid content were 8.53% and 56.23% respectively. Preliminary characterization was performed via Fourier transform infrared spectroscopy (FT-IR), size exclusion chromatography (SEC) and Gas Chromatography-coupled with mass Spectrometry (GC–MS). Pectin is a suitable polymeric matrix for the elaboration of edible films intended as active food packaging. The Pectin film was obvious defects such as poor barrier and mechanical properties. In this context the objective of this study was to develop and characterize films based on blends of chitosan and pectin containing essential oil was by casting in order to modify the functional properties of the films [2].

Key words: Pectin, *Citrus Limon*, extraction, biopolymers, biodegradable films

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From imidates toward N1-ethylacetate-1,2,4-triazoles

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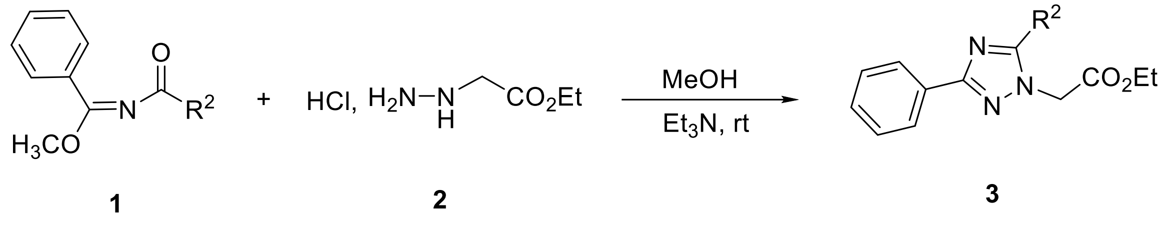
Triazoles are five-membered heterocycles with three nitrogen atoms. They are of great interest because of their numerous applications in the pharmaceutical[1], agricultural[2] and material science[3] fields.

In this work we describe the strategy for the synthesis of N-ethylacetate-1,2,4-triazoles from the reaction of hydrazinoacetate on ethoxycarbonylated, acylated and sulfonamide imidates.

Key words: Imidate, Hydrazine, Triazole



R^2 = OEt
R^2 = Alkyl
R^2 = Vinyl
R^2 = $NHSO_2R$

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Synthesis, spectroscopic characterization, thermal analysis and DFT calculation of a new hybrid compound $(C_{11}H_{10}N)_2[ZnCl_4]$

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The crystallization and characterization of a new hybrid compound $(C_{11}H_{10}N)_2[ZnCl_4]$ by powder and single –crystal X-ray diffraction**,** thermal analysis DTA-TGA and X-ray micrography and microanalysis (SEM / EDX) are described. A complete spectroscopic study has been carried out; it was accompanied by a comparative DFT theoretical study, carried out by Gaussian 09 software. The molecular unit of the compound is formed of two independent phenylpyridinium, $(C_{11}H_{10}N)^+$, monoprotonated organic cations and an tetrachlorozincate(II), $[ZnCl_4]^{2,-}$ inorganic anion. The compound structure can be described as a succession of organic-inorganic layers parallel to the (001) plane. The cohesion and stability of the studied material is ensured by N-H···Cl hydrogen bonds between the organic and inorganic layers as well as by van der Waals interactions leading to a three-dimensional network Three-dimensional Hirshfeld surface (3D-HS) **[1]** and two-dimensional fingerprints (2D-FP) **[2]** reveal that the structure is dominated by Cl···H/H···Cl, H···H and C···H/H···C contacts.

Keywords: Organic-inorganic hybrid; Tetrachlorozincate(II); XRD; DFT study; Hirshfeld surface, Two-dimensional fingerprints, Thermal analysis.

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Phenolic constituents, α-amylase inhibitory activity of *Pinus pinea* L. growing in Tunisia: An *in vitro* and *in silico* study

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α-Amylase is a key enzyme of starch digestion, playing an important role in deciding glucose releasing amount. Inhibition of the enzyme activity by polyphenols is suggested as a potential approach in controlling starch digestion and regulating postprandial hyperglycaemia.[1]

The aim of this study was to characterize and quantify the polyphenolic constituents in ethyl acetate and methanol extracts from the trunk bark of *Pinus pinea* L. and to assess its α-amylase properties. The phenolic profile of extracts was determined using LC-HRMS method. Eighteen constituents were identified in both extracts with *trans*-taxifolin and ellagic acid, as the main compound, respectively. EtOAc and MeOH extracts inhibited α-amylase with IC_{50} values of 9.16 and 8.33 µg/mL, respectively. This activity was supported by molecular docking analysis of some major compounds of both extracts. The selected compounds showed a low binding energy, and they could bind with the key amino acid residues of α-amylase.

Key words: *Pinus pinea* L, polyphenolics, LC-HRMS, anti-α-amylase, molecular docking

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Magnetic solid-phase extraction based on Date Stones Biochar for the determination of nonsteroidal anti-inflammatory drug residues in water

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Biochar (BC) derived from agro-wastes has attracted much attention due to its excellent adsorption capacities, ability for functionalization, low cost, and the possibility of renewability. BC represents ideal adsorbents for solid-phase extraction techniques.

This study deals with the potential of biochar, as sorbent for the microextraction of nonsteroid anti-inflammatory drugs (NSAIDs) from aqueous solution. Magnetic solid phase extraction of NSAIDs and their determination by liquid chromatography coupled to mass spectrometry were considered. Magnetic date stones biochar was synthetized and characterized by TEM/EDX, FTIR and XRD. An experimental design was applied for the optimization of magnetic solid phase extraction process. A two-level full factorial design was used for optimizing experimental conditions such as extraction time, sample volume, eluent volume and adsorbent mass. The suitable conditions were 10 mL of sample solution, 4 min of extraction time, 3.5 mL of elution solvent and 10 mg of adsorbent. For validation linearity, LOD, LOQ and precision were evaluated. The limit of quantification and limit of detection were from 0.20 to 0.37 µg L^{-1} and from 0.061 to 0.111 µg L^{-1} with inter day and intra-day precisions less than 3.2%. The recoveries of NSAIDS were higher than 92.60 %. The MDSBC can be reused five times without any decrease in adsorption capacity.

Key words: Biochar, magnetic solid phase extraction, NSAIDs, chemometrics.

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Photodegradation Activities of Cu_9S_5, SnS_2, and Cu_2SnS_3 Nanoparticles Synthesized from Precursor Complexes

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Nanoparticle of Cu_9S_5, SnS_2 and Cu_2SnS_3 have been prepared by a one-pot thermal decomposition of copper(II) bis (N-methyl-N-paramethoxyphenyl) dithiocarbamate, dimethyltin (IV) bis (N-methyl-N-paramethoxyphenyl) dithiocarbamate, and the co-thermal decomposition of both complexes in oleylamine, respectively. The crystal structures of the studied compounds have been confirmed by X-ray powder diffraction. The microstructures have been verified and studied using scanning electron microscope (SEM) and transmission electron microscopic (TEM) techniques. The absorption in the visible to near infra-red region of has been determined using the absorption spectroscopy. The visible-light photocatalytic evaluation of these nanomaterials showed good activities for the photo-enhanced degradation of methyl orange (MO), with the SnS_2 and Cu_2SnS_3 exhibiting comparable properties (>90% removal efficiency) and better than the Cu_9S_5 nanoparticles with < 90% efficiency.

Keywords: Copper sulphide, Tin sulphide, Copper tin sulphide, Photocatalysis, Methyl orange.

Parameters effect of manual electric welding on structural and mechanical properties of assembled steels

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Welding is the technic of assembling more metal parts with or without bring metal. The several welding processes have been regrouped into a group of fusion welding. This last is based on the principles of heat application to assemble the materials to be welded. Different welding processes are determined by the thermal energy source whether it results from electrical, chemical and mechanical energy, with a variety of different techniques available. The aim of this work is to study the effects parameters of electrical manual welding as current, arc voltage and type of chamfer on the structural and mechanical properties of welding seam of steel parts assembled by manual arc welding was investigated in this study. Three types of current, three types of potentials and three types of chamfers were chosen during this study. After analyzing by various characterization technics of all samples assembled by the welding process mentioned, the three technological parameters of current, arc voltage and chamfer kind selected in this study were optimized.

Key words: welding, steel, electric arc, current intensity, voltage

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Tetrathiafulvalene derivatives: Synthesis, x-ray structure, electrical and magnetic properties, and theoretical study

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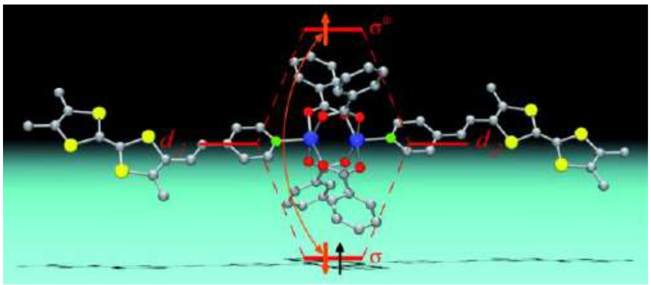
A few asymmetrically substituted tetrathiafulvalene were successfully synthesized as precursors of conductor and magnetic materials. The chemical structures of these compounds were investigated using spectroscopic methods (IR), RMN^{1}H, RMN^{13}C, and Masse spectra. Electrochemical properties have been investigated by cyclic voltammetry at ambient temperature. The crystal structures of these ligands and their complexes have been determined by single-crystal X-ray diffraction (SCXRD). The electrical conductivity of these materials measured by two points methods shows the conduction properties of these synthesized materials. Magnetic studies revealed a paramagnetic behavior.



Keywords: unsymmetrical TTF molecules; redox potentials; synthetic methods; X-ray.

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Recycling of reverse osmosis membranes for use in wastewater treatment

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This study focuses on the possibility of recycling RO membranes from a seawater desalination plant and reusing them to purify wastewater. A composite reverse osmosis (RO) membrane, reference BW30-400-FR, manufactured by Dow FilmtecTM was used for all the tests. The cutting of the module is done by cutting it into three discs: the inlet and the middle then the outlet. For the degradation of the active layer of the RO membrane we tested three solvents such as $KMNO_4$, NaOH, H_2O_2 and the mixture of NaOH with $KMNO_4$. At the end of the proposed treatment, the treated films are recovered and rinsed with distilled water. After drying, the films are analyzed by scanning electron microscopy (SEM), and the clogging powder is analyzed by EDX, to estimate the compounds, which are responsible for the clogging. A frontal filtration of wastewater by these modified membranes has been carried out. An analysis of the physico-chemical properties of the filtrate was made by spectrophotometer. The efficiency of the recycled membranes was verified by measuring the flow of wastewater and by determining the quantity of suspended solids in the wastewater. The obtained results show the efficiency of the treatment for the degradation of the active layer of the waste osmosis membranes in order to transform it into a microfiltration and/or ultrafiltration, and to reuse them in order to improve the quality of the wastewater treatment discharged into the natural environment.

Key words: Membrane, Reverse osmosis, Frontal filtration, Wastewater, SEM

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Multiobjective optimization of wastewater treatment by electrochemical 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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Down-Shifting in Ce^{3+}-Tb^{3+} co-doped phosphate glasses

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The Down-Shifting (DS) of UV photons into the visible range has been attracting much attention for lighting appliances and solar cells. This work reported the DS luminescence in Ce^{3+}-Tb^{3+} co-doped phosphate glasses. Photoluminescence and decay curves were measured and analyzed. According to the emission spectra, it was noticed a decrease in emission of the Ce^{3+} peak intensity, whereas the visible Tb^{3+} transitions intensity increase, indicating an energy transfer from Ce^{3+} to Tb^{3+}. Moreover, it was observed that the blue emission of Tb^{3+} decreases, while the green emission enhances by gradually increasing of Tb^{3+} concentration. According to the decay curves of Tb^{3+}, this result can be explained by cross relaxation between Tb^{3+} ions. The experimental temporal evolution of the green emission of Tb^{3+} ions obtained under excitation the Ce^{3+} ions at 280 nm is well simulated using a proposed model.

Keywords: Photoluminescence; lanthanide ions; Energy transfer; Cross relaxation.

Geochemical characterization of Meknassy gypsum and exploitation forecasts

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After the start exploitation of the phosphate Meknassy site, it is important to strip a very large gypsum mass which can reach a thickness of 600 meters, considered as sterile.

Geochemical studies of this gypsum; in particular in the Jebbas area, shows results that comply with the European standard (EN 13279-N); such as the degree of purity, yield, density, spreading and setting time achieved on the coating to be sprayed. The chemical analyzes carried out in the laboratories interest to the contents of SO3 and CaCO3 which constitute the basic formula of gypsum (CaSO4 2H20). These analyzes are also focused on the contents of soluble salts such as chlorides and other oxides (sodium oxides and ferric oxides).

Other physical analyzes are also applied to this gypsum in the plaster state, such as the whiteness index, the mechanical resistance to bending and the setting time; Thus this primary material can be the object of gypsum exploitation by factories in the region and which constitutes an important reserve which exceeds 50 10^6 tons (according to the Gafsa phosphate company).

Keywords: Meknassy, Gypsum, geochemical studies, European standards, reserve.

Crystal structure, optical studies, experimental and theoretical characterization of novel antibacterial benzimidazolium-tellurate hybrid compound.

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Tellurate hybrid compounds are considered among the most interesting materials in the chemical industry because of their attractive properties [1, 2]. In a bid to improve this real estate, new benzimidazoluim-tellurate hybrid compound was intended and synthesized by slow evaporation at room temperature. X-ray diffraction on single crystal identified a monoclinic cell of space group $P2_1/m$ with good reability factor. The structure is organized by an alternation of chlorotellurium polyhedra and benzimidazolium plane, stabilized with hydrogen bonds and week interactions which make the building of the crystal [3].

Exhaustive optical study was evaluated by UV-Vis spectroscopies which presented, in the ultraviolet area, three absorption signals. Some experimental results are supported theoretical DFT calculations, which confirm the strong interactions between constitutive moieties and the perfect stability of the material. Furthermore, the synthesized product was also screened for in vitro antimicrobial activities, which reveals their favorable antibacterial properties against Escherichia coli and Staphylococcus aureus stains. Satisfied antibacterial properties were found after incubated in bacterial suspensions for 24 h at 37 °C.

Key words: benzimidazole, tellurium, X-ray, hydrogen bonds, UV-Vis, DFT, antibacterial properties.

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Investigations on synthesis and electrical properties of the $La_{1.85}Ca_{0.15}CuO_{3.5}$ prepared by topotactic reduction with CaH_2

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The present work reports on the reaction of a cuprate $La_{1.85}Ca_{0.15}CuO_4$ with CaH_2 which yields $La_{1.85}Ca_{0.15}CuO_{3.5}$, a new oxygen-vacancy-ordered arrangement of cooperatively-distorted Cu_2O_3 planes containing 4-coordinate Cu^+ sites. This new compound has been characterized by X-ray diffraction, electron paramagnetic resonance (EPR), differential scanning calorimetry (DSC) and impedance spectroscopy. The powder X-ray diffraction data have shown that $La_{1.85}Ca_{0.15}CuO_{3.5}$ adopts a face-centered monoclinic crystal structure (A2/m, a = 8.6224(6) Å, b = 3.8446(2) Å, c =13.0179(10), $\alpha = \gamma = 90°$ et $\beta = 109.690(5)°$) with anion vacancies located within the CuO_2 ($CuO_{1.5}\Upsilon_{0.5}$, where Υ represents an anion vacancy) layer of the phase. Concerning the EPR measurements, they have shown the presence of Cu^{2+} cation and a hyperfine structure suggesting a pronounced hybridization of the copper-oxygen bond. The impedance spectra were analyzed in terms of equivalent circuits involving resistors, capacitors and constant phase elements (CPE). The re-oxidization under mild conditions at 420 °C in oxygen atmosphere transforms $La_{1.85}Ca_{0.15}CuO_{3.5}$ phase to T'-$La_{1.85}Ca_{0.15}CuO_4$. This phase transition is confirmed by DSC and impedance spectroscopy. The significance of this reaction relates to its mechanism, as it implies low temperature oxygen mobility realized in a solid oxide, which has technological importance for oxygen membranes of SOFCs.

Keywords: Non-stoichiomic oxides; Reduction *via* hydride method; Oxygen mobility; Electron paramagnetic resonance; Electrical properties; Equivalent circuits.

Nanoparticles from *Arum arisarum* extract as innovative antimicrobial and wound healing agent

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In the recent years, the medical sector is getting increasingly interested in the wound dressing materials that contain medicinal herb instead of metal nanoparticles to impart antibacterial or other desirable properties. Several plant extracts and their phytoconstituents are known as a promising alternative for wound healing agents due to the presence of diverse active components. The development of nanotechnological methods can help to improve the efficacy of different therapeutics as well as herbal-based products.

Arum arisarum, is a medicinal plant used traditionally for the management of wounds and infections by algerian population.

The main goal of our study was to evaluate the healing and antibacterial potential of a nanodressing based on the plant extract via *in vivo* circular wound excision model with inoculation of the wound by *Staphylococcus aureus.* The ethanolic extract was analyzed by HPLC-UV-ELSD-ESIMS. The *in-silico* methods will be used in strategies for the discovery of new molecules with a therapeutic aim based on pharmacophoric models and docking methods to guide and prioritize the synthesis of molecules of various structures and original, likely to have the best affinities for the targets studied.

Phytochemical results showed a high content of active components inducing an efficient wound healing effect determined by an *in vivo* study. The nanoparticle-based wound dressing materials have the potential to reduce both the healing time of wounds and bioburden. Topical therapy using wound dressing is used in the conventional approach to manage wound, prevent infection, and promote good wound healing.

Key words: *Arum arisarum*, HPLC-UV-ELSD-ESIMS, nanodressing, *In vivo* wound healing, *Staphylococcus aureus*

Hydrogen production over the Spinel $CoFe_2O_4$ under visible light

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In this work, the Spinel FeCo2O4 prepared by co-precipitation was characterized photo-electrochemically in order to assess its performance for the hydrogen production. The X-ray diffraction revealed a single phase crystallizing in the spinel structure with an average particle size of 35 nm. The UV–Visible spectrum of the black product exhibits a direct optical transition at 1.53 eV. The inverse of the square of the capacitance as a function of the potential (C-2 - E) exhibited a line negatively slopped, characteristic of p-type. The conduction band (-0.6 VSCE) made up of Co3+: 3d orbital is more cathodic than the H2-level (-0.70 V) leading to its spontaneous evolution under visible irradiation. The H2 production was realized under visible light (29 mW cm-2) with a liberation rate of 0.58 µmol H2 / h-1 /g. The chemical stability of FeCo2O4 was demonstrated by its regeneration then its use again under the same experimental conditions; the volume of hydrogen (1.6 ml) of the second test is practically the same as that of the first.

Key words: Spinel $FeCo2O_4$, Co-precipitation, Hydrogen; Visible light

Physical characterizations of Ag_3PO_4 and $Ag_4P_2O_7$. Degradation of methyl orange on Ag_3PO_4, $Ag_4P_2O_7$ and Ag_3PO_4/Ag_4PO_7 under visible and solar lights

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The present study is devoted to the physical characterization and photocatalytic performances of Ag_3PO_4 and $Ag_4P_2O_7$ under visible and solar lights. Ag_3PO_4 and $Ag_4P_2O_7$ were successfully synthesized by chemical precipitation route. Their structural, optical and electrochemical properties were determined using different techniques. The X-ray diffraction revealed the existence of well-crystallized phases in hexagonal and cubic systems respectively. The optical study showed direct electronic transitions for Ag_3PO_4 and $Ag_4P_2O_7$ materials, their optical gap values are respectively 2.46 and 3.16 eV. The photoelectrochemical measurements were used to determine the conduction, valence and flat band potentials, the latter is equal to -0.13 and -0.19 V respectively for both materials. The oxidizing power of Ag_3PO_4, $Ag_4P_2O_7$ and their heterojunction ($Ag_3PO_4/Ag_4P_2O_7$) under visible and solar lights were demonstrated by the photodegrdation of Methyl Orange (MO); under solar light, the MO degradation performances over the heterojunction ($Ag_3PO_4/Ag_4P_2O_7$) were much improved (75%) compared to those obtained under visible light (50%) during 80 min.

Key words: Ag_3PO_4, $Ag_4P_2O_7$, Precipitation, MO photodegradation, visible light.

Study dose and phase syntheses on Au-Ni using Swift heavy ion

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The Au-Ni system is one of the bimetallic nanoparticles important, which has significant magnetic and optical properties, which allow us to use it in different domains like applications of electrical contact material and contact materials, in the catalytic field etc. In the present work, we examine the interface modification and phase formation in [Au (20nm)/Ni (20nm)]5/Si multilayer irradiated by 100 MeV of Au ions with different fluence in range of $5 \times 10^{12} - 1 \times 10^{14}$ ions/cm^2. The FESEM image for the 100 MeV swift heavy Au ion irradiated sample revealed a similar grainy morphology of the pristine sample even for the highest dose. The XRD results show there is no peak asymmetry feature and emergence of intermediate peak upon ion fluence increase, which exclude Au-Ni solid solution or metal alloy formation, and therefore, eliminate any possibility of ion beam mixing due to high-energy irradiation. This is in good agreement with SEM observation that showed no surface modification even at the highest irradiation fluence.

Keywords : Swift heavy ion irradiation, FESM, XRD, Phase synthesis.

Development of nanosuspension for enhancing oral bioavailability of a poor water-soluble drug

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The objective of this work is to contribute to the improvement of the bioavailability of curcumin; an active principle used in the pharmaceutical field for its strong biological and therapeutic activities. The adopted strategy is the formulation of nanosuspensions. The micrometric size of curcumin was reduced into à nanometric size using the Nano-edge process with optimal proportions of natural excipients. This nanometric size has been confirmed by DRX, SEM and DLS. The stability of the nanosuspension was evaluated by measuring the zeta potential for a period of 8 days. The freeze-dried nanoscale powder showed an improvement in solubility, biological activities compared to its initial micrometer size. In vitro dissolution tests have shown a remarkable improvement in solubility and bioavailability.

Key words: curcumin, nanosuspension, nanoparticle, bioavailability, solubility, antioxidant, antibacterial, anti-inflammatory, in vitro dissolution test.

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Valorization of *Citrus* waste in the region of Blida (Algeria) by extraction of essential oils

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The purpose of this study is the valorization of *Citrus* Limon peel by extraction of essential oils (the method used is microwave-assisted hydrodistillation), the results of the volumes of essential oils obtained according to the particle size of the peels show that the maximum yield (2.9%) is reached for particles of diameter (200 to 300 µm). According to the results obtained by studies of several researchers, which aims for the extraction and characterization of essential oils from different varieties of citrus fruits by different extraction methods, we note the method of distillation assisted by microwaves, offers significant advantages over alternatives, namely shorter extraction times and higher yields.

Key words: waste, recovery, extraction, citrus fruits, essential oils.

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SOLID PHASE EXTRACTION AND ANALYSIS OF EMERGING ANTIBIOTICS IN EFFLUENT

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The presence of trace amounts of antibiotics in the environment and the risk they represent have made the scientific community aware of the real need to establish strategies for the identification, quantification and elimination of these micropollutants in the environment.

The presence of these micropollutants in the various environmental compartments in trace amounts makes their monitoring and the determination of their level of contamination difficult.

Among these techniques of elimination of micropollutants, the adsorption by porous materials resulting from the valorization of biomass such as the stone of dates was recognized as the most effective process in the treatment of water, because of its simplicity, its moderate cost and its performances.

The presented study contributes to the development of a detection method for two antibiotics by HPLC-UV. Several parameters were studied: the nature of the solvent, the elution solvent volume and the sample volume.

Key words:
Micropollutant, SPE, liquid chromatography, biomass.

Effect of Cu_2ZnSnS_4 (CZTS) thin film thickness on Al/p-Cu_2ZnSnS_4/Mo Schottky diode properties

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The aim of this study is to investigate the effect of the CZTS thin film thickness (d) on structural, morphological and electrical properties of Al/p-Cu_2ZnSnS_4/Mo Schottky diodes (d=219 nm and d=326 nm).X-ray diffraction analysis reveals a polycrystalline CZTS powder preferentially oriented along a (112) plane. Analysis of the Al/CZTS/Mo junction shows that the crystallinity of the films improves with increasing thickness, in accordance with XRD and SEM analysis. Raman spectroscopy enables to verify the vibrational modes in CZTS. In addition, a series of diode factors, namely the ideality factor (η) and the series resistance (Rs), were assessed based on I-V measurements. The impedance analysis revealed a decrease in resistance with increasing temperature, suggesting a thermally activated process. With increasing thickness, a decrease in the diameter of the semi-arc can be detected, suggesting an increase in conductivity and a better crystallinity which with correlate structural and morphological analyses.

Keywords: CZTS, Schottky diode, Structural properties, Impedance spectroscopy, Current Voltage (I-V) measurements.

Influence of NiO doping on the microstructure of SnO_2 thin films for NO_2 Gas Sensor

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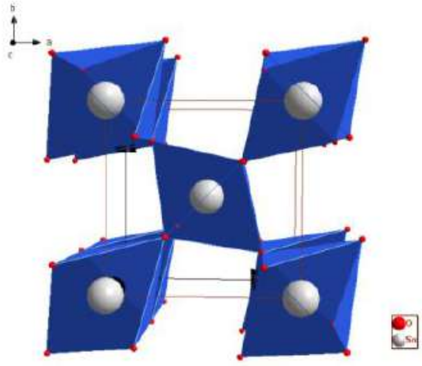
Nitrogen dioxide (NO_2) is the major reason for acid rain and respiratory illness in humans. Therefore, rapid, portable, and effective detection of NO_2 is essential. Herein, a novel and simple method to construct a NiO-SnO_2 thin films is investigated.

Tin (IV) oxide (SnO_2) and Nickel doped tin oxide thin films (NSO) were deposited by spray pyrolysis technique from an aqueous solution for an eventual gas sensing application. X-ray diffraction analysis confirmed the tetragonal structure of pure SnO_2 and Ni-doped films. The lattice parameters calculated for (NSO) decreased with increasing the Ni ratio. The average crystallites sizes deduced from scherrer formula are between 5 and 8 nm. The FE-SEM reveals that films surface is relatively homogeneous with good coverage of the substrate surface without any cracks. Increasing the Ni content causes the appearance of cauliflower aggregation structures of around 100 nm diameter and be denser at a high percentage of Ni. The Raman spectroscopy indicates the formation of SnO_2 nanostructures and increases defects and vaccines by increasing the Ni contents.



Key words: Thin film mixed oxide, Ni-doped SnO_2, Microstructure study, NO_2 gas sensor.

Evaporation of desalination brines: simulation vs. experimental work

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Sodium chloride is mainly produced either through an ancient process in which seawater gets concentrated by naturel evaporation or by forced water extraction processes, driving the precipitation of halite crystals. Traditionally, after salt harvesting from concentrated seawater brines, a residual by-product depleted in sodium chloride, known as bittern, is discharged into the sea [1]. This waste stream has severe negative environmental impacts on the receiving water body. On the other hand, both brines and bitterns are highly concentrated solutions rich in various minerals, some of which are on the top list of strategic compounds as demonstrated by the intensive research activity on the field [2]. In this work, seawater evaporation has been simulated using PHREEQC software, which is able to predisct the physico-chemical properties and species activities through the full Pitzer model. For each sparingly soluble salt during the evaporation process, once supersaturation is reached, the solution is allowed to deplete through precipitation of single or multiple species. Simulation will focus on the evolution with mass concentration factors of the following properties: density, electrical conductivity and the quantity of salts precipitated. Simulation results are compared to the experimental ones obtained by forced water evaporation using seawater and desalination brine.

Key words: Desalination process, seawater evaporation, brine, salts precipitation, PHREEQC simulation, experimental evaporation, physico-chemical properties.

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Validated RP-HPLC/UV method for determination of Vitamin B12 in multivitamin dietary supplement tablets

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Vitamin B12 has an important role in cellular metabolism especially in DNA synthesis, methylation and mithochondrial metabolism. A deficiency may lead to disruption of DNA and cell metabolism and have serious clinical consequences. Vitamin B12 is found naturally in a wide variety of animal foods but some people have trouble absorbing it from food. The body absorbs vitamin B12 in a two-step process. First, hydrochloric acid in the stomach separates vitamin B12 from the protein that it's attached to. Second, the freed vitamin B12 then combines with a protein made by the stomach, called intrinsic factor, and the body absorbs them together. In dietary supplements, vitamin B12, usually in a form called cyanocobalamin, isn't attached to protein and doesn't require the first step. However, it does need to combine with intrinsic factor to be absorbed.

A reliable reversed phase high performance liquid chromatographic method was validated and applied for the determination of vitamin B12 in a multivitamin tablets «Tetra B». Chromatographic separation was achieved isocratically on Waters C18 column (25mm, 4.6mm DI; 5µm DP) and the mobile phase consisted to Methanol/Acetonitril/Acetic acid/Water (10/10/0.8/qsp 100). The flow rate was 1ml/min and the detection was carried out at 361nm. The method was validated in terms of specificity, linearity, precision and fidelity.

Linearity was tested in the range of 0.5 to 5µg/ml and R^2 was found equal to 0.9998. Relative standard deviation was RSD = 0.11% and CV= 100.87%. LOD is in order to 0.1µg/ml. The method extensively validated was found precise, linear and faithful. It was then successfully applied for determination of Vitamin B12 in dietary supplement «Tetra B».

Key words: Vitamin B12, HPLC, Validation

Antioxidant, anti-inflammatory and anti-nociceptive effects of chondroitin sulfate from marine origin

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Chondroitin sulfates (CS) have attracted considerable interest in recently years due to their potential therapeutic applications and structural heterogeneities [1]. Indeed, the CS from marine origin *(Centrophorus granulosus, Scyliorhinus canicula)* was isolated, characterized and essayed for antioxidant activity, anti-inflammatory activity and anti-nociceptive activity. Chondroitin sulfate was extracted from the species by digestion with papain followed by precipitation with cetylpyridinium chloride and ethanol and was subjected to electrophoresis on cellulose acetate, then the structure was characterized by FT-IR and physicochemical procedures, Molecular weight measurements were performed by SEC-MALLS. The antioxidant activity was studied by three tests (DPPH, ABTS and FRAP). Then, the *in vivo* anti-inflammatory activity was evaluated by the paw edema test in rats and finally test the anti-nociceptive activity in rats using the Von Frey test. The results showed that the chemical structure of this CS is also characterized by a remarkable negative charge density due to the abundance of sulfate groups and by a weight average molar mass (Mw). The results of the study of the biological activities of the CS show that this polysaccharide in the two species is endowed with a remarkable antioxidant, anti-inflammatory, anti-nociceptive activity. Extracts show different anti-radical activities depending on their origin. Thus, they constitute an antioxidant molecule and can have valuable anti-inflammatory properties in the field of osteoarthritis pathology.

Keywords: Chondroitin sulfate, *Centrophorus granulosus, Scyliorhinus canicula*, antioxidant activity, anti-inflammatory activity *in vivo*, anti-nociceptive activity.

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Fe_3O_4 nanomaterials: synthesis, optical and electrochemical properties

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Sidi Thabet, 2020 Tunis, Tunisia

The magnetite Fe_3O_4 nanoparticles were synthesized via the hydrothermal process in the presence of sodium dodecyl sulfate (SDS) and cetyltrimethylammonium bromide (CTAB) as surfactants. The obtained products were characterized by X-ray powder diffraction, transmission electron microscopy, and ultraviolet-visible absorption spectroscopy. The electrochemical study of these products as advanced electrodes for supercapacitors was done using cyclic voltammetry (CV) and galvanostatic charge/discharge tests. The specific capacity values deduced from the cyclic voltammetry experiments were found to increase in the following order: Fe_3O_4/without surfactant (34 F g^{-1}) < Fe_3O_4/CTAB (44 F g^{-1} <Fe_3O_4/SDS (63 F.g^{-1}). The latter exhibited a specific discharge capacitance of 60 F.g^{-1} that remained stable after 700 charge/discharge cycles [1]. The improved electrochemical performance of Fe_3O_4/SDS may be due to the particle size and shape effects [2]. As a result of the enhanced electrochemical performance, Fe_3O_4/SDS hybrids could be regarded as a promising electrode for Li/Na-ion batteries and supercapacitors.

Keywords : Fe_3O_4 nanoparticles. TEM. Cyclic voltammetry. Galvanostatic charge/discharge

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Synthesis and Antioxidant Activity of 4-Aryl-3,4-dihydro-2*H*-benzo[*g*]chromene-2,5,10-triones

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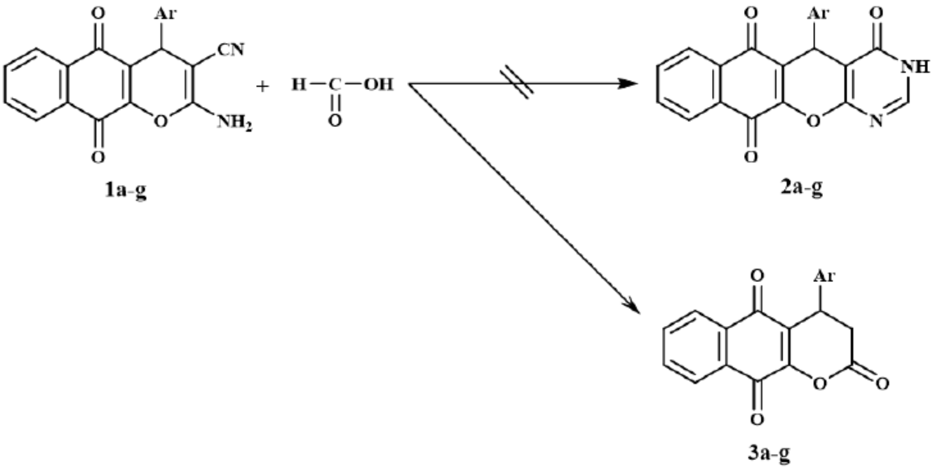
In this work, we studied the condensation of 2-amino-4*H*-benzo[*g*]chromene-3-carbonitriles **1a-g** as precursors with formic acid, in mild reaction conditions. The objective was the synthesis of new 5-aryl-3,5-dihydro-4*H*-benzo[6,7]chromeno[2,3-*d*]pyrimidine-4,6,11-triones **2a-g**, while the isolated products which were characterized by the different spectroscopic analysis (IR, NMR, HRMS) and elemental analysis, showed exceptionally the structures of 4-aryl-3,4-dihydro-2*H*-benzo[*g*]chromene-2,5,10-triones **3a-g**. The synthesized compounds were evaluated on their antioxidant activity *in vitro* using ascorbic acid as standard.



Key words: benzo[*g*]chromene derivatives, 2-amino-4*H*-benzo[*g*]chromene-3-carbonitriles, antioxidant activity, formic acid

Synthesis of new
5-methyl-2,8,10-triarylpyrimido[5,4-e][1,2,4]triazolo[1,5-c]pyrimidine

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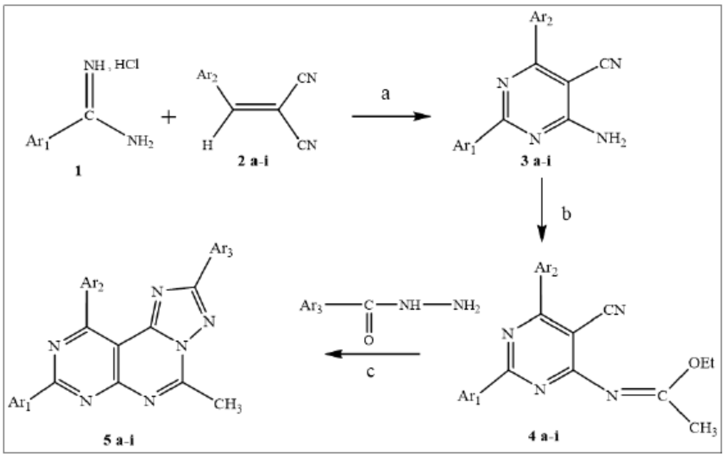
In the present work, it is proposed to describe the synthesis of 5-methyl-2,8,10-triarylpyrimido[5,4-e][1,2,4]triazolo[1,5-c]pyrimidine derivatives via several steps.

In the first, the benzonitrile is converted to benzamidine hydrochloride 1. After that, the reactivity of this product with different arylidenemalononitriles 2a-i offered the 4-amino-5-cyanopyrimdine derivatives 3. Then, these compounds 3a-i was treated with triethyl orthoacetate and the mixture was heated under microwave irradiation (MWI) to afford the desired imidate 4a-i with good yields.

Finally, we transformed these imidates 4a-i into news triazolopyrimidopyrimidines via treatment with arylhydrazide.



Scheme 1: Synthesis of triazolopyrimidopyrimidines 5a-i, Reagents and conditions:
(a) CH_3COONa, EtOH-Water (V/V), Reflux, 3h (b) $CH_3C(OEt)_3$, CH_3COOH, MWI, 45 min,
(c) Toluene, CH_3COOH, Reflux, 2h.

All new compounds are identified and characterized by spectroscopic techniques ^1H NMR, ^{13}C NMR, FTIR and HRMS.

Process Simulation of Biodiesel Production and Purification from Microalgal Oils

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In this work, three process scenarios to produce biodiesel from microalgae oil by trans-esterification via basic catalysis have been proposed and simulated using SuperPro Designer® software. To investigate the effect of raw materials on the process performance, oil of two species of microalgae (*Chlamydomonas reinhardtii* and *Dunaliella salina*) was represented in the simulator by a multicomponent mixture identified from the triglyceride composition found in the literature, where the first species was represented by nine triglycerides and the second specie was represented by fourteen triglycerides. The flowsheets contained an oil pretreatment unit linked together with a unit for the production and purification of biodiesel. The pretreatment unit aimed at obtaining an adequately deacidified oil, which can then be directed to the next unit of production and purification of biodiesel. The oil pretreatment unit differed from one process flowsheet to other because three different operations were tested: (a) esterification with methanol, (b) esterification with ethanol, and (c) physical deacidification. The results showed that, for a set amount of raw algal oil (8 tons/h), the physical deacidification process using *C. reinhardtii* showed the lowest production of biodiesel. The esterification with ethanol, showed the highest consumption of alcohol, with 16,180 and 16,115 tons/year for *C. reinhardtii* and *D. salina*, respectively. In the case of esterification with the methanol, results showed the highest amount of water consumption, with 240,849 and 241,756 tons/year, for *C. reinhardtii* and *D. salina*, respectively. Finally, equipment and their operating conditions employed during this work allow the achievement of biodiesel properties as specified by European biodiesel standard EN 14214, with emphasis on properties such as density, flash point, and viscosity.

Keywords: Process simulation, Microalgae, Transesterification, Fatty acids, Lipids.

Comparison of the Sustainability of Biodiesel Production from Microalgae

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In recent years, the cultivation of microalgae has gained interest due to its high productivity of lipids, the main raw material employed for the production of biodiesel. In the present work, process design alternatives were designed for the production of biodiesel from microalgae. The process starts with the stage of microalgae flocculation, then the concentration of microalgae, followed by the extraction and purification of lipids, to then evaluate and compare their sustainability through an economic, energy, and environmental analysis. Various technological alternatives were evaluated for each stage, using SuperPro Designer® software for process simulation, based on parameters and operational data published in various scientific sources related to the subject. Energy consumption, operational and investment costs were calculated and analyzed, together with the productivity of each evaluated alternative, for each stage and the whole process, thus obtaining for each scenario respective results for the specific energy consumption (kWh/unit of product), the specific variable cost (€/unit of product) and the net present value (€). It was determined that the production of biodiesel from microalgae is currently technically feasible, but not profitable. From the analysis, more research progress should be dedicated to eliminating the drying stage to obtain an energetically profitable product. The best economic performance was obtained using a biodiesel sales price equal to or greater than €2.6 to be profitable, far from the current sales value of biodiesel in Europe (€0.86 per liter). The profitability of the production of biodiesel from microalgae could be achieved through the parallel production, and sale, of other products derived from these microorganisms, mainly those that have a high market value, such as proteins, carotenoids (red algae), and other chemical compounds.

Key words: Process simulation, Extraction, Unit operations, Fats, Profitability.

Synthesis of new Tetrazole derivatives

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In recent years, Thiophene and its derivatives have known an increasing importance as intermediates to biologically active compounds and in organic synthesis. 2-Amino-3-functionally substituted thiophene derivatives have been studied as probe molecules in chemical biology and drugs or hits in medicinal chemistry. Our laboratory interested in the development and functionalization of heterocyclic compounds with promising biological and pharmacological activities including some new concept of green chemistry; as a part of our research, different types of 2-aminothiophenes were achieved in good yields that are then used to prepare tertazole derivatives.

Keywords: Thiophene; 2-aminothiophene; Gewald; tertazole; biologically active compounds

The research teams of our laboratory focus their efforts on the synthesis of new heterocyclic compounds with promising biological and pharmacological activities via modern and ecofriendly strategies. As a part of our research, we prepared 2-aminothiophenes derivatives which will be used to prepare tertazole derivatives **(Figure 1)**.

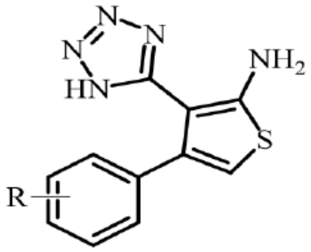

Figure 1: 4-phenyl-3-(1H-tetrazol-5-yl)thiophen-2-amine derivatives.

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New magnetic refrigerant for application in magnetic refrigeration

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We present a new refrigerant $La_{0.7}Ca_{0.15}Sr_{0.15}Mn_{1-x}Ga_xO_3$ (x = 0.0-0.1) manganites. These compounds were prepared by sol-gel method. The refinement of the X-ray diffraction reveals that all samples crystallize in a rhombohedral structure (space group $R\bar{3}c$). Detailed measurements of the magnetization as function of temperature and magnetic applied field M (μ_0H, T) were carried out. From the M(μ_0H, T) curves, we have calculated the magnetic entropy change (ΔS_M) according to the Maxwell relation.

The temperature dependence of the magnetization M(T) reveals a decrease of M when increasing the x content. The magnetic entropy change (ΔS_M) reaches a maximum value near room temperature. It was also found that these compound exhibits a large magnetocaloric effect MCE which increase when decreasing Ga concentration. So, the studied compounds could be considered as a potential material for magnetic refrigeration application.

Keywords: Magnetic measurements; Rietveld refinement; magnetic refrigeration; magnetocaloric effect

Synthesis and characterization of $CuTiO_3$ by hydrothermal method

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[b)] Ecole Normale Supérieure d'Enseignement Technologique de Skikda, Algérie

In this work, we aimed to investigate an efficient and low-cost system performance of $CuTiO_3$. which was prepared by a hydrothermal technique. The synthesized photocatalyst were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), ultraviolet-visible spectroscopy (UV-Vis) and photocatalytic methods. The experimental analysis shows that after calcinations at a temperature of about 800°C, the NiTiO3 phase is well crystallized with a preferential orientation of the grains along the direction (.....). The micrographic images revealed a homogenization of the grain size according to the magnification. The energy dispersive X-ray analysis (EDX) analysis shows characteristic peaks and composition of $CuTiO_3$ powder. The optical measurements showed that the band gap is about 2,2eV.

Key words: $CuTiO_3$, Hydrothermal Method, Microstructure, Optical measurement.

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Extraction of pectin from Tunisian artichoke *(Cynara scolymus)* : Physico-chemical characterization and biological evaluation

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In recent years, polysaccharides derived from artichokes have attracted increasing attention in medicine [1], herbiculture, food [2], and many other industries. In the present study, PSG and PSV polysaccharides were extracted from the bracts of two varieties, "Blanc Oranais" and "Violet d'Hyères," of **Cynara scolymus** with hydrochloric acid (1 M) at 80 °C. The structures of PSG and PSV were characterized by ultraviolet-visible (UV-Vis), Fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR) spectrometry, Gas Chromatography-coupled mass spectrometry (GC-MS), and size exclusion chromatography SEC/MALS/VD/DRI. Importantly, the biological evaluation of PSG and PSV revealed that the two polysaccharides present an interesting anti-radical potential. Moreover, PSV showed a higher antiproliferative potential than PSG against the proliferation of HepG-2 liver cancer epithelial cells, and the inhibitory activity test of the -amylase enzyme showed that the two polysaccharides have an interesting inhibitory power.

Key words: pectin, artichoke, physico-chemical characterization, antiproliferative effect.

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Elaboration and study of antitumoral activity of a novel decavanadate complex

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Vanadium presents a potential biological, pharmacological, and physicochemical property. The growing interest is mainly due to the use of vanadium in the bioinorganic field such as the treatment of diabetes by regulating the blood glucose level of animals and diabetic patients, viral infection and cancer. Recently, several articles have been published regarding the antitumor activity of decavanadate. Also, the family of N-heterocyclic compounds is an important class of compounds in medicinal chemistry. In this context, we focused our work on the synthesis, characterization and study of the antitumor activity of a novel decavanadate complex. The resolution of the structure leads after several cycles of refinements followed by a few Fourrier-Differences to accepted values of reability factors. The structure consists of a three-dimensional supramolecular assembly, where $[V_{10}O_{28}]^{6-}$ units interact with the cationic ligand, the hexahydrated Magnesium polyhedron and the water molecules of crystallization through hydrogen bonds. The structure was characterized by various experimental techniques, including X-ray powder diffraction and IR and UV-visible spectroscopy. In this study, the cytotoxic and antiproliferative activities of the synthesized complex on human cancer cells were investigated, showing that the latter could be a valuable candidate for the development of a novel highly active chemotherapeutic drug for brain cancer.

Keywords: decavanadate; X-ray diffraction; antitumural activity

Square-Based Bipyramid Tetraaza Macrocyclic Complexes: Characterization, Complexation and TD-DFT Modelisation

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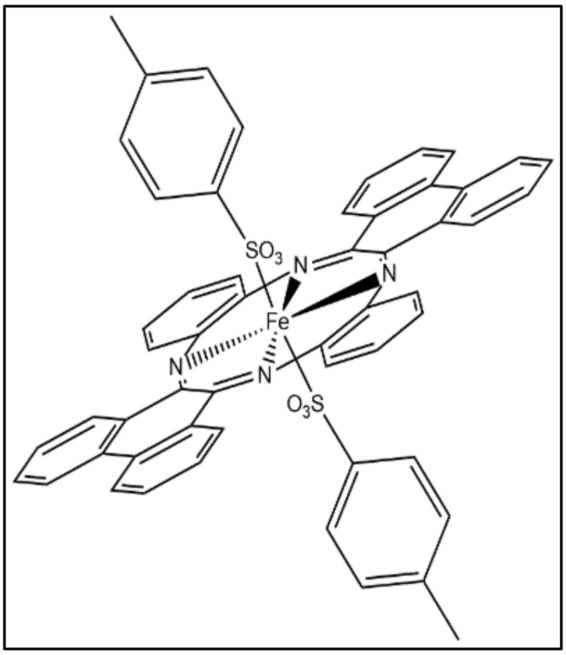
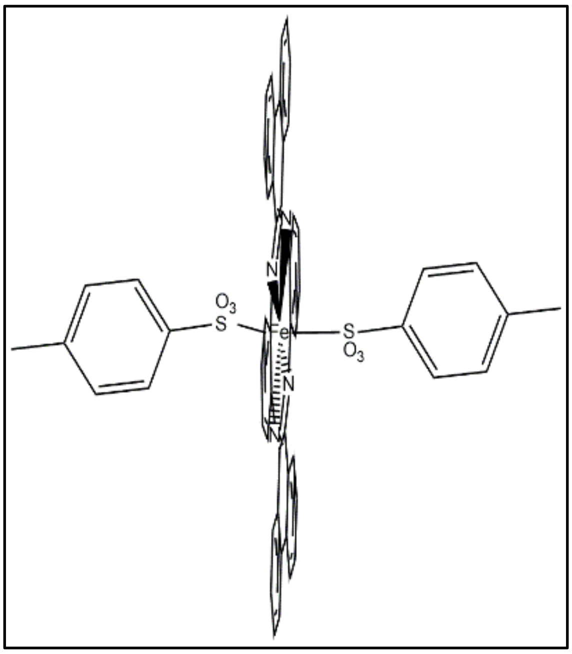
This study proposes a synthesis of a novel Square-Based Bipyramid tetraaza macrocyclic Schiff base ligand ($C_{40}H_{24}N_4$) involving M = Co, Fe, and Para-Toluene Sulfonic Acid PTSA inside the cavity. New obtained complexes are characterized by ^{1}H and ^{13}C NMR, UV–Vis and FT-IR spectroscopy. Besides, the structure properties and the energetically stability are carried out using DFT/B3LYP method with 6-311++G(d,p) as basis set.





Keywords: Schiff base, Tetraaza macrocyclic, ligand, Modélisation DFT.

Synthesis, structural and electrical study of a new double perovskite $(La_{2/3}Sr_{1/3})_2$ $(Sn_{1/3}Cu_{1/3}Fe_{1/3})_2O_6$.

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The triple substitution in the B-site simultaneously with the single substitution in the A-site of the perovskite SrSnO3 has allowed the synthesis of a new double perovskite $(La_{2/3}Sr_{1/3})_2$ $(Sn_{1/3}Cu_{1/3}Fe_{1/3})_2O_6$. The sol-gel process was adopted in the elaboration of this material.

The X-ray crystallographic analysis and Rietveld structural study of the developed material, based on a structural model, [1] showed that $La_2SrSnCuFeO_9$ crystallizes in the quadratic system (space group I4/m), with lattice parameters a = 5.62258(5) Å, b = 5.62258(5) Å, c = 7.95001(8) Å. The structure of this compound shows a (1:1) order at the B sites. Specifically, the octahedral sites are divided into two subsets which occur alternately in 3 dimensions throughout the structure in a checker-board pattern: $(Sn_{2/3}$, $Cu1_{1/3})$, $(Fe_{2/3}$, $Cu2_{1/3})$. The resulting cationic distribution can be illustrated by the crystallographic formula $[SrLa_2]_A[(SbCu_{0.5})_{2a}(FeCu_{0.5})_{2b}]_BO_9$.

The electric properties of the material have been studied through the variation of the conductivity, dielectric constant and dielectric loss in function of the frequency and temperature besides the study of the impedance spectroscopy. According to the results, it has been revealed that $(La_{2/3}Sr_{1/3})_2$ $(Sn_{1/3}Cu_{1/3}Fe_{1/3})_2O_6$ is characterized by a semiconductor character.

Keywords: Perovskite, cationic distribution, Rietveld refinement, sol-gel, Electric properties, Impedance spectroscopy, Environment and green material.

Acknowledgements: A special appreciation dedicated to all the researchers working in the Materials and Environment for Sustainable Development Laboratory LR18ES10, ISSBAT.

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Elaboration and characterization of new materials based on oxides: Electrical, dielectric and optical properties

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$Li_{0.3-x}Ce_xAl_{0.3}Si_{0.7}O_{2\pm\delta}$ (x=0; 0.03; 0.05; 0.07 and 0.1) powders were prepared via the mechanical milling reaction method [1]. The phase identification and morphology were studied by X-R diffraction (XRD) and transmission electron microscopy (TEM).

The vibrational absorption bands are identified by infrared spectroscopy (IR).

The electrical conductivity was studied by impedance spectroscopy. Measurements were carried out in an open circuit using two electrodes with a signal amplitude of 50 mV and a frequency band ranging from 5 Hz to 13 MHz.

The Ce^{4+} doping has a remarquable influence on structural and electrical properties.

Key words: mechanical milling process, doping ceria, impedance spectroscopy.

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Phenolic compounds extraction from Olive mill wastewater and identification using LCMS/MS

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The recent studies were directed towards valorizing wastes and industrial effluents specifically olive mill wastewater (OMW) which are liquid effluents generates from the olive oil extraction process. These effluents are very well known for being a source of pollution due to their high concentration in organic matter, However, they are also rich with phenolic compounds which are bioactive molecules very known with their antioxidant capacity that makes them a huge interest of many industries.

For that matter, our study is based on studying the extraction of phenolic compounds from Olive mill wastewater and the effect of the extracting method and the solvents. The olive mill wastewater (OMW) samples were collected from the Cap Bon, Tunisia after being stored for 3 months in evaporation baths. The phenolic compounds were extracted using three different methods: maceration, liquid-liquid, and steam distillation. For the maceration method different solvents were used; Ethanol, methanol, acetonitrile, dichloromethane, chloroform, cyclohexane, petroleum ether, in addition to two solvent mixtures: methanol, chloroform (1:1) and acetonitrile, chloroform (1:1). The comparison of the extraction methods revealed that the liquid-liquid method using ethyl acetate as a solvent is the most effective method followed by the maceration using a mixture of chloroform and methanol, their polyphenol contents are respectively in the range of 1.17 g EAC/L of OMW and 1.07 g EAC/L of OMW. However, the steam distillation did not show any relevant results. In addition, an identification of the phenolic compounds using ultra high-performance liquid chromatography coupled to mass spectroscopy (UHPLCMS/MS) was initiated using two samples, we noticed that those two samples have different profiles. However, this has allowed us to identify in both cases many bioactive compounds that are anthocyanins. four other bioactive compounds were identified as well, like are flavan-3-ol, 1-Acetoxypinoresinol and p-DHPA-EA.

Key words: Olive mill wastewater, extraction, phenolic compounds, UHPLCMS/MS, anthocyanins

Self-assembly of new cobalt thiocyanic complex based on histamine, Synthesis, Empirical, Antioxidant activity, and Quantum theory investigations

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The cobalt complex has been synthesized from the reaction of the histamine with metallic salt $CoCl_2.6H_2O$ and thiocyanate ion (SCN^-) as a ligand in H_2O/ethanolic solution and processing by the evaporation crystal growth method at room temperature to get crystals. The synthesized complex has been fully characterized by single-crystal X-ray diffraction. UV-Visible, FTIR spectroscopy, TGA analysis, and DFT circulations were also performed. The crystal structural analysis reveals that the solid $\{[Co(SCN)_4](C_5H_{11}N_3)_2\}\cdot 2Cl$ crystallizes in the monoclinic space group $P2_1/m$.

Metal cations are joined into corrugated chains parallel to the b-axis direction by four thiocyanate anions. Different interactions pack the system into a ring formed by N-H···Cl and N-H···S hydrogen bonds. Hirshfeld surface analysis cum 2D fingerprint plots visualize the main intermolecular interactions with their contributions in the solid-state phase. The molecular geometry of the complex was used for quantum chemical calculation. Here, frontier orbital analysis and electrostatic potential illustrate the chemical reactivities of the metal-organic complex. QTAIM and NCI analysis reveal the strength of interactions at the electronic level.

Keywords: Metal complex, Cobalt thiocyanate, Crystal structure, Physico-chemical study, Hydrogen bonds, Hirshfeld surface analysis, DFT studies.

Molecular Interactions between Glyphosate and H_2O and Isomerisation Reaction Paths from Non-ionized to Zwitterion Species in Aqueous Solution

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The molecular interactions between glyphosate (N-phosphonomethylglycine) [1] and water molecules and the reaction paths from zwitterion to the neutral species were studied by the use of density functional theory calculations. Models of glyphosate-$(H_2O)_n$ (n=1-9) have been adopted. The hydrogen-bond network in ionized (zwitterions) and non-ionized forms was examined. Ready isomerization was thought to be associated with reasonable hydrogen bond directionality. Isomerization via a proton exchange process with an ion-pair intermediate was discussed.

Key words: Glyphosate, Tautomerization, H-bonds, DFT, Solvation

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Study of salt effects on the aggregation behavior of ionic liquid 1-allyl-3-methylimidazolium bromide in aqueous solution

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Because of their special properties, room-temperature ionic liquids (RTILs) are used as new solvents in chemical processes and have been the target of numerous scientific investigations. Many ILs with advantageous properties over "traditional" molecular solvents have been described for this application. Imidazolium-based ILs are of great interest for solvents, phase transfer catalysts, and electrochemical applications. Many of these applications require mixing ILs with polyelectrolytes (PE) or salts. In the present work, we investigate the effect of inorganic potassium salts (KPF6 and KBF4) on the aggregation of the free ionic liquid with the salts in the pre-micellar region using conductometry, densimetry, and viscosity measurements at three different temperatures. The results were confirmed by UV spectroscopy. The aggregation behavior of the 1 allyl-3-methyl imidaolium bromide AMIMBr is interpreted considering the complex and competitive nature of the interactions between the ionic liquid, the inorganic salt and water. All parameters show that strong synergistic interactions were observed in the aqueous medium in the mixed systems studied and the presence of salt can be explained by interactions between counter-ion and salt ion.

Key worlds: ionic liquid, salt effect, self-aggregation, ionic conductivity, density.

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

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

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

Crystal Structure, Spectroscopic Characterization, and Optical Properties of the Hybrid Compound $(C_7H_{11}N_2)_2[CdCl_4]\cdot0.5H_2O$

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A preparation procedure for the title compound $(C_7H_{11}N_2)_2[CdCl_4]\cdot0.5H_2O$ ($C_7H_{11}N_2$= 4-(dimethylamino)pyridinium) was developed and gave good yields and purity. The Cd(II) ion is coordinated in a slightly distorted tetrahedral environment by four chlorides. The crystal arrangement shows a layered structure with alternating organic and inorganic layers parallel to the (001) plane and located at $x=n+1/2$ ($n \in Z$). In the crystal, the organic and inorganic layers are linked by C—H…Cl, C—H…O, N—H…Cl and N—H…O hydrogen bonding interactions. Hirshfeld surface analysis and fingerprint plots of the structure reveal that molecular packing is governed by hydrogen bonds and π-stacking. The UV-Vis diffuse reflectance spectrum allowed us to determine a direct band gap of 3.596 eV with a semiconducting character, using the Tauc-extrapolation method. The observed photoluminescence band with a maximum at 562 nm is assigned to excited π - π* states in the 4 - (dimethylamino) pyridinium cation.

Key words: chlorocadmates(II), 4-(dimethylamino)pyridinium, crystal structure, Hirshfeld surface analysis, photoluminescence

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Synthesis of new oxadiazoles from imidates

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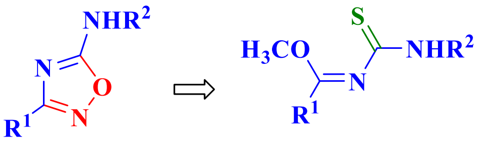
The oxadiazoles are privileged heterocyclic structures in medicinal chemistry. They are often considered as ester and amide bioisosteres in drug discovery research. Continuing investigations into their biological activities as antimicrobial, anticancer, anticonvulsants, and anti-inflammatory agents highlight their significant and growing impact within drug discovery programs.[1] Oxadiazoles are versatile and can be performed starting from most nitriles.[2] As part of the synthesis of new oxadiazole from imidate, this communication deals with the synthesis of new oxadiazole from thiocarbamoyl imidate.



R^1 = Ph, Bn, iPr, mMePh.
R^2 = Ph, CH_2-CH=CH_2, CH_2cyclohexyl.

Figure 1. Synthesis of new oxadiazoles.

Key words : Oxadiazole, Thiocarbamoylimidate.

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Investigation on molecular structure, thermal behavior, theoretical calculation and biological properties of a novel thiocyanate complex $(C_{14}H_{15}N_2)_2[Co(NCS)_4]$

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The slow evaporation technique was used to synthesize a novel crystalline complex, $(HPhPip)_2[Co(NCS)_4]$,by combining cobalt chloride, potassium thiocyanate and 1-phenylpiperazine.According to the crystallographic study, the Co^{2+}ion is surrounded by four NCS^- anions, forming a distorted tetrahedron geometry. The $[Co(NCS)_4]^{2-}$ anions and 1-phenylpiperazinium cations are linked together through N–H…S, C–H…S and C–H···π intermolecular interactions, resulting consequently a three-dimensional network. The vibrational modes analysis is developed via FTIR spectroscopy. A theoretical investigation has been performed by DFT that allows the determination of the molecular frontiers orbitales and the Molecular Electrostatic Potential maps.Thus, the band gap energy between HOMO and LUMO explains the eventual charge transfer interactions. The Hirshfeld surface, 2D fingerprint plots and enrichment ratio were investigated. Moreover, the robust thermal stability was tested by ATD/ATG. Finally, the bacterial potency has been surveyed against some pathogenic bacteria and fungal strains. Antioxidant capacity towards $DPPH^{\bullet+}$ radical cation is assessed as well.

Keywords: Coordination chemistry, Crystal structure, Bacterial strains, Metal complex.

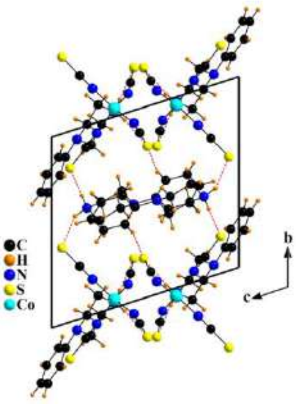

Figure.1: Projection along the *a*-axis of the structure of $(HPhPip)_2[Co(NCS)_4]$. Dotted lines indicate hydrogen bonds.

New fluorescent material based on anthracene and triazole for blue organic light emitting diode: A combined experimental and theoretical study

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A new anthracene-based functional material (an-tri-van) has been prepared by a click chemistry reaction for use as an emitter in blue OLEDs. A combined experimental and theoretical study was carried out to better understand the optoelectronic properties of the new organic material An-Tri-Van. Its molecular structure was confirmed by proton nuclear magnetic resonance (^{1}H-NMR) and Fourier transform infrared spectroscopy (FT-IR). Thermal analysis was determined by DSC and showed that the material has good thermal stability up to 200°C. The UV-Vis absorption and photoluminescence (PL) optical properties of an-tri-van were studied in dilute solution and as a thin film. The HOMO and LUMO energy levels were estimated by cyclic voltammetry analysis. The structural, optical and charge transfer properties of the organic material studied were evaluated by density functional testing (DFT) and time dependent density function (TD-DFT). The B3LYP method with the basis sets 3-21g(d), 6-31+g(d) and 6-311++g (d, p) was successfully applied to reliably compare the predicted vibrational, structural, electrochemical and optical properties. The studied molecule exhibited a non-planar structure with an energy band gap of about 3.4 eV and a vibronic structure with absorption in the near visible ultraviolet region with an absorption maximum of 402 nm, which is attributed to the $\pi \rightarrow \pi*$ electronic transitions mainly of the anthracene group. The excited an-tri-van showed pure blue color emission. Based on the Marcus theory and from the analysis of the charge transfer properties, we found that the An-Tri-Van molecule has an interesting hole and electron transport capability. Furthermore, the current-voltage (I-V) characteristic of a typical tri-layer OLED (ITO / NPB/An-Tri-Van/ Alq3/ Al) was generated by simulation, and the threshold voltage is estimated to be 5.4 V. The prepared an-tri-van molecule has tunable electronic and physical properties, which present the most favorable characteristics for blue OLED emission.

Keywords: Anthracene; Click chemistry; Triazole; Opto-electronic properties; DFT/TD-DFT; Organic Light-Emitting Diodes

Conductivity study of carboxymethylated cellulosic polyelectrolytes XCMC. A Test of different Models

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We present in this poster the detailed experimental and theoretical results relative to the conductivities of KCMC, NaCMC, LiCMC and CsCMC aqueous polyelectrolytes in order to complete the text content of our oral contribution entitled “Influence of Dielectric friction on the dependency of the Mobility of Carboxymethylated cellulosic chains with the nature of their counterions”.

The different theoretical chain models used for the interpretation are: The Manning’s thread-like chain model, the Pearl-Necklace-like chain model and the general Ellipsoidal model, characterized by the structural length L_S = 3877A°, the structural charge number $|Z_S|$ = 750; and by four different degrees of substitution DS.

Calculation for each model of the degree of counter-ion condensation, and hydrodynamic, electrophoretic, ionic relaxation and dielectric friction effects, allows the comparison between experimental and calculated conductivities, in a concentration range between $5\ 10^{-4}$ to $5\ 10^{-2}$ equiv l^{-1}.

This analysis permits to find the most probable chain configuration, to calculate its corresponding degree of the ionic condensation and to compare for each conformation, the different friction effects and their dependence on the concentration, on DS, and on the nature of the counterions.

A one pot synthesis of new highly substituted-allyl carbamates

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Allylic carbamates are of considerable interest due to their important role in various areas. Indeed, they belong to the structural or functional part of many approved drugs[1] and prodrugs[1], which are used for the treatment of several diseases such as Alzheimer's disease[2]**,** cancer[3], hepatitis C[4], and epilepsy[5]. They are found to be important raw materials in the synthesis of polyurethanes[6], pesticides, herbicides, insecticides and fungicides[7]. They are also used as intermediates in numerous organic synthesis[8] and heterocyclic compounds synthesis[9]. In this work, we report the one-pot synthesis of new variously substituted γ-chloro-γ,β-allylic carbamates from β-chloro-α,β-unsaturated aldehydes. The new compounds and the corresponding intermediates, the γ-chloro-γ,β-allylic alcohols were fully characterized by (^{1}H and ^{13}C) NMR, IR and HRMS spectroscopic techniques. The crystal structures of two allylic carbamates were established by single-crystal X-ray diffraction.

Keywords: β-chlorovinylaldehydes; allylic alcohols; allylic carbamates; X-ray diffraction.

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Assess the performance of microstructural and optoelectronic properties of dual porous silicon decorated by ZrO_2/Al_2O_3 nanoparticles.

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Nanoparticles of Al_2O_3 and ZrO_2 were deposited in dual Silicon nanopores by chemical vapor deposition (CVD). This work presents a study of the integration effect of the alumina nanoparticle on morphological and opto-electronic properties of a porous Sidp/ZrO_2 composite. Various techniques have been used such as scanning electron microscope, energy dispersion X-ray spectroscopy, X-ray diffraction, spectroscopic ellipsommetry and impedance analyzer techniques for coroled between morpho-structural and opto-electronic properties. After correlating the opto microstructural and electrical properties, we find this process simple, easy and efficient to produce high quality Sidp/ZrO_2/Al_2O_3 thin films for optoelectronic applications.

Keywords: ZrO_2 /Al_2O_3, dual porous Silicon, Morpho-structurale, opto-electronic properties.

Effects of hydroalcoholic extracts from Okra (*Abelmoschus esculentus* L.) Leaves, Fruits and Seeds on European sea bass (*Dicentrarchus labrax*) leucocytes, and their cytotoxic, bactericidal and antioxidant propreties

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M. Ángeles Esteban, Mehrez Romdhane

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Abelmoschus esculentus L. (okra) leaves, fruits and seeds contain phenolic compounds which have remarkable health benefits. The *in vitro* effects of ethanolic extracts obtained from okra's different parts on European sea bass (*Dicentrarchus labrax*) were estimated in this study. Phytochemical screening of okra's different parts hydroalcoholic extracts revealed an important content of phenolics and flavonoids. Significant effects on *Dicentrarchus labrax* immunostimulant activities (viability, phagocytic ability and capacity, respiratory burst, and peroxidase) were detected. Middle concentrations of different extracts showed a significant increase in the phagocytosis ability and capacity and respiratory burst activity of HK leucocytes. However, middle concentrations of leaves and fruits ethanolic extracts significantly decreased the peroxidase activity. In addition, all okra ethanolic extracts produced a marked a significant cytotoxic activity at middle and higher against *DLB-1* and PLHC-1 cell lines. Moreover, all doses of seeds and leaves extract at higher concentrations of fruits highlighted significant bactericidal activity on two fish pathogenic bacteria. Finally, the antioxidant activity (ABTS assay) of *Abelmoschus esculentus* L. extracts was determinate.
Overall, the results highlights the possibility of using *Abelmoschus esculentus* L. leaves, fruits, and seeds extracts in the aquaculture farm as an alternative to chemical compounds.

Keywords: *Abelmoschus esculentus* L. extracts, Immunostimulant, Cytotoxicity, Bactericidal activity, Antioxidant, Aquaculture

Effects of synthetic routes on structure and physico-chemical properties of phosphates nanoparticles

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In the present work we describe a new approach for the synthesis of phosphates materials. Pure $M_2P_2O_7$ (M=Mn, Co) phases with a high crystallinity have been sonochemically synthesized. X-ray Powder Diffraction (XRD) characterizes the resulting nano-sized particles. The materials crystallize in the C2/m monoclinic structure. IR absorption spectroscopy reveals the various vibrational modes relating to P-O groups. The fluorescence emission spectra present the different emission bands of the divalent transition metals in the phosphate matrix. The results suggested that phosphates type $M_2P_2O_7$ are good multi-functional materials for both catalytic and energy storage applications.

Key words: Sonochemistry, phosphate materials, various vibrational modes.

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Investigations of sintered dry-pressed alumina using synthesized organic copolymer

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Polyelectrolytes containing 35 mol % of the carboxylate groups and 65% of hydroxyl functions are synthesized to provide the dual function of dispersant and binder for dry pressed alumina.

The incorporation of synthesized copolymers in the ceramic formulation improves tensile strength of pressed products from low concentrations (1wt%), indicating a good binding effect. Synthesized polyelectrolytes are characterized by a low glass transition temperature, maintaining a plastic character, which provides good compaction for green bodies. This result ensured a high relative green density (around 63%) after compaction under 190 MPa.

Homogeneous and dense microstructure of the green parts containing synthesized copolymer leads to a good densification at the end of sintering. Such property makes synthesized copolymer more promising than the industrial additives (99.2% against 97.7% in the presence of commercial PVA + PEG at 1650 °C).

Minimizing the amount of organic additives in the alumina formulation prevents microstructure defects during sintering, and improves the mechanical properties of sintered parts to reach tensile strength of 357.5 MPa at T=1700°C with the addition of 2wt% of copolymer.

Reactivity of 3,5-dicyanothiophene and Structure-Reactivity Relationships

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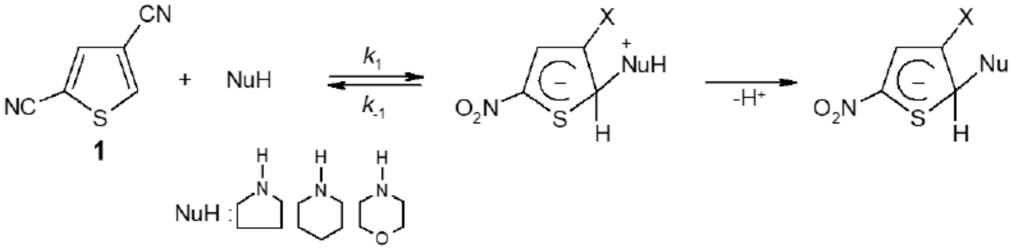
Though the linear free energy relationship log k = *s* (*N* + *E*) (Angew Chem., Int. Ed. Engl. 1994, 33, 938-957), the electrophilicity parameter *E* of 3,5-dicyanothiophene **1** has been determined, at 20 °C, by kinetic investigations of their electrophilic addition reactions to a series of secondary cyclic amines in aqueous solution.

The derived *E* parameter of thiophene **1** (*E* = -22.63) has been integrated into the electrophilicity scale established by Mayr and it is shown that these thiophene has a *E* value which is roughly 9 orders of magnitude less reactive that the 3,5-dinitrothiophene (*E* = -13,42) and 10 orders of magnitude less reactive that the 1,3,5-trinitrobenzene (*E* = -13.19), the common reference aromatic electrophile in nucleophilic addition or substitution processes.



Reaction of 3,5-dicyanothiophene with secondary cyclic amines in water at 20 °C.

Key words: Electrophilicity / Kinetics / Mayr's Equation / 3,5-dicyanothiophene / LFER.

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Wooden tips as sustainable supports in liquid phase microextraction: a closer view of the influence of wood matrix.

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Micro-extraction techniques are a natural evolution of classical sample processing techniques and are characterized by the reduction of the quantity/volume of the extractant phase used. This reduction brings obvious advantages such as the minimization of costs and the reduction of the environmental impact of these techniques.

In the context of techniques using wood tips as substrates in liquid phase microextraction. The porosity of the tips is used to host an organic solvent on the pores. 1-octanol has been selected as solvent as it is a classical extractant in microextraction, and its extraction ability is fully characterized. In fact, the octanol-water partition coefficient is well reported for many compounds as it is used as a polarity index in extraction. In this article, the extraction capabilities of octanol-coated wooden tips have been studied using non-steroidal anti-inflammatory drugs as model analytes. Their extraction has been optimized considering the effect of three main variables: pH, ionic strength, and extraction time. The impact of the wood matrix compounds on determining the analytes by mass spectrometry has also been studied. Although the direct infusion-mass spectrometry analysis resulted in a rapid and efficient approach for determining the drugs at therapeutic levels, the ion suppression effect induced by the wood matrix reduces its potential. In this context, liquid chromatography allowed to improve the performance. Working under the optimal conditions, the proposed method permits the determination of the drugs with limits of quantification as low as 8-32 µg/L, precision (expressed as relative standard deviation) better than 21.3 %, and accuracy (defined as relative recoveries) in the range of 80 to 114 %.

Keywords: Wooden toothpicks, Liquid-phase microextraction, Mass spectrometry, non-steroidal anti-inflammatory drugs (NSAIDs), 1-octanol, Saliva.

Electrocatalytic reduction of hydrogen peroxide over Au- Cu(111) alloys Theoretical approach to establish structure -activity relationship

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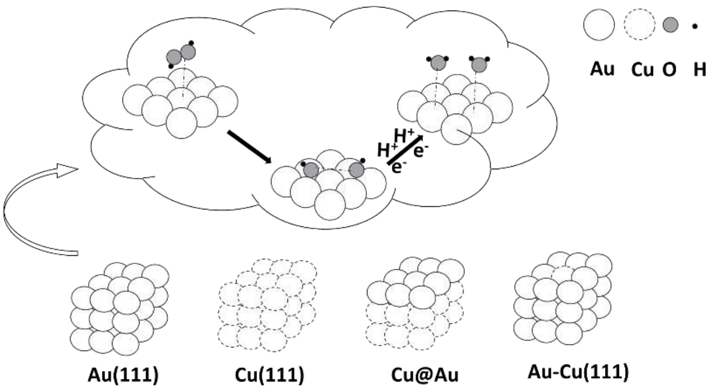

Theoretical approaches have been demonstrated to be powerful to establish structure-activity relationship when using metallic nanoparticles as the active site in heterogeneous catalysis. In this work, we targeted the hydrogen peroxide reduction reaction (HPRR), which is key to detect H_2O_2 even at traces in water. For this study we adopted the grand-canonical density functional theory (DFT). Two HPRR mechanisms have been studied on four surfaces ; bare Au(111) [1] and Cu(111)[2] surface, and for the alloys Cu@Au (Core/shell) and Au-Cu (single atom doped),the first mechanism involved O–O bond breaking in H_2O_2* followed by Hydrogen-transfer reactions between various reaction intermediates and the second mechanism pathway involved the addition of H* to $H_2O_2^*$ coadsorbed on the surface. Compared to pure Au(111) and Cu(111), the elementary steps corresponding to H_2O_2 reduction are significantly improved over Cu@Au(111) and Au-Cu(111) surfaces and the rate determining step is considered to be $OH + H^+ + e^- \rightarrow H_2O$. Detailed DFT calculations on Au, Cu and Au-Cu model alloys reveal a positive role of Cu on Au by favoring the adsorption of H_2O_2 and its intermediates on the catalyst surface compared to pure Au, as well as by slightly reducing the negativity of its onset potential (-0.1 V). Among the studied surfaces, the core/shell surface shows the highest reactivity, and the suitable mechanism is shown to be first pathway which includes O-O bond cleavage.

Key words: Bimetallic Cu@Au, hydrogen peroxide reduction, Density functional theory, Reaction mechanism

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Study of the catalytic wet air oxidation of p-hydroxybenzoic acid on a fresh Ru catalyst supported by different oxides

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Environmental remediation has become more effective when using nanotechnologies [1]. In this study, the catalytic wet air oxidation (CWAO) reaction of p-hydroxybenzoic acid (p-HBA) was realized in a batch reactor at 140 °C at a fixed pressure of 50 bar of air over Ru-based catalysts. Four support materials were employed: TiO_2, CeO_2–TiO_2, ZrO_2–TiO_2, and La_2O_3–TiO_2, which present mesopores in their texture, and exhibit adsorption capacities for pollutants. Those supports were prepared by sol-gel method and impregnated to 3 wt.% of Ru. Those catalysts were characterized by different techniques: adsorption-desorption of N_2, XRD, XPS, H_2–TPR, NH_3-TPD, TEM, and HRTEM. The relationship between catalytic activity and physicochemical properties was discussed. A higher specific surface area BET, large amount of active surface oxygen, and Lewis acidity sites were obtained on catalysts containing cerium (Ru/CeTi). The Ru catalysts containing cerium showed higher activity than the Ru/TiO_2, Ru/ZrTi, and Ru/LaTi. It is assumed that the acid sites and surface oxygen are acting like a tramp for the p–HBA molecule increasing the conversion on the Ru particles joined to an additional oxygen supply by cerium redox process (Ce^{3+}/Ce^{4+}). The presence of cerium inhibits the deposit of carbon on the Ru surface catalyst.

Keywords: CWAO, p-HBA, Ru catalysts, support effects, Sol-gel processing

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Effect of compost addition on phytoremediation of a soil by oleander (*Nerium oleander* L.)

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Contamination by trace metals has become a major environmental problem. This work aims to study the plant potential and the effect of compost addition in the remediation of soils contaminated by trace metal elements, especially by zinc (Zn) and copper (Cu).

All the experiments are taken place under greenhouse for 36 days, using *Nerium oleander* as an in-situ phytoremediation agent. These plants are grown in two different substrates (sand and sand + compost). Metal stress is applied to the plants with the nutrient solution containing increasing concentrations of Cu and/or Zn. The results obtained showed that the addition of compost to the growing medium leads to a slight decrease in pH and an increase in its electrical conductivity. The lowest metal contents in the plant and in the soil residues, were found in a growing medium containing compost. In addition, *Nerium oleander* accumulated substantial amounts of zinc and copper mainly in its roots. The overall results confirmed that *Nerium oleander* is a phytoremediator of heavy metal in the contaminated areas and that compost help the bio-decontamination process.

Key words: phytoremediation, *Nerium oleander*, compost, zinc, copper

Validation of analytical method for the determination of 16 pesticides residues on a tomato matrix

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Validation of analytical procedures is the process of determining the suitability of a given methodolgy for providing useful analytical data. It's the formal and systematic proof that a method compiles with the requirements for testing a product when observing a defined procedures. In the present work an analytical methodology for quantification of the pesticides: Dichlorovos, Ethoprophos, Disulfoton, Alpha HCH, Gamma HCH, Propyzamide, parathion-methyl, Ronnel, Fenitrothion, Chlorpyrifos, Alpha endosulfane, Tokuthion, DDT, Endosulfane Sulfate, Bifenthrin, Cypermethrin residues in tomatoes was developed and validated using Gas Chromatography with a Electron Capture Detector (GC-ECD). The validation parameters studied, in accordance with the requirements of SANTE/12682/2019 guideline [1] of the European Commission, focused on the matrix effect, linearity, specificity, limit of quantification and accuracy of the method. The possibility of a matrix effect was studied.

Key words: analytical validation, pesticide residues, GC-ECD

References

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Alluaudite Phases as electroactive material for sodium ion batteries

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Energy production and storage have become key issues concerning our welfare in daily life. Present challenges for batteries are twofold. In the first place, the increasing demand for powering systems of portable electronic devices and zero-emission vehicles stimulates research towards high energy and high voltage systems. In the second place, low cost batteries are required in order to advance towards smart electric grids that integrate discontinuous energy flow from renewable sources, optimizing the performance of clean energy sources. Na-ion batteries can be the key for the second point, because of the huge availability of sodium, its low price and the similarity of both Li and Na insertion chemistries. The electroactive orthophosphate phases ont été préparés par autocombustion méthode assistée par la glycine. Structural, morphology thermal, thermal and electrical properties have been investigated.

Its structures were determined using X ray powder diffraction and Rietveld method refinements. The two compounds $Na_2M^{2+}{}_2Fe^{3+}(PO_4)_3$ (M = Mn and Co) are alluaudite-type. Both compounds crystallize in monoclinic system with the space group C2/c and similar parameters: a = 12.0337(3) Å, b = 12.6268(3)Å, c = 6.5070(1) Å, β = 114.563(2)° for $Na_2M^{2+}{}_2Fe^{3+}(PO_4)_3$ (NMFP) and a = 11.7597(3) Å, b = 12.4579(3) Å, c = 6.4607(1) Å, β = 113.968(1)° for $Na_2Co_2Fe(PO_4)_3$ (NCFP). The $NaNiFe_2(PO_4)_3$ (NNFP) compounds crystallize in orthorhombic system with the space group Imma and unit cell parameters: a = 10.3993(1) Å, b= 13.1966(1) Å, c = 6.4955(1) Å. The composition and morphology of the compounds were checked by energy dispersive spectroscopy coupled with scanning electron microscope. The thermal analysis confirmed the allotropic transition of the three materials from monoclinic to orthorhombic symmetry with the changing of divalent transitions metal ion. The electrical conductivity results of indicated that NNFP has the lowest value of activation energy of value= 0.63 eV owing to the large size of open channels existed in the orthorhombic symmetry.

Corrosion inhibition of carbon steel in 1M HCl using ethyl acetate extract of a species belonging to Apiaceae family

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Corrosion is material damage caused by chemical, electrochemical, and biological reactions. The global estimate for corrosion cost is in the region of US$ 2.5 trillion [1]. To overcome this problem, researchers focus on plant extract to develop alternative low-cost and environmentally benign corrosion inhibitors [2-3]. In this work, the inhibition of the corrosion of carbon steel in a 1 M HCl solution by the ethyl acetate extract of a species belonging to the Apiaceae family was evaluated by potentiodynamic polarization (PDP) and electrochemical impedance (EIS). The results show that the extract gives 89,32% inhibition efficacy at 500 mg L^{-1}. Inhibitory efficacy increased with increasing inhibitor concentration and decreased with increasing temperature. Polarization curves showed that these extract act as mixed-type inhibitors for anodic and cathodic reactions.

Key words: Corrosion, inhibitor, carbon steel, EIS, PDP.

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Synthesis, Structural and spectroscopic studies, thermal characterization and Hirshfeld surface analysis of Cobalt (II) organic-inorganic hybrid material $(C_{12}H_{22}N_2)[CoCl_4]$

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In this work, a new cobalt hybrid compound $(C_{12}H_{22}N_2)[CoCl_4]$ was synthesized as single crystals by slow evaporation at room temperature. The physico-chemical characterizations of the prepared compound were done by various experimental techniques: powder and single crystal X-ray diffraction, spectroscopic studies (IR and UV-visible) and thermal analysis (TG).
The single crystal X-ray diffraction study showed that the compound crystallizes in the orthorhombic system with the space group $Pna2_1$. The final values of the veracity factors are: R1= 0,0578 for 8422 reflections, wR2 = 0.853 and S = 0.803. The asymmetric unit of the studied complex includes two protonate 1,3-phenylenebis(N,N-dimethylmethanamine) organic cations and two $[CoCl_4]^{2-}$ tetrahedra. The cohesion of the structure is ensured by hydrogen bonds N-H...Cl and Cl…Cl interactions. Thermal analysis was performed to display the different steps of weight loss relative to the title compound. The analysis of the Hirshfeld surfaces (d_{norm} and aspect ratio) associated to 2D fingerprint plots has been done in order to strengthen and consolidate the study of the elaborated complex it helped quantifying the relative contributions of the inter-molecular interactions in the crystal structure.[1]

Key words: hybrid compound, crystal structure, Hirshfeld surface analysis, thermal analysis.

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Molecular structure, spectroscopic studies, thermal behavior, DFT calculations and antimicrobial activity of a Co(II) coordination polymer $^{1}_{\infty}[Co(\mu\text{-}L)(\mu\text{-}Cl)(H_2O)_2]Cl$

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In this study we report a combined experimental and theoretical study of a new Co(II) coordination polymer $^{1}_{\infty}[Co(\mu\text{-}L)(\mu\text{-}Cl)(H_2O)_2]Cl$ based on 4-amino-4*H*-1,2,4-triazole (L). Single crystal X-ray diffraction revealed that the title compound crystallizes in the orthorhombic space group *Pnma* and the Co(II) ions are coordinated by two N atoms of the bridging 4-amino-1,2,4-triazole ligand, two *trans*-oriented bridging Cl^- ligands and two O atoms from coordinated water molecules in a distorted octahedral geometry. Intra and intermolecular N–H···O and O–H···Cl hydrogen bonding interactions stabilize the crystal structure. The experimental IR and Raman spectra showed good agreement with the calculated ones using density functional theory (DFT) on the monomolecular model $[Co(L)_2Cl_2(H_2O)_2]$ at B3LYP/6-311++G(2d,2p) level [1, 2]. TGA and DSC experiments coupled with mass spectrometry under an argon atmosphere in the temperature range from 25 to 950 ºC showed thermal stability till about 100°C. The title compound exhibited selective activity against selected bacterial strains and yeasts in agar diffusion experiments with maximal activity of 20 mm at a concentration of 2.5 mg/mL.

Keywords: Co(II) coordination polymer, 4-amino-1,2,4-triazole (L), crystal structure, thermal properties, DFT calculations, antimicrobial activity.

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In vitro and in silico analysis of the antidiabetic activity of a new triazole-based functionalized chitosan

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Overweight and obesity are widely regarded as serious health problems worldwide. It is classified as a primary chronic metabolic health problem. However, the availability of effective agents for the prevention and/or therapy of obesity is still limited. For this reason, many promising works for the development of several natural substances such as polysaccharide derivatives are reported, which are applied for the treatment and prevention of obesity as well as for all related health problems. Polysaccharides containing heterocyclic moieties have attracted great interest, especially triazole derivatives, which are of great interest due to their wide range of biological activities. Chitosan is the second most abundant renewable polysaccharide on earth after cellulose. Chitosan and its derivatives have been shown to possess various biological activities. In the present work, we report the successful synthesis and characterization of a new chitosan derivative that was synthesized by click chemistry. for a biological purpose such as anti-obesity activity.

This material found its solubility in the common organic solvents. Its structure was confirmed by XPS and IR-FT. Thermal characterization of the chitosan derivative was performed by differential scanning calorimetry (DSC). The analysis of the antidiabetic activity of the elaborated biomaterial based on triazole was performed in vitro and using a molecular docking.

Key words: chitosan, triazole, click chemistry, anti-obesity

Removal of tartrazine dye from agro-food wastewater by raw biomaterial

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Application of raw sawdust (SD) for the removal of tartrazine has been investigated. The materials were characterized via elemental analysis, BET, pH of zero charge, Boehm titration, Fourier transform infrared spectroscopy and scanning electron microscopy. The effects of various parameters such as pH, contact time, agitation speed, adsorbent mass, initial dye concentration and temperature on the removal of the dye were studied. The highest removal percentages were found to be 47.88 %. Langmuir saturation adsorption capacity was equal to 0.8 mg/g at 298 K. Even if SD shows a more limited efficiency in tartrazine removal, it can be used as it is, without any activation step, therefore it can be a convenient alternative to the activated material. In conclusion, SD is promising, biodegradable, eco-friendly, cost-effective and efficient adsorbent for the removal of tartrazine from wastewater effluents.

Keywords: Sawdust, Tartrazine removal, Biosorption, Isotherm modelling.

Preparation and green application of Tunisian acid-activated clays

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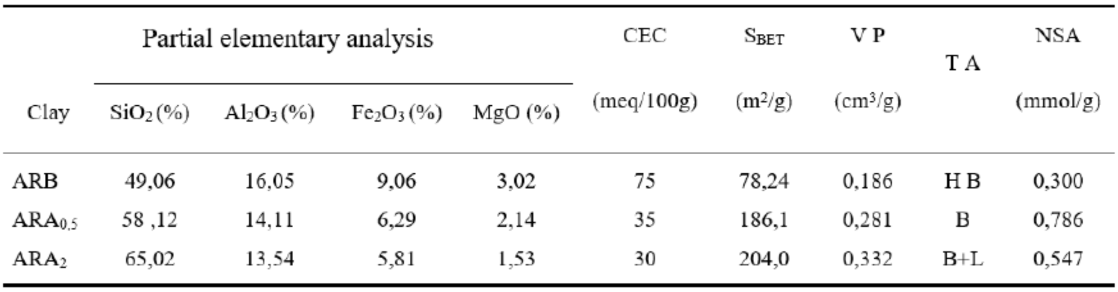
Clays belong to the group of phyllosilicate minerals exhibiting a wide variety depending on several factors. They are renowned for their physico-chemical properties. Natural or modified they are used effectively in a wide range of chemical reactions.

Our work will be devoted to the characterization of Tunisian clay in its raw and purified state. The acid activated clays thus prepared are characterized and used in the synthesis of 1,3-dioxolanes with a series of ketones, using these catalysts under green chemistry.

Table 1 : Main physico-chemical characteristics of raw and acid-activated clays.



	Partial elementary analysis				CEC	S_{BET}	V P	T A	NSA
Clay	SiO_2 (%)	Al_2O_3 (%)	Fe_2O_3 (%)	MgO (%)	(meq/100g)	(m^2/g)	(cm^3/g)		(mmol/g)
ARB	49,06	16,05	9,06	3,02	75	78,24	0,186	H B	0,300
$ARA_{0,5}$	58 ,12	14,11	6,29	2,14	35	186,1	0,281	B	0,786
ARA_2	65,02	13,54	5,81	1,53	30	204,0	0,332	B+L	0,547

CEC : Cation Exchange Capacity ; S_{BET}: Specific Surface; V P : Porous Volume; NSA: Number of Acid Sites

TA : Type of acidity; H B: Hydrogen bond; B: Bronsted Sites; L: Lewis sites

Key words: Heterogeneous catalyst, acid activated clay, green chemistry

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Validation of an analytical method for the dosage of five antihypertensives with the accuracy profile

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Drug association for the treatment of arterial hypertension give hope for improving the life expectancy of hypertensive patients. [1] To this end, there are several pharmaceutical specialties marketed or under development which contain various combinations of antihypertensives. The purpose of this study was to validate a new HPLC-UV method for the routine analytical control and post marketing control of 5 antihypertensive drugs: hydrochlorothiazide, bisoprolol, perindopril, valsartan and lercanidipine.[2–5]
Chromatographic separation of active substances was performed on an Intersil C8 column (250 x 4.6 mm; 5 µ) using a mobile phase consisting of phosphate buffer 6.74 mmol/L (pH 4) and acetonitrile in gradient mode at a flow rate of 1 mL/min and a temperature of 45 °C. Active species were monitored at 223 nm. The obtained drug retention times were 3.39, 4.21, 5.48, 10.56 and 14.06 minutes, respectively, and the resolution of all active substances was greater than 2. The developed method was validated according to accuracy profile methodology. An acceptance limit of ±5% of theoretical concentration has been set. For all active substances, good linearity (correlation coefficient > 0.999), high precision (relative standard deviation [RSD] values, both for repeatability and intermediate precision, were < 2%) and acceptable accuracy (relative biases were found to be < 2%). The accuracy profile shows the validity of our method for the determination of hydrochlorothiazide in the concentration range studied (0.163-0.244 mg/mL), bisoprolol in the concentration range studied (0.168-0.247 mg/mL), perindopril in the concentration range studied (0.165-0.245 mg/mL), valsartan in the concentration range studied (0.163-0.236 mg/mL) and lercanidipine in the concentration range studied (0.163-0.245 mg/mL).
The proposed HPLC-UV method is a reliable, fast, simple, and accurate method that can be conveniently used for the routine quality control of these active substances.

Key words: Antihypertensives, Drug association, HPLC, Validation, Accuracy profile

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New anthracene-based polymer containing tetrazole units for fluorescent sensors

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This communication covers the conception of new soluble and filmogene conjugated polymer (**PAnSCN-Tet**) for heavy metal sensing application. The prepared material is based on the highly emissive anthracene chromophore and contain tetrazole and cyanide groups in their molecular chain backbones. The effect of the electron withdrawing groups on photophysical properties and the chelating abilities of the elaborated organic material were investigated. The optical analysis shows that the the steric hindrance of tetrazole units dominates their electronic effects leading to a blue-shift of its absorption spectrum. Also, the electrochemical study reveals a considerable electronic affinity increase following the incorporation of tetrazole units in the conjugated system of polymer. DFT calculations has been employed to estimate the optimized macromolecular structure of elaborated polymer and a notable change in geometry in terms of planarity was observed depending on the incorporated withdrawing group. The synthesized polymer was studied as optical sensors. The changes in the photoluminescence intensity were used to evaluate the binding affinity of the semiconducting material to different metal ions. The obtained results showed considerable decrease in photoluminescence (quenching) responses with Mn^{2+} cations a short time after adding the cations to **PAnSCN-Tet** solutions with good sensitivity and selectivity.

Keywords: Organic semiconductors, Click chemistry, Tetrazole, Mn^{2+} detection, Fluorescent chemosensor.

Structural, Physicochemical Characterization and Antimicrobial Activities of a new Tris(8-Hydroxyquinoline)Cobalt (III) Ethanol

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Trischelate oxyquinoline octahedral metal complexes (Mq_3) have been widely studied for their potential applications in organic solar cells, light emission diodes (OLEDs), data storage and communication devices [1,2]. 8-HQ is derivative of quinoline which is considered as a "privileged structure" in medicinal chemistry [3].

In this context, our investigation has focused on the synthesis, the characterization of a new species of the formula $[Co(C_9H_6NO)_3].(C_2H_6O)$ and evaluating its antimicrobial potentialities.

This compound has been characterized by single crystal X-ray diffraction, IR and UV-VIS spectra and in vitro antimicrobial activity.

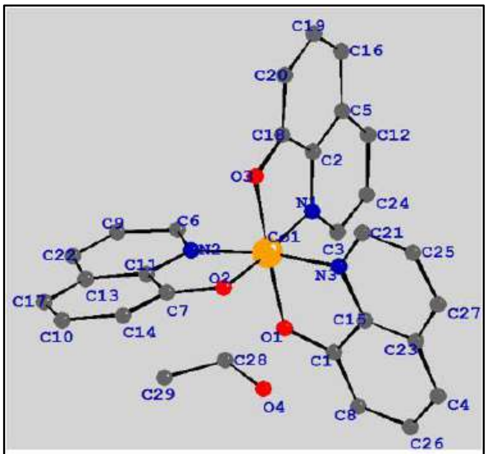

Fig.1 Représentation du complexe $[Co(C_9H_6NO)_3].(C_2H_6O)$

This compound was crystallized in monoclinic system, space group $P2_1/n$ with a=11.261(1)Å, b=13.113(1)Å, c=16.615(1)Å, $\beta = 94.082(1)°$ and refined to R = 0.0284 and wR = 0.0774.

The monomeric cobalt complex crystallizes together with an ethanol molecule which is not included in the coordination sphere of cobalt. The Co(III) atoms were six-coordinated and surrounded by three deprotonated QL ligands showing a distorted octahedral geometry (Fig. 1). Structural cohesion is established essentially by π-π interactions between the neighbouring rings of quinoline groups and intermolecular hydrogen bonds connecting the cobalt complex entities and uncoordinated ethanol molecules. Significant antibacterial activity against *K pneumoniae* and *E coli*, in addition to superior antifungal actions illustrated against *Candida* compared to the positive standard.

Keywords: Cobalt (III) complex, crystal structure, antibacterial activity, spectroscopy studies.

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Extraction, structural characterization and biological properties of polysaccharides from food waste: A review

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Recently, the recovery of agro- residues food represents an attractive economic option as food wastage was becoming a critical problem around the globe due to the continuous increase in the world population. Indeed, the exponential growth in food waste is imposing serious threats such as health risk and environmental pollution. Therefore, numerous studies are now exploring the possibility of the transformation of bioactive compounds, mostly polysaccharides, isolated from food waste into ingredients that can be incorporated in various pharmaceutical, food or cosmetic products. Previous studies have shown that polysaccharides are very important biologically active compounds of food waste, with numerous biological activities effects. The main purpose of this review is to appraise available literature describing the extraction, purification, structural characterizations and biological properties of polysaccharides isolated from food waste. This review also provides a foundation for the further investigation, production and application of these polysaccharides as functional foods and therapeutic agents.

Key words: Food waste; Polysaccharides; Extraction; Physicochemical characterizations; Biological activities

Comparative study of carbon nanotubes and C-18 sorbents for solid-phase extraction of pharmaceuticals substances from water samples.

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Increase in global demand for drugs has made pharmaceutical industry one of the major 26 polluters of solid wastes and effluent into the environment [1]. Sampling and analysis methods for these substances are increasingly efficient and have made it possible to acquire a large amount of data. An analytical method based on Solid Phase Extraction (SPE) with cartridges packed with multiwalled carbon nanotubes (MNWTCs) and C-18 bonded silica combined with ultra-performance liquid chromatography-diode array detection (UPLC-DAD) was established for the determination of eight pharmaceuticals substances (antihistaminic and antimigraine drugs) in environmental and industrial water samples.

For the separation of the eight studied pharmaceuticals products, nature of stationary phase, wavelength detection, composition and pH of mobile phase were optimized. The characteristics for consideration during the validation of the analytical procedure are specificity, linearity, precision, accuracy, limit of detection and limit of quantification. Factors affecting the extraction efficiency including sample volume, the elution solvent type and its volume were optimized. The developed method was successfully applied to the analysis of environmental and industrial water samples. The recoveries of pharmaceuticals substances spiked in water samples ranged from 60 % to 83 %. According to our experimental results, the C-18 silica cartridge has good analytical potential for the extraction of medicinal substances, and it is more efficient than the MNWTCs cartridge.

Key words: carbon nanotubes; SPE; UPLC-DAD; pharmaceuticals substances.

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Michael addition of 1,3-dicarbonyl compounds catalyzed by iron oxide nanoparticules

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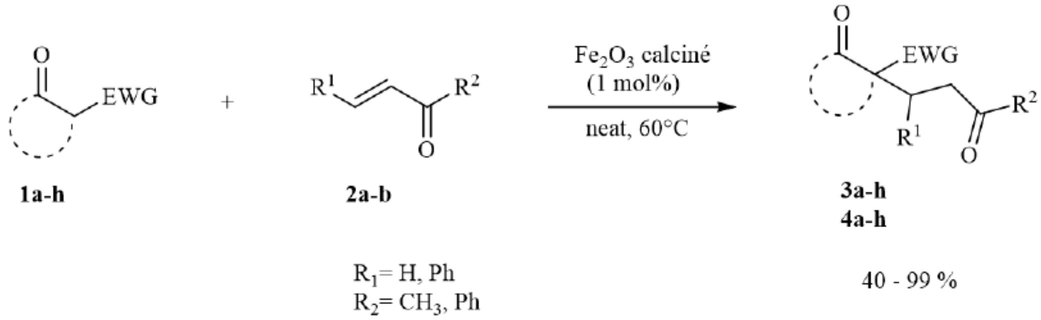
The Michael reaction of the 1,3-dicarbonyl compound **1** and the enones **2** is classically a high yielding base-mediated process (1) and can even be performed with high stereoselectivity (2). However, there are some disadvantages with base catalysis, including side reactions of the starting materials and subsequent reactions of the Michael products **3** and **4**. Recently, we have been able to synthesize several iron oxides (including core-shell) nanoparticules (Fe_2O_3@Fe_2O_3, Fe@Fe_2O_3, GO@Fe_2O_3 and calcinated Fe_2O_3) and asses their potential catalytic activity for C-C bond formation through Michael addition.



Scheme 1. Michael addition of 1,3-dicarbonyl onto α,β-unsaturated carbonyl compounds

It appeared that calcinated Fe_2O_3NP are the most efficient catalysts for Michael addition of various 1,3-dicarbonyl compounds onto α,β-enones at low catalyst loading (1 mol%) under neat conditions.

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Synthesis of new derivatives of 3-amino-hydantoins and study of their antibacterial activity

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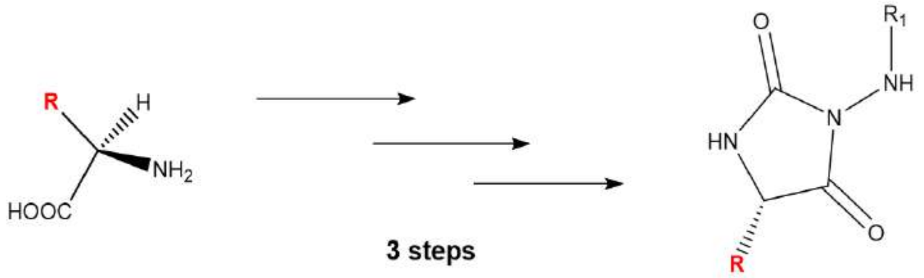
Antibiotics have been shown to be extremely effective in the fight against bacterial diseases that affect both humans and animals. Antibiotics' increasing therapeutic use has led to a rapid emergence of multi-resistant bacterial strains.

To keep improving our ability to combat multi-resistant bacteria, our team at the laboratory of the faculty of pharmacy of Monastir has been interested in creating new basic structures with the scaffold "3-aminohydantoin" and testing their antibacterial activity.

In this work, we have synthesized a series of ten optically pure chiral 3-aminohydantoins in three steps. Optically pure amino acids have been used as starting substrates for the preparation of these structures. The process of synthesizing these derivatives is confidential since this work is part of a research project for new drugs. Then, we tested their antibacterial activity. Some of these products are mostly active on enterobacteria. The study of antibacterial activity showed us the activity potential of these products.

The results obtained are encouraging to continue the synthesis of these derivatives by introducing new modifications by introducing the functional groups and the variation of their topology to improve this activity.



Key words: amino acids, chirality, 3-aminohydantoin, anti-bacterial activity.

Polyelectrolyte complexes for wastewater treatment

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Pôle Technologique de Sidi Thabet, 2020 Sidi Thabet, Tunisia.
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Water pollution control has become increasingly important in recent years. In fact, the release of contaminants, such as dyes, into aqueous effluents could have teratogenic, carcinogenic and mutagenic effects on aquatic organisms and human beings. Consequently, the treatment of aqueous effluents is essential in order to comply with legislation and standards relating to dyes. To date, several methods have been implemented to remove dyes, such as adsorption, ion exchange, chemical precipitation, membrane separation, and reverse osmosis. In recent years, the use of polyelectrolytes has become a promising alternative for the removal of dyes and metal ions from contaminated water. In fact, the interaction of a dye with a polyelectrolyte of opposite charge in aqueous solution results in a change in the absorbance or fluorescence spectrum of the dye, known as metachromasy. In this context, we investigated the efficiency of PE complexes for the retention of either cationic or anionic dyes, leading to the formation of a tri-compound complexes.

Keywords : polyelectrolytes ; polyelectrolyte complexes ; dyes removal/retention ; metachromasy ; tri-compound complexes.

Synthesis of a new polyoxovanadate and their applications

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Nowadays, with the growing problem of water contamination from discharged effluents by the increasing expansion of textile, leather, paper and ink industries and the problems related to pathogenic microorganisms causing diseases, the need for a substance with antimicrobial, anticancer and photocatalytic activity is very high. Decavanadate compounds have attracted the attention of several research groups due to their application in a variety of fields ranging from environmental to medicinal applications, which include wastewater treatment and cancer therapy. During the last decades, a significant number of the new decavanadates have been synthesized and explored intensively. In the present work, the compound $(C_5H_8N_2)_6V_{10}O_{28}.2H_2O$ was prepared by slow evaporation from an aqueous solution. The structural, vibrational, optical, electrical and electrochemical properties have been studied. X-ray diffraction analysis revealed that the compound $(C_5H_8N_2)_6V_{10}O_{28}.2H_2O$ crystallized in the triclinic system with the space group *P*-1. The vibrational study by confirms the existence of functional groups. The diffuse reflectance was recorded to determine the band gap. The material studied has been used for the main areas of research which include photocatalytic materials for wastewater treatment and biological applications in the development of anticancer drugs. The prepared compound acts as a photocatalyst for the removal of methylene blue (MB) dye under visible light irradiation. It also demonstrated a highly selective anticancer effect against U87 cells compared to other cell lines (IGR39, MDA-MB-231). The performances of these materials as electrode materials have been tested.

Keywords: Decavanadate, Synthesis, Infrared spectroscopy, Band gap, Photocatalytic activity, Anticancer activity.

Synthesis, empirical and theoretical studies of a new compound histaminium bis(trioxonitrate)

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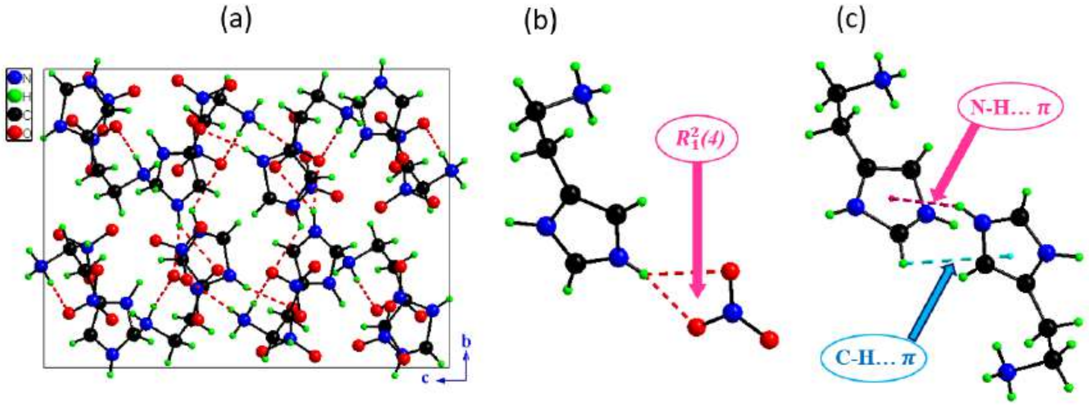
We report in this work, a novel organic-inorganic hybrid material, histaminium bis(trioxonitrate) with general chemical formula $(C_5H_{11}N_3)(NO_3)_2$, denoted by HTN. This compound have been elaborated and crystallized to the monoclinic system with space group $P2_1/c$ and the lattice parameters obtained are: a = 10.4807 (16) Å, b = 11.8747 (15) Å, c = 16.194 (2) Å, β = 95.095 (6)°,V = 2007.4 (5)Å^3 and Z = 8. The atomic arrangement of the title compound can be described by three-dimensional framework. In HTN structure organic cations and nitrate anions are linked via N-H...O and C-H...O hydrogen bonds. Hirshfeld surfaces and two-dimensional fingerprint plots estimate the intermolecular interactions accountable for the generation of crystal packing. The infrared spectrum of this compound reported from 4000 to 400 cm^{-1} confirmed the presence of the principal bands assigned to the internal modes of the organic cation and nitrate anions. This compound was also investigated by visible ultraviolet spectrometry and spectrofluorimetry. DFT calculations were carried out to analyze the structure and properties of HTN. HOMO and LUMO analyses explain the charge transfers within the molecule. Topological analysis, RDG, molecular electrostatic potential (MEP) have been processed to calculate the intermolecular H-bonds interactions in detail.



Projection along the $\vec{a}$ axis of atomic arrangement of HTN **(a)**. N-H ... O hydrogen bond graphs **(b)**. Interactions between organic cations **C-H…π** and **N-H…π** stacking **(c).**

Keywords: Organic-inorganic hybrid, Three-dimensional network, Hirshfeld surface, Infrared spectrum, visible ultraviolet spectrometry and spectrofluorimetry.

Regioselective Heck coupling reaction on dialkyl allyloxymethylphosphonate

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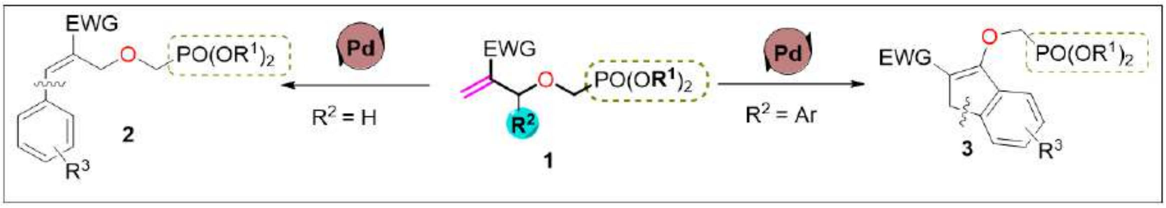
In this communication, we present the synthesis of new phosphonated ethers *via* palladocatalyzed Heck coupling reactions. First, we describe the synthesis of new cinnamyléther-methylphosphonates **2** substituted-aryl groups through intermolecular coupling reactions. Then, our attention turned to the intramolecular cyclization process that allowed us to synthesize indene **3**. Additionally, our approach has been further extended to 1,4-*bis*-cinnamyléther-methylphosphonates.



Scheme: Heck coupling reaction on dialkyl allyloxymethylphosphonate

Key words: Heck coupling, allyloxymethylphosphonate, β-H-elimination.

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Synthesis, crystal structures, and optical properties of rare earth silicate oxyapatite

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A novel series of apatite phosphors with a formula of $Na_{1-2x}La9(SiO_4)_6O_2$:xSm^{3+} were synthesized through a solid-state method. The crystal structures, photoluminescence, and cathodoluminescence were investigated systemically. In this work, the approach is demonstrated the efficient incorporation of Sm^{3+} in $Na_{1-2x}Sm_xLa_9(SiO_4)_6O_2$ apatite and evaluates if the structure and composition of the apatite host matrix can influence the luminescent properties of Sm^{3+} activator regarding the structure of these apatites [1], the concentration of the dopant and the annealing temperature may affect the distribution of Sm3+ ions at the M1 and M2 sites with the C3 and Cs local symmetries, respectively. The results of the XRD analysis show an oxyapatite structure with the space group P63/m. Samarium can occupy crystal matrices and enter nonequivalent crystallographic positions in a lattice, thus forming various optical centers. The PLE and PL spectra demonstrate that the prepared phosphors can be excited efficiently by the commercial u-NV chip and emit intense orange-red light. The concentration quenching is determined to be exchange coupling. The relative emission intensity of NLSO:$0.1Sm^{3+}$ at different temperatures indicates that it has more excellent thermal stability than that of commercial NLSO: Ce^{3+} phosphor.

Keywords: Synthesis, Characterization, X-ray diffraction, emission.

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The anti-aging, antituberculosis and antioxidant potential on Saudi Arabia extracts of Oleaeuropaea Leaves

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The olive leaf extract and olive leaf indicated a high potential for application in food additive and foodstuff [1]. It could be these bio-products useful and important in condition therapy related with oxidative stress and can use it to develop functional foods and to improve the food's shelf life. Therefore, the aim of this work is to valorize Olea leaves extract collected from Aljouf region in Saudi Arabia.

The olive leaf chemical composition of *Oleaeuropaea* L. grown from eljouf in Saudi Arabia, using solvents of increasing polarity cyclohexane, dichloromethane, chloroform ethyl acetate, methanol and ethanol was determined using by GC/MS. Furthermore, the antioxidant activity (diphenylpicrylhydrazyl (DPPH) anti-aging and anti-tuberculosis of olive leaf extracts was evaluated. The results indicated that extract of *oleaeuropaea L.* have a considerable continent in polyphenols (hydroxytyrosol, oleuropein and their derivatives) regarding its antioxidant effects.

KeyWords: Anti-Aging, antituberculosis, antioxidant, extracts, Oleaeuropaea L. leaves, phenolic content

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Continuous column adsorption of Indigo Carmine using activated carbon derived from date palm

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Activated carbon obtained from petiole of *Phoenix dactylifera* (AC-Pt) by chemical activation was used as an efficient adsorbent for the removal of indigo carmine dye (IC) from aqueous solutions. The four most popular breakthrough models, namely, Adams–Bohart, Thomas, Yoon–Nelson and Yan were used for the correlation of breakthrough curve data. The experimental breakthrough data, including the saturation adsorption capacities, breakthrough times, for the studied pollutant were evaluated by varying the flow rate. The Bohart-Adams model fit perfectly to the initial part of the breakthrough curve ($C_t/C_0<0.5$), and the hole curve was well fit by the Yoon-Nelson and Thomas model.

Key words: Activated carbon, *Phoenix dactylifera*, indigo carmine, Continuous adsorption.

DIASTEREOSELECTIVE SYNTHESIS OF 3-AMINOPYRROLIDIN-2-ONES 4-CARBOXYLATES

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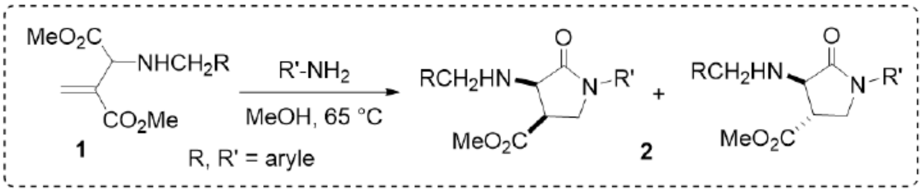
Nitrogen-containing heterocyclic products are prevalent in a multitude of natural and unnatural products.[1] 3-Aminopyrrolidines are a subset of this molecular class that have been used widely as chiral ligands[2] and as common building blocks in the preparation of bioactive compounds.[3,4] The aim of this communication is to present and discuss a convenient alternative for the diastereoselective conjugate addition of primary amines to dimethyl 2-(arylamino)-3-methylenesuccinate **1[**5] has been used as the key step in a simple and efficient protocol for the preparation of 3,4-disubstituted aminopyrrolidin-2-ones **2** in medium to good yields. In this approach, the construction of the heterocyclic ring **2** was based on an efficient coupling of one equivalent of primary amines with the allylamine **1** in methanol at 65 °C, involving two-step sequence: conjugate addition followed by heterocyclization to provide both *anti*- and *syn*-3-aminopyrrolidin-2-ones 4-carobxylates **2**.



Key words: 3-Aminopyrrolidin-2-ones 4-carboxylates, allylamine, diastereoselective synthesis.

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Synthesis and characterizations of biobased furanic polyesters based on itaconic acid

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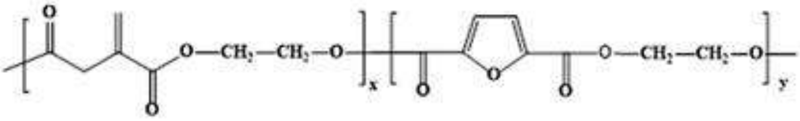
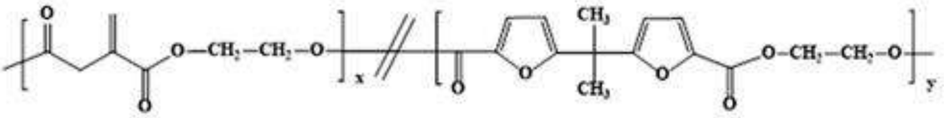
In recent years, chemical components from renewable resources have become increasingly important as an alternative to chemicals from petrochemical resources. The trend towards the research for these derivatives was simulated by the abundance of biomass, the diversity of available structures and its renewal. In this context, The investigation of furanic monomers and itaconic acid (IA)[1] offers interesting potential for the synthesis of new bio-based polyesters[2]. Herein, we report two series of polyesters from *(i)* IA, 2,5-furandicarboxylic acid (FDCA) and ethylene glycol (EG) *(ii)* IA, 5,5'-Isopropylidene-bis(ethyl 2-furoate) (DEF) and EG, synthesized by a bulk polycondensation. The structures were identified by FT-IR and ^{1}H NMR. The thermal properties and cristallinity behaviour were evaluated using TGA, DSC, DMTA and XRD. These polyesters display excellent thermal stability and they are amorphous. Studies are now in progress to explore their mechanical properties and degradation.





Key words: biobased polyesters, bulk polycondensation, amorphous, thermal stability.

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Electrophilic Reactivity of 2,1,3-benzothiadiazole

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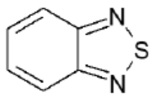
In earlier work we have reported that the 4-nitrobenzochalcogenadiazoles represent an another class of neutral electrophiles whose C-electrophilicity can be quantitatively described by the linear free enthalpy relationship (1).

$$\log k\,(20\ °\mathrm{C}) = s_{\mathrm{N}}\,(E + N) \qquad (1)$$

We will now report on the kinetics of the reactions of the 2,1,3-benzothiadiazole **1** with a series of secondary cyclic amines in various solvent and demonstrate that the second-order rate constants *k* of these reactions follow Eq (1). As can be seen, the electrophilicity parameter *E* of these benzothiadiazole **1** has been evaluated and included them into comprehensive electrophilicity scale of Mayr. In addition, theoretical electrophilicity index (ω) for 4-nitrobenzochalcogenadiazoles **2** and benzothiadiazole **1** are calculated in order to elucidate general relationship between experimental electrophilicity (*E*) and theoretical electrophilicity index (ω).



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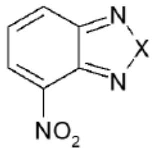

2

X = O, S and Se

Key words: Kinetics / Mayr's Approach / Lewis basicities / Nucleophilic addition / Structure-Reactivity Correlations.

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

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

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

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

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Due to biological importance and industrial applications of aminopyrimidines [1,2], we report the synthesis, the single crystal X-ray diffraction analysis, the Density Functional Theory (DFT) calculations and the spectroscopic study of the new hybrid compound (2-amino-4-methoxy-6-methylpyrimidinium) bis(μ_2-chloro)-tetrachloro-di-copper(II). DFT is a quantum-mechanical approach for calculating the electronic structure of atoms, molecules, and solids in chemistry and physics and it is very important for organic and inorganic molecules. The DFT calculations which perform in this study include the calculation of Mulliken loads, Frontier Orbitals, Molecular Electrostatic Potential (MEP) surfaces and determination of the optimized structure.

The AutoDock Vina program was used to perform molecular docking between complex ligand and HSP90/PDB: 5LRZ. The title molecule was the most promising hit chemical, and the receptor PDB: 5LRZ (2.00 Å) proved to be a better receptor for this study, maybe due to its higher resolution value. We can say that it is very effective in inhibition PDB: 5LRZ.

Drug-likeness profile and *in silico* ADME features of the compound were examined. The investigated compound exhibits a strong pharmacokinetic property, with oral bioavailability and good absorption, according to drug-likeness and ADME properties and no violation of Lipinski rules occurred or results satisfied the Lipinski's rule of five.

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

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Green synthesis of mesoporous photocatalyst based on ZnO-modified local iron-ores and their photocatalytic activity

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The impact of manufacturing in the textile industry on the environment is considered unsafe at a high level [1]. Wastewater from textile companies is considered the most polluting by taking into account the composition and the volume of the effluent generated [2]. In this work, we have reported the green synthesis of ZnO nanoparticles and coupled ZnO-iron oxide nanocomposite by sol-gel method using local iron-ores as iron oxide origin collected from the Tamra deposit (Tunisia). Investigated photocatalysts were tested in the treatment of real textile dyeing effluent. Experiments were conducted on a lab-scale prototype using UV lamp as an artificial light source and solar irradiation as a natural light source. ZnO-iron oxide nanocomposite shows much higher photocatalytic performance with 95 % and 91 % of color and COD removal within 2 h of UV light irradiation-than iron oxide and ZnO nanocomposite. Under solar irradiation, all photocatalysts present high activity for effluent photodegradation compared to UV irradiation and coupled semiconductor ZnO-iron oxide achieves 98.6 % and 92 % of color and COD removal, respectively in the presence of H_2O_2.

Keywords: real textile effluent, sol-gel method, solar irradiation, ZnO nanoparticle, iron-oxide.

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Synthesis and characterization of Fe^{3+} doped TiO_2 nanoparticles and their photocatalytic performance for azo dye degradation

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Metal doping is a popular method to improve the photoreactivity of TiO_2 semiconductors under UV-Vis illumination [1]. Amongst a variety of metals, iron has been considered an appropriate candidate for incorporation in TiO_2 structure [2]. In this study, Fe-doped TiO_2 (Fe-TiO_2) was prepared by sol-gel method using Titanium tetraisopropoxide ($Ti(OC_3H_7)_4$ as precursors and $Fe(Cl)_3$ as the dopant. The as-prepared samples were characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), X-ray diffraction (XRD), N_2 adsorption-desorption isotherms and UV-Vis spectroscopy. The photocatalytic activity of prepared samples was investigated for the photodegradation of Congo red azo dye under UV light irradiation. Obtained results show that prepared photocatalysts by this method have high specific surface areas, mesoporous structure, and excellent photocatalytic performance for Congo red degradation under UV light irradiation.

Keywords: Fe-TiO_2, sol-gel method, azo dye, UV irradiation, characterization, photodegradation.

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Indirect electrochemical process oxidation of auramine dye: Application to textile industrial wastewater treatment

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In this study, electrochemical oxidation of Auramine dye was studied in an aqueous medium (pH = 3) by electro-Fenton process (EFP). This electrochemical process generates in a catalytic way hydroxyl radicals (OH°) which are powerful oxidant species ($E^0(OH°/H_2O)$ = 2.8 V/NHE) used for the oxidation of organic pollutants. The kinetics of Auramine degradation and the mineralization efficiency of its process are investigated through the effect of some operating parameters. The value of 300 mA as applied current, Fe^{2+} as a catalyst with a concentration of 0.2 mM and a temperature of 40 °C are found to be the optimum operating parameters. The reaction kinetic follows a pseudo-first order. The efficiency of EFP is confirmed by the decrease of the molecule concentration during the treatment until its total disappearing. The chemical oxygen demand (COD) analyses indicate after 8 h a mineralization degree of 90% for the Auramine synthetic solution, 91% for the effluent provided from a small Tunisian textile industry and 41% for the wastewater provided from a medium one. The energy consumption per unit COD mass (EC_{COD}) of the EFP is determined for the treatment of Auramine synthetic solution and for the two real effluents.

Validation of an RP-HPLC method for the quantification of an anti COVID 19 drug substance, the Favipiravir in its pharmaceutical form

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An antiviral is a molecule that disrupts the replication cycle of one or more viruses. It acts at a specific moment in the replication cycle of a virus and therefore, it slows down the infection by limiting the multiplication of viral particles. Favipiravir, or 5-fluoro-2-oxo-1H-pyrazine-3-carboxamide is an antiviral derived from pyrazine used against RNA viruses. This molecule has been shown to be effective against influenza pandemics and the Ebola virus [9]. It appears to have a marked tissue distribution in the lungs, which results in faster viral clearance in the respiratory tract. For that reason, the favipiravir becomes, in 2020, one of the antivirals used in the treatment of the coronavirus. The development of a reliable, robust and fast analytical method for the quantification of favipiravir in a pharmaceutical form is part of general control efforts against the coronavirus pandemic in order to guarantee the quality of medicines. A reversed phase high performance liquid chromatographic method was developed for the determination of favipiravir in its pharmaceutical form. An adequate chromatographic separation was achieved using a Waters column ODS3V (250 mm W x 4.6 mm DI; 5 µm DP) maintained at a temperature of 40°C ± 2°C. The mobile phase is debited in isocratic mode at 1mL min-1 and consists of acetonitrile/methanol/Sodium perchlorate buffer 10Mm at pH=3 (20, 30, 50 v/v/v). The detection wavelength is 210 nm. The developed method has been validated in term of specificity, linearity, accuracy, fidelity, LOD and LOQ. The results obtained show that the method is linear with a correlation coefficient R2 equal to 0.9997, just with a CV equal to 0.51% and faithful with an RSD equal to 0.38%. The method is validated and could be used in routine analysis to assess the quality of favipiravir-based drugs.

Key words: Antiviral, Coronavirus, Favipiravir, HPLC, Validation.

Phytochemical compounds contents influenced antioxidant activities, α-amylase and acetylcholinesterase inhibition of Tunisian *Nitraria retusa* extracts.

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Nitraria retusa (ghardeq) has long been considered in folklore medicine as a medicinal plant. Hence the aim of this study was to assess the analysis of different phytochemicals compounds contained in the methanolic leaf extracts collected from different bioclimatic zones of Tunisia and then tested for their antioxidant, antidiabetic and antialzeimer activity. The chemical differentiation among populations occurs regardless their eco-geographic appurtenances. The levels of polyphenols (221.33± mgEAG/gDW for Gabes to 16±6 mgEAG/gDW for seliana) and flavonoids (132.293±1.285 to 77± 1.113 mgER/gDW for the same populations respectively) in leaf extracts showed moderate condensed tannins, and anthocyanin content significantly varied among populations (15,45± and 10 15..66to 10 for Gabès and Siliana respectively) The antioxidant activity was assessed by using three method namely DPPH scavening activity, reducing power assay and fer chelation. Analysed leaf extracts among populations revealed excellent antioxidant activity DPPH scavenging activity respectively.

Extracts were found to possess important capacity to inhibit the α-amylase and acethylcholinesterase activities which was correlated to their Phenolics contents Therefore, *N. retusa* can be used as a natural source of bioactive compounds in food and pharmaceutical industries

Key words: *Nitraria retusa*, phenolic compounds, antioxidants activities, acethylcholinesterase inhibition, α-amylase inhibition

Metallic pollution effects on the leaf anatomic structure of some native mediterranean species

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Plants growing in the industrial areas and near the major roads can accumulate pollutants in their leaves. Anatomical analyses in leaves, indicated foliar injuries of plants exposed to stressful air conditions. In this study, histological changes induced by air pollutants (from a cement factory combined with the pollution generated by human activities) in *Nitraria retusa and Atriplex halimus leaves* were followed. Our plant species have been identified to be able to absorb, detoxify and tolerate high levels of pollution. The tolerance degree is indirectly correlated with the intensity of injuries which occur in plant structure. Leaf thickness, height of palisade cells, diameter of the spongy cells, height and width of the upper epidermis cells, the thickness of the external wall of the upper epidermis cells, histological sections caused damage and / or total destruction of epidermal cells in some section of the underside of leaves in particular for leaves of both plant. Completely collapsed epidermal and mesophyll cells are observed in the leaves of the two species. Changes in the anatomical structures of plant species often report the intensity of metallic stress in contaminated environments.

Key words: *metallic pollution, epidermis, leaf structure, native plant species*

Synthesis, structural characterization of $Na_2Li_2(H_3O)_2[V_{10}O_{28}]^{\cdot}18H_2O$ compound

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A novel decavanadate compound with two monovalent inorganic cations, $Na_2Li_2(H_3O)_2[V_{10}O_{28}]^{\cdot}18H_2O$, was synthesized by slow evaporation at room temperature.
The $Na_2Li_2(H_3O)_2[V_{10}O_{28}]^{\cdot}18H_2O$ compound has been characterized by monocrystalline X-ray diffraction, Transform-Infrared (FT-IR), thermogravimetric analysis (TGA-DTGA). The $Na_2Li_2(H_3O)_2[V_{10}O_{28}]^{\cdot}18H_2O$ compound crystallizes in the triclinic system, space group P-1, with cell parameters: a = 8.523(2) Å, b = 10.632(3) Å, c = 11.868(2) Å, α = 105.67(1)°, β = 101.77(2)°, γ = 99.43(1)°, V = 985.88(4) Å^3 and Z = 2. The formula unit is formed by: a centrosymmetricdecavnadate group $[V_{10}O_{28}]^{6-}$, a $[NaO_2(H_2O)_3(H_3O)]^{2+}$ group, a $Li(H_2O)_4^+$ tetrahedral, two ions hydronium $[H_3O]^+$ and eighteen water molecules. The structure is stabilized by O-H...O hydrogen bonds.

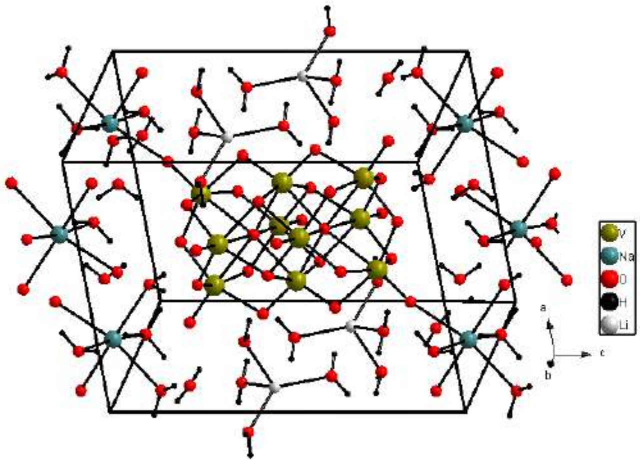

Figure 1. Unit cell of $Na_2Li_2(H_3O^+)_2[V_{10}O_{28}]^{\cdot}18H_2O$ compound

Keywords: Decavanadate, structure, characterization,

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Development and validation of a stability indicating method for simultaneous determination of two antiviral recently approved grazoprevir and elbasvir by RP-HPLC

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Hepatitis C virus (HCV) related liver disease is a major global health problem. The treatment of this virus, discovered in 1989, has long been based on a combination of interferon alpha and ribavirin. The response rate of this treatment way did not exceed 50%. A better understanding of HCV replication mechanisms has led to the development of several new direct-acting antivirals (DAAs). These new drugs have revolutionized treatment by obtaining a virological cure of more than 90% for the majority of patients. However, given the high cost of treatment, access to these drugs is still limited in many situations. Grazoprevir (GZR) and elbasvir (EBR) are new DAAs which, in combination, have demonstrated excellent efficacy on genotypes 1, 4 and 6, including in patients whose previous treatment with other DAAs has failed.

In order to support the quality control of GZP and ELB-based drugs, a reversed-phase high-performance liquid chromatography (RP-HPLC) method has been developed for the simultaneous determination of ELB and GZP and their degradation products under conditions of hydrolysis and oxidative stress. Adequate chromatographic separation was obtained using a Waters Spherisorb phenyl column (150 mm x 4.6 mm ID, 5 µm particle size) maintained at a temperature of 40°C ± 2°C. The mobile phase is acetonitrile: 5 mM ammonium formate buffer (+0.1% v/v trimethylamine, pH = 3.2) (60:40 v/v) at a flow rate of 0.8 mL min -1. The stability indication criterion of the developed method is successfully verified by a study of forced degradation of these active ingredients under hydrolysis and oxidation conditions. No interference was observed between ELB, GZR and degradants. The identification of the molecular structure of the degradation products was carried out by coupling liquid chromatography-mass spectrometry (LC-MS).

Key words: Hepatitis C virus, Grazoprévir, Elbasvir, LC/MS, Forced Degradation, Accuracy profil.

Structural and Mechanical properties of Co_2MnGa: Density functional theory

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Heusler compound Co_2MnGa is proposed from calculations within density functional theory (DFT) using full potential linearized augmented plane wave (FP-LAPW) method as implemented in the Wien2k code. The ground state structure exhibits significantly high magnitude bulk modulus placing Co_2MnGa in the range of hard materials. In this case, it is best to verify this by calculating the set of elastic constants and its derivatives. Moreover, the stiffness constant of the spin wave and the Curie temperature are calculated. This theoretical study provides detailed information on the compound Co_2MnGa, in different aspects and can also provide information on the application of this material.

Keyword: Co_2MnGa; Mechanical properties; Density functional theory; First-principle calculation.

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New decavanadate compounds as potential therapeutic agents against chronic myeloid leukemia

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Decavanadates have been widely investigated because of their many interesting properties and their potential use in several applications. In this work, we synthesized the vanadium complex, $(C_9N_2H_{24})_3V_{10}O_{28}\cdot 7H_2O$ (**CI**), to study its potential effect in comparison to previously reported $(C_4N_2H_7)_4(C_6N_2H_{10})V_{10}O_{28}\cdot 2H_2O$ (**CII**) and $(NH_4)_4Li_2V_{10}O_{28}\cdot 10H_2O$ (**CIII**). Interestingly, the hemolytic assay showed high blood compatibility of the three decavanadate compounds making possible their intravenous administration. Thus, the presented work show a great potential of decavanadate compounds to be developed into novel anti-leukemia agents applicable also in the malignant cells resistant to the current conventional drugs.

Keywords: Synthesis, Decavanadate, Chronic myeloid leukemia, Therapeutic agents.

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Enhanced Proton Conductivity of a Sulfonated Polyether Sulfone Octyl Sulfonamide Membrane via the Incorporation of Protonated Montmorillonite

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Hybrid membranes consisting of sulfonated poly (ether sulfone) octyl sulfonamide (SPESOS) cast together with protonated montmorillonite (H-MMT, 1, 3, and 6 wt.%) were fabricated and characterized. The FT-IR spectra of the H-MMT/SPESOS composites confirmed that no chemical reactions occurred between the SPESOS and clay. The XRD diffractogram showed a significant shift in the major peak of SPESOS at $2\theta = 15.5°$ due to the incorporation of H-MMT. Furthermore, SEM confirmed a homogeneous structure of the composite, and the TGA results revealed that the addition of H-MMT promoted water absorption via the decrease in the loss of composite mass during evaporation. The SPESOS with H-MMT had higher water retention, contact angle, and proton conductivity values than pristine SPESOS. The proton conductivity of the hybrid membranes, however, improved at 100 °C from 42 mS/cm in pure SPESOS to 787, 350, and 300 mS/cm for the 1, 3, and 6 wt.% H-MMT hybrids, respectively. These results demonstrated that the incorporation of the H-MMT is a viable strategy to boost the performance of SPESOS to construct a possible membrane for applying in fuel cells.

Keywords: SPESOS, · Proton Conductivity, · Protonated Montmorillonite, · Composite membrane, · Fuel cells

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Synthesis of a 1D/0D CdS@ZnS nanocomposite as an electrochemical sensor for hydrogen peroxide detection

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In this work, an electrochemical hydrogen peroxide (H_2O_2) sensor, based on CdS/ZnS nanocomposite was reported. In addition, we mentioned the synthesis of CdS/ZnS nanocomposite by combining the hydrothermal route with a homogeneous precipitation process. The physiochemical proprieties of these nanomaterials were characterized by X-ray diffraction (XRD), Energy-dispersive X-ray Detector (EDX), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). These techniques showed that ZnS is of cubic structure having a nanorod shape, while CdS is of hexagonal structure with a spherical shape. The H_2O_2 sensing merit of the nanocomposite was investigated using cyclic voltammetry and amperometry in a 0.1 M NaOH solution. The proposed sensor displays good electrocatalytic activity towards H_2O_2 with a sensitivity of 430 µA mM^{-1} cm-2 ($R^2 = 0.999$) and has a wide linear response, ranging from 1 to 1870 µM. It also demonstrates a rapid detection time of 1 s and a very low detection limit of 0.35 µM. Likewise, the proposed nonenzymatic sensor exhibited a high selectivity towards hydrogen peroxide detection. These observed promising results confirm that the as fabricated modified electrode could potentially serve as an effective alternative method and a suitable sensor for multianalyte detection with a nanostructured sensing electrode in many biological systems and complex materials.

Keywords: Hydrogen peroxide, electrochemical sensor, Hydrothermal synthesis, Zinc sulfide, Cadmium sulfide, nanocomposite.

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Wide bandgap small molecules for semi-transparent organic photovoltaic devices

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We describe the synthesis of two new dumbbell-shaped small molecules used as near ultra-violet absorbers for transparent organic solar cell application. The electron-donor TAT units, sandwiching the central chromophore, constitute very efficient π-stacking platforms that are nevertheless highly soluble thanks to the presence of three alkyl chains. The TAT units are used in combination, with a small central electron donor unit, either a carbazole or a thieno[3,2-*b*]thiophene (TT) unit. The two new dumbbell-shaped small molecules including only electron-donor units are strongly absorbing in the near UV range, due to the reduced electronic conjugation. Combined with a suitable hole mobility, the most conjugated thieno[3,2-*b*]thiophene-based derivative, when used as electron-donor component in a bulk heterojunction organic solar cell, exhibits a 48% of average visible transmittance with a power conversion efficiency close to 2%.

Keywords : Transparent organic solar cells, Near Ultra-Violet organic dyes, wide bandgap organic materials.

Development and validation of a method for analyzing ibuprofen in the raw state and after grinding by X-ray diffraction

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As part of our work, we are interested in developing and validating a method of analysis by X-ray diffraction - XRD and laser granulometry according to the ISO / IEC 17025 standard and in the reduction of the particle size of the ibuprofen by the grinding input.

To do this, a comparative study was carried out by optical microscopic techniques, DRX, DSC and FTIR were used to characterize the solid state of ibuprofen before and after grinding under different conditions.

Laser granulometry is an analysis method that allows you to determine the size particles (0.02 to 2000 µm) suspended in liquid or air based on the principle of laser diffraction by the theory of Fraunhofer and Mie.

The results found allow us to carry out the reduction in the size of the ibuprofen particles and we can characterize the microstructural and structural changes induced during the processes of reduction of the size of the particles of ibuprofen.

So, Ibuprofen is a nonsteroidal anti-inflammatory drug used especially in inflammation. This drug is practically insoluble in water. The particle size distribution of ibuprofen affects their solubility as well as their rate of dissolution. We have developed a method analyzing ibuprofen in the raw state and after grinding by X-ray diffraction.

Key words:

Ibuprofen, Development, Validation, Laser Granulometry, DRX, FTIR.

Carboxymethyl cellulose from Tunisian *Opuntia* (Cactaceae)

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In this work, *Opuntia* (Cactaceae) is used as a renewable resource for carboxymethyl cellulose (CMC) production. The cellulose fibres were extracted from Opuntia (Cactaceae) by applying an eco-friendly delignification process based on the use of green treatment with sodium hydroxide/hydrogen peroxide mixtures. The extracted cellulose fibers were carboxymethylated using sodium hydroxide and MCA in an ethanol medium. The chemical composition of fibers obtained from *Opuntia* (Cactaceae), such as cellulose, holocellulose, lignin and ashes was determined. The high quality carboxymethyl cellulose produced from *Opuntia* (Cactaceae) cellulose was characterised by scanning electron microscopy. The thermal and structural characteristics were evaluated. The obtained results prove that *Opuntia* (Cactaceae) fibres can potentially serve as a suitable source for high quality CMC.

Key words: *Opuntia*, fibres, cellulose, carboxymethyl cellulose.

Voltammetric simultaneous quantification of p-nitrophenol and hydrazine by using magnetic spinel $FeCo_2O_4$ nanosheets on reduced graphene oxide layers modified with curcumin-stabilized silver nanoparticles

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A sensor based on a screen-printed carbon electrode loaded with curcumin-stabilized silver nanoparticle-coated reduced graphene oxide magnetic spinel ($FeCo_2O_4$) nanosheets was constructed. For this purpose, the surface of the working electrode was modified sequency with reduced graphene oxide modified with $FeCo_2O_4$ nanosheets and curcumin functionalized curcumin nanoparticles. The choice of the used nanomaterials is based to their high surface to volume ratio and their high electrocatalytic activities. The later enable sensitive simultaneous quantification of hydrazine and p-nitrophenol. The respective working potentials typically are at +0.15 V for hydrazine and at -0.75 V for p-nitrophenol (both vs. pseudo-Ag/AgCl), and the detection limits are 23 nM and 18 nM (at S/N = 3). Moreover, good selectivity, repeatability, reproducibility and storage stability are shown. As far as the real sensing tests, spiked samples of river water and industrial wastewater were used to assess the applicability of the designed platform and findings showed great recovery rates from 98.3 to 102.7 %.

Keywords: $FeCo_2O_4$ nanosheets, Curcumin, Hydrazine, P-nitrophenol, Electrocatalytic activity, Simultaneous sensing.

Synthesis, microstructure, and luminescence properties of Er-doped $LaAsO_4$ nanoparticles: An experimental and theoretical study.

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Er-doped $LaAsO_4$ samples have been prepared using the combustion method. All picks are indexed in the monoclinic system, space group $P2_1/n$. The highly crystalline powders with nanometric size have been confirmed by X-ray powder diffraction measurements and by the scanning electron microscopy. The measured excitation and emission spectrum have been obtained for λ_{em}= 378 nm and λ_{ex}=1530 nm respectively. The electronic structure and optical properties of the title compounds have been calculated using the DFT method via the two approximations GGA+PBE and GGA+PBE+U for the undoped and doped compounds receptivity. The bond structure and the density of the states show the intercalation of the states 4f of the Erbium in the forbidden band of $LaAsO_4$ which allows the decrease of the optical gap. The different electronic transition in the doped and undoped compounds have been deducted from the dielectric function curves and the density of states and confirm the emission of the doped compound in the infrared region.

Key words: combustion method, DFT, bond structure, density of states, dielectric function, photoluminescence Properties.

Green and ultrasound-assisted synthesis of 1,3-diaryl-2-propenones catalyzed by Amberlyte IRA-410 and Amberlyte IRA-400 basic resins

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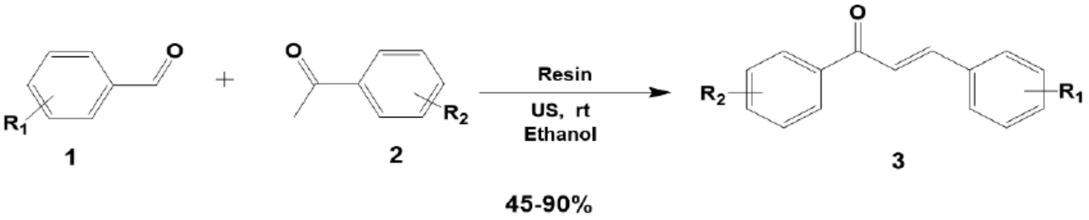
Recently, chalcones have been a very wide field of research, due to their antidiabetic [1], anti-bacterial [2], anti-inflammatory, anticancer and antipyretic properties. For this reason, their synthesis presents a challenge for chemists, especially in the organic chemistry. They are obtained via an aldol condensation reaction. This method can be regarded as valuable and worthwhile as it proved to be green, safe and easy synthesis of *trans*-chalcones under ultrasound irradiation in the presence of anionic resins. Several *trans*-Chalcones have been obtained following an environmentally friendly methodology by using Amberlyte IRA-410 and Amberlyte IRA-400 resins as heterogeneous and efficient catalysts. The products of the condensation reaction were synthesized, in general, in good yields and the analysis confirmed well their structures.

Key words: Anionic resins, Ultrasound irradiation, *Trans*-chalcones, Amberlyte IRA-410, Amberlyte IRA-400.



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A Theoretical Study of Molecular Interactions in glyphosate Dimers: The importance of H-bonds in the stabilization of zwitterion pairs

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In this work, the molecular properties and the strengths of the H-bonds intermolecular systems in glyphosate dimers (Fig.1) were inspected and analyzed at the B3LYP-D3/6-311++G(2d,2p) level in the gas phase and in aqueous solution using the density based solvation model (SMD) in order to get insight into the importance of the various noncovalent binding interactions and of their interplay. The high capability of (OP)-O-H….O-(CO) and N-H….O-(CO) in changing drastically the conformational orientations of monomeric units in intermolecular systems of glyphosate dimers is illustrated. Computations allow to show that in addition to the H-bonds network, the electrostatic attraction, and also their mutual interactions are responsible for the high stability of zwitterion ion pairs of glyphosate dimers.

Key words: Glyphosate, Dimerization, Noncovalent interactions, H-bonds, DFT, Empirical dispersion correction, SMD Solvation Model

Molecularly imprinted curcumin nanoparticles decorated paper for electrochemical and fluorescence dual-mode sensing of bisphenol A

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A molecularly imprinted paper-based analytical device (MIP-µPAD) was developed for the sensing of bisphenol A (BPA). The platform was screen-printed onto a filter paper support, where the electrodes and the fluorescence µPADs were designed. Owing to its dual electrochemical and fluorescence responses, molecularly imprinted curcumin nanoparticles were used to sense BPA. The µPAD design was characterized by transmission electron microscopy, scanning electron microscopy, fluorescence spectroscopy, and electrochemical techniques. The sensor design comprised a wide linear range from 1 to 200 µg.L^{-1} with limits of detection of 0.47 ± 0.2 and 0.62 ± 0.3 µg.L^{-1} (LOD, S/N = 3) for electrochemical and fluorescence sensing, respectively. Furthermore, the system showed good analytical performance such as selectivity, stability, and reproducibility. The feasibility of the MIP-µPAD was demonstrated for the sensing of BPA in seawater, foods, and polycarbonate plastic packaged water with recovery values of 97.2 and 101.8%.

Keywords: Molecular imprinted nanoparticles, Bisphenol A, Dual-mode sensing, Microfluidic paper.

Regioselective Palladium-Catalyzed Cross-Coupling Reactions of Ethyl 2,6-Dibromopyrazolo[1,5-*a*] pyrimidine-3-carboxylate

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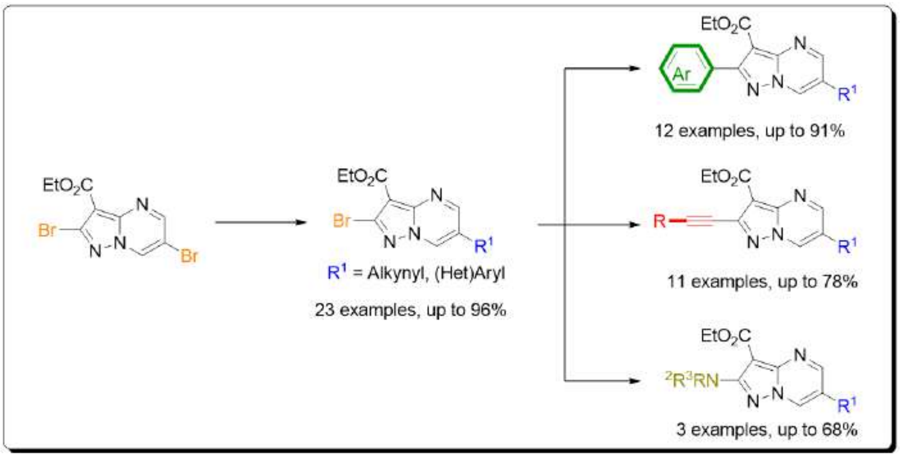
An efficient and original synthesis of various 2,6-disubstituted pyrazolo[1,5-a]pyrimidines is reported. A library of compounds diversely substituted in C-2 and C-6 positions was easily prepared via sequential site-selective cross-coupling reactions of 2,6-dibromopyrazolo[1,5-a]pyrimidine [1]. The Suzuki-Miyaura and Sonogashira regio-controlled reactions performed with excellent selectivity in favour of the C6-position after careful optimization of the cross-coupling conditions. The monobrominated compounds, obtained on a large scale, were subjected to a second arylation, alkynylation or amination, leading to a new series of ethyl 2,6-disubstituted pyrazolo[1,5-a]pyrimidine-3-carboxylate. These unprecedented results constitute the first regioselective approach for diversification of the chemically and biologically interesting pyrazolo[1,5-a]pyrimidine heterocycles at C2 and C6 positions.



Scheme 1 : Metal-catalyzed selective couplings of 2,6-dibromopyrazolo[1,5-a]pyrimidine

Keywords : 2,6-dibromopyrazolo[1,5-a]pyrimidine, cross-coupling reactions, regioselective, 2,6-disubstituted pyrazolo[1,5-a]pyrimidines.

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Structural study, optical and vibrational properties, DFT calculations, Hirshfeld surface analysis and thermal characterization of Zinc (II) organic-inorganic hybrid material $(C_8H_{14}N_2)_2[ZnCl_4]_2$

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The title organic-inorganic hybrid compound, $(C_8H_{14}N_2)_2[ZnCl_4]_2$, was synthesized by slow evaporation at room temperature and characterized using elemental analysis, X-ray powder diffraction, FT-IR, UV-Vis, impedance spectroscopies and thermal analysis. Single-crystal X-ray diffraction **[1]** analysis indicates that this compound crystallizes in the monoclinic system, P21 space group while the asymmetric unit of the title compound consists of two tetrahedral $[ZnCl_4]^{2-}$ ions and two diprotonated organic cations $(C_8H_{14}N_2)^{2+}$. The cohesion of the structure is achieved by N-H…Cl hydrogen bonds, and Cl…Cl interactions. Powder XDR analysis confirms the phase purity of the crystalline compound and scanning electron microscopy (SEM-EDX) verify the composition of the phase. The optical properties were studied using optical absorption UV-Vis spectroscopy. FTIR spectroscopy was carried out to study the functional groups present in the crystal structure. Electrical analysis of our compound has been investigated using complex impedance spectroscopy (CIS) at different temperatures and frequencies. Thermal behavior (DTA/TGA) of this complex was also performed. Hirshfeld surface analysis **[2]** reveals that the structure is dominated by H…Cl/Cl…H (70.9%) contacts. Electronic properties HOMO and LUMO were analyzed by density functional theory (DFT).

Keywords: Organic-inorganic hybrid; XRD; Hirshfeld surface; DFT.

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Combined experimental and theoretical studies of a new organic-inorganic arsenate: Molecular docking and DFT approach.

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Due to their structural diversity, organic-inorganic hybrid (OIH) materials have been extensively studied in the last few years **[1-4]**. The assembly of the organic and inorganic components on a molecular level offers new features that potentially combine the properties of the two parts. Designed hybrid materials possess exceptional physical properties such as optical properties for applications in the fields of optoelectronics and energy. An experimental and theoretical study of the molecular structure of an organic arsenate templated by 4-aminopyridine is presented. The optimized geometry, vibrational frequencies and various thermodynamic parameters of the title compound calculated using DFT methods are in agreement with the experimental values. The theoretical calculations were performed using density functional theory (DFT) method at B3LYP/6-311++G (d,p) basis set levels. A detailed interpretation of the IR and Raman spectra were reported. Electronic stability of the compound arising from hyper conjugative interactions and charge delocalization were investigated based on the natural bond orbital (NBO) analysis. The molecular docking simulation results showed an excellent agreement with the experimental findings and satisfactory support the antiviral effects, the druggability and pharmacokinetic properties of the compound.

Key words: DFT; HOMO-LUMO; NLO; Thermodynamic functions; Vibrational frequencies.

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GENERAL AND EFFICIENT TRANSESTERIFICATION OF β-KETO ESTERS WITH VARIOUS ALCOHOLS USING Et_3N AS A BRØNSTED BASE ADDITIVE

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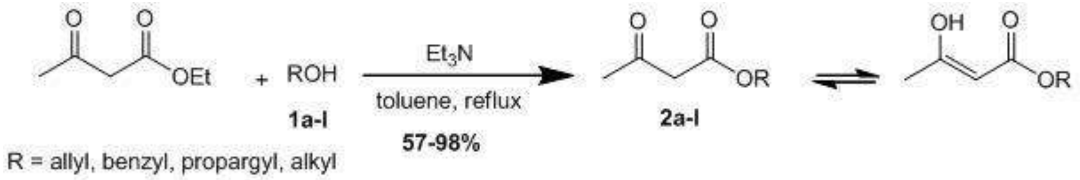
Transesterification is a transformation of an ester into another through interchange of the alkoxy moiety. This synthetic transformation has attracted much attention in organic synthesis and biodiesel fabrication.[1,2] A large number of acid or basic catalysts have been used for this purpose but none of these methods reported that Et_3N could catalyse transestrification of β-keto esters with alcohols.[3]

We report herein our results dealing with this topic involving a variety of allyl, benzyl, propargyl, and alkyl alcohols as well as Morita-Baylis-Hillman ones,[4] using commercially available and inexpensive Et_3N for the first time as a Brønsted base additive.

All β-keto esters were obtained in moderate to excellent yields[5] with no trace mounts of the Carroll decarboxylative rearrangement ketones (Scheme 1).



Scheme 1. Et_3N-mediated transesterification of ethyl acetoacetate with various alcohols

Key words: Alcohols; Brønsted base; β-keto esters; transesterification

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Green synthesis and characterization of ZnO nanoparticles: Effective Catalyst for the Degradation of Basic Fuchsin in Industrial Dye Wastewaters

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In view of advantages of green synthesis, a novel green route for synthesis and stabilization of zinc oxide nanoparticles (ZnONPs) using an aqueous extract of fruites as capping agent.

The ZnO nanoparticles that followed were characterized by UV-visible spectroscopy, FT-IR spectroscopy, X-ray diffraction and dynamic light scattering. the synthesized NPs are wurtzite hexagonal structure with include an average size of about 64.51 nm. Thus, due to the outstanding catalytic results, nearly 87% removal degradation was achieved in 120 min after 90 min sonication time at room temperature, which is better than without catalysts. these ZnO nanoparticles with lowcost and high performance, should be applied in the practical degradation of industrial waste water.

Keywords: Green synthesis ; ZnONPs ; Characterization ; Photocatalyst

Figure Caption

Schematic diagram of photocatalysis mechanism of ZnONPs.

Development and characterization Polymer/NaxCoO_2 for application as electrodes in energy storage systems

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The lamellar oxide "NaxCoO_2" is the most beneficial material for use as a positive electrode for sodium-ion accumulators, despite the success of sodium cobaltite, which is currently the most widely used. In addition, its structural modification that limits the insertion-disinsertion phenomenon motivated us to design and synthesize a new composite material «Polymer/NaxCoO_2» whose capacity of oxide alone was tried to improve which is about 150 mAhg^{-1}, by the presence of a conductive polymer.

Great interest is given to conductive polymers which have found their applications in different industrial fields thanks to their typical stabilities, their simple and inexpensive syntheses, as well as its structure which provides a maximum degree of conjugation hence the ability to give high electrical conductivities.

Our work aims to improve the electrochemical performance of materials used as cathode in the sodium-ion battery, using a conductive polymer that serves to protect the spray electrode during electrochemical reactions. The lamellar oxide NaxCoO_2 was synthesized by the soil-gel method[1] using a complex agent. Polymerization was produced by oxidative polymerization of the monomer and ammonium persulphate in a HCl[2] solution. Polymerization was carried out by varying the amount of starting monomer in order to modify the thickness of the polymer layer on the oxide surface.

Various characterization techniques such as X-ray diffraction (DRX), thermogravimetric analysis (ATG), differential scanning calorimetry (DSC), Fourier transform spectroscopy (FTIR), UV-spectroscopyVisible and Raman spectroscopy and scanning electron microscopy (SEM). The analyses showed that all the materials developed have the same structure including the P6/3mmc space group. All materials also showed similar morphology and nanometric particles.

Keywords: conductive polymers, polymer/NaxCoO_2 composites, sodium-ion batteries.

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Structural characterization, phase transition and electric and dielectric proprieties of $(H_2Piper)_4$ $[(FeF_6)_2FeF_5(H_2O)(H_2O)_4]$.

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A new organic–inorganic hybrid compound based on iron fluoride, $(H_2Piper)_4$ $[(FeF_6)_2FeF_5(H_2O)(H_2O)_4]$ (Piper = Piperazine) was synthesized by hydrothermal method [1] and characterized by X-ray single-crystal diffraction, differential scanning calorimetric (DSC), electric and dielectric measurements. Single-crystal X-ray study revealed that the title compound crystallizes in $P\bar{1}$ space group with lattice parameters: a = 12.5535(5) Å, b = 12.8715(4) Å, c = 22.2774(8) Å, α = 92.321(3)°, β = 95.957 (3)°, γ = 91.946(3)°, V = 3574.6 $Å^3$ and Z = 4. In the molecular arrangement, $[FeF_6]^{3-}$ and $[FeF_5(H_2O)]^{2-}$ anions are linked to $[H_2Piper]^{2+}$ cations and free water molecules through hydrogen bonds (O–H···F and N–H···F) generating 3D network. DSC confirmed the presence of two phase transitions of the hybrid material. The complex impedance of $(H_2Piper)_4$ $[(FeF_6)_2FeF_5(H_2O)(H_2O)_4]$ was investigated in the temperature range 410-530 K and in the frequency range 200-2.10^6 Hz. Furthermore, an electrical equivalent circuit was reported to explain the impedance results [2]. The variation of the dc and ac conductivity verified two phase transitions of the title compound. The temperature dependences of dielectric permittivity indicated a relaxation process and highlighted the good protonic conduction of this material [3].

Key words: iron fluoride, hydrothermal method, phase transitions, electrical equivalent circuit, and relaxation process.

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Synthesis, characterization and quantum study of an α- aminophosphonate derivative.

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To solve certain health problems, for millennia, diseases around the world have been treated with phosphonate-based medicines.

Hence the need to develop new active compounds with a new structure for the fight against chronic diseases that remain a public health problem.

We looked at the synthesis of α-aminophosphonates, which are new molecules for which biological tests have been found.

Our main objective is the synthesis of aminophosphonates and is part of the logic of finding new molecules of variety ability having in their structure a pattern N-C-P and $P(O)(OC_2H_5)_2$.

In this work:

- A synthesis of α-aminophosphonate ester according to the reaction of Kabachnik-Fields.
- This synthesized ligand has been confirmed by the UV-Vis, FT-IR, and NMR ^{1}H, ^{13}C, and ^{31}P spectrals.
- The geometric properties of this synthesized molecule were studied by the DFT method using the Gaussian 09 software.

Thermophysical properties of N,N-Dimethylacetamide with 1-pentanol and 2-pentanol

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This work reports thermophysical properties measurements of binary mixtures of N,N-Dimethylacetamide with 1-pentanol and 2-pentanol. Density, speed of sound, refractive index, and kinematic viscosity were measured over the whole composition range at the temperatures (283.15, 298.15 and 313.15) K and at atmospheric pressure (0.1 MPa). Experimental data were used to calculate the following properties: excess molar volume, excess isentropic compressibility, refractive index deviation and viscosity deviation. Excess molar volumes were positive for both mixtures although there are some slight negative values for the system containing 1-pentanol at lower temperatures and at lower mole fractions. Refractive index deviation behavior against composition was sigmoidal at lower temperatures and negative at T=313.15 K for (N,N-Dimethylacetamide + 1-pentanol), on the other hand negative values were obtained for the mixture (N,N-Dimethylacetamide + 2-pentanol). Excess isentropic compressibilities and viscosity deviations were negative for both systems. The results obtained were interpreted based on both structural and energetic effects.

Key words: Density, Speed of sound, Refractive index, Kinematic viscosity, Binary mixtures

Synthesis, characterization and optic properties of a new hybrid polyoxometallate salt : $(NH_4)_3(CN_3H_6)_2[HV_{10}O_{28}].2H_2O$

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New hybrid polyoxovanadate salt : $(NH_4)_3(CN_3H_6)_2[HV_{10}O_{28}].2H_2O$ was synthesis from metavanadate and guanidine hydrochloride in an aqueuse solution, characterized by single crystal X-ray diffraction, infrared and UV-vis spectroscopy and and photoluminescence property. The struture of $(NH_4)_3(CN_3H_6)_2[HV_{10}O_{28}].2H_2O$ was composed of one $(HV_{10}O_{28})^{5-}$ cluster, three $(NH_4)^+$, two $(CN_3H_6)^+$ cation and two water molecules. The structure was crydtzllized in the triclinic system, P-1 space group with a = 9.932 Å, b = 10.407 Å, c = 10.731 Å, $\alpha = 72.04°$, $\beta = 62.61°$, $\gamma = 61.98$ and Z=1. In the crystal, molecules are linked into a three-dimensional network by N-H ··· O_w, N-H ··· O, O_w-H ···O and C-H ···O hydrogen bonds involving water molecules, organic molecules, and Van der Waals interactions. The prevalence of these intermolecular interactions was confirmed by an analysis of the Hirshfeld surface. The relative contribution of different interactions is associated with O···H/H···O intermolecular interactions. The optical survey of $(NH_4)_3(CN_3H_6)_2[HV_{10}O_{28}].2H_2O$ has been used to determine the optical band gap and to provide the blue and orange fluorescent behavior of grown crystals.

Keywords: Inorganic-organic hybrids, polyoxometalate, Decavanadate, X-ray Diffraction; IR, UV-visible Spectroscopies, photoluminescence property.

Comparison of effects of three sulfated glycosaminoglycans from Tunisian and Brittany seashore biodiversity on dermal fibroblast proliferation and matrix metalloproteinases secretion

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Sulfated glycosaminoglycans are major players of tissue remodeling and tissue homeostasis. Thus, these compounds could be regarded as interesting drugs or actives for health [1]. Unfortunately, it is difficult to synthetize them chemically. Indeed, they are often extracted from mammalian tissues which can pose sanitary, regulatory, and technical problems. Therefore, the use of sustainable marine resources to replace those molecules could be an alternative solution. We assessed the biological properties of three different sulfated polysaccharides extracted from marine biodiversity of Tunisia and Brittany. Thus, a chondroitin sulfate from sea cucumber and a dermatan sulfate from sea urchin showed a great potential for regenerative growth factor protection against proteolysis, and a low molecular weight fucoidan from brown algae, displaying some heparan-mimetic properties can be regarded as a tissue regeneration booster, promoting growth factors signal. Our preliminary results showed that these marine polysaccharides can be considered as interesting compounds for regenerative medicine or cosmetics.

Key words: Sulfated glycosaminoglycans, Marine biodiversity, Biological properties.

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Comparative study of aqueous extracts from olive and mulberry leaves: Antioxidant and protective properties against cadmium toxicity in colorectal cancer and renal cells

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Aqueous extracts of freeze-dried olive and white mulberry leaves was studied for protective potential and antioxidant power against Cd toxicity in colorectal cancer and renal cells. The results exposed that mulberry aqueous extract (MAE) has the highest extraction yield, contents of polyphenols and flavonoids about 26.45%, 45.53 mg gallic acid equivalents/g of dry extract and 36.40 mg rutin equivalents/g of dry extract, respectively, in comparison with olive aqueous extract (OAE). Furthermore, biological properties were determined by radical scavenging capacity, ferric reducing power and total antioxidant capacity. Moreover, the cytoprotective effect of extracts were assessed using the mitochondrial activity testing method, malondialdehyde, and reactive oxygen species production. Data revealed that the highest reducing and antiradical power as well as the greatest total antioxidant capacities were obtained by the aqueous mulberry extract. Additionally, results indicated that MAE have a better (i) proliferative with a remarkable decrease in cell viability after 24hxof incubation and (ii) cytoprotective effect than OAE on colorectal cancer and renal cells against metal toxicity. These outcomes suggest that the MAE could be employed as an easily accessible source of natural antioxidants and as potential phytochemicals against renal and colon cancers.

Key words: *Olea europaea* L.; *Morus alba* L.; Cadmium (Cd); Cytotoxicity; Oxidative stress; renal and colorectal cancer cells.

Synthesis and characterization of novel metal tungstate/g-C_3N_4 nanocomposite as highly performing ascorbic acid electrochemical sensor

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The electrochemical detection of ascorbic acid (AA) using an ITO electrode modified with a $CuWO_4/NiWO_4/g\text{-}C_3N_4$ (CNWG) nanocomposite is the subject of this paper. Through various spectroscopic investigations, including DRX, FTIR, SEM, and TEM, the as-synthesized nanoparticles were examined and described. Different electrochemical techniques, including cyclic voltammetry, chronoamperometry, and amperometry, were used to assess the electrochemical performance of CNWG/ITO towards ascorbic acid detection in N_2-saturated 0.1M NaOH aqueous solution. The results illustrate that ascorbic acid is identified with a low detection limit of 0.1µM for a linear range of 0-1000µM with a sensitivity of 0.4µAµM^{-1}cm^{-2}. The sensor is selective, stable and satisfyingly reliable in real sample experiments. The findings show that the synergistic features of each component in the nanocomposite materials give the CNWG/ITO electrode exceptional sensing capabilities. It is highly interference-resistant and selective for the detection of cysteine, stearic acid, citric acid, urea, CsCl, and $CuSO_4$. It has been established that the sensing electrode's low cost and environmental friendliness make them potentially useful in biological industries. Ascorbic acid determination on real samples reveals that the recommended method would be effective for routine AA analyses used in clinical settings.

Keywords: Nanocomposite, Electrochemical sensing, electrode, Ascorbic acid, cyclic voltammetry, amperometry.

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Synthesis, Crystal Structure and characterization of a New Decavanadate.

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A new decavanadate compound was synthesized by slow evaporation at room temperature. The molecular structure was investigated by single-crystal X-ray diffraction. It crystallizes in the triclinic system, (P-1) with the cell parameters are : a=11.282(5) Å, b=10.424(3) Å, c=8.502(1) Å, α=112.81(2)°, β=87.25(2)°, γ=111.49(5)°, V=852.4(5) Å^3, and Z=2. The formula unit of compound is formed by an acidic decavanadate group $[H_4V_{10}O_{28}]^{2-}$, a $Na_2(H_2O)_{10}^{2+}$ dimer, and four molecules of water. The cohesion of the structure is ensured by hydrogen bonds and van der Waals interactions. The study of the Hirshfeld surface shows that O…H/H…O and H…H interactions dominate the structure.

Keywords: Decavanadate, Synthesis, Crystal structure and Hirshfeld surface analysis.

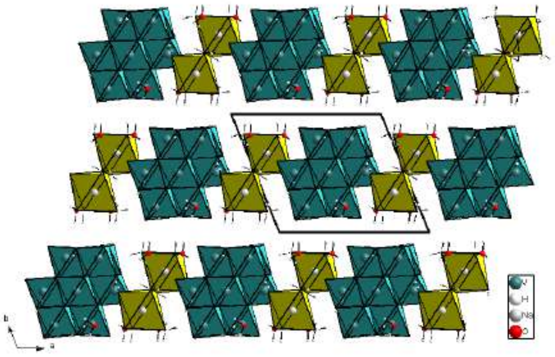

Fig.1 : Projection of the structure according to the *c* axis.

Synthesis of $CuTe_2O_5$ nanoparticles doped with x%Er_2O_3 and their antibacterial activities

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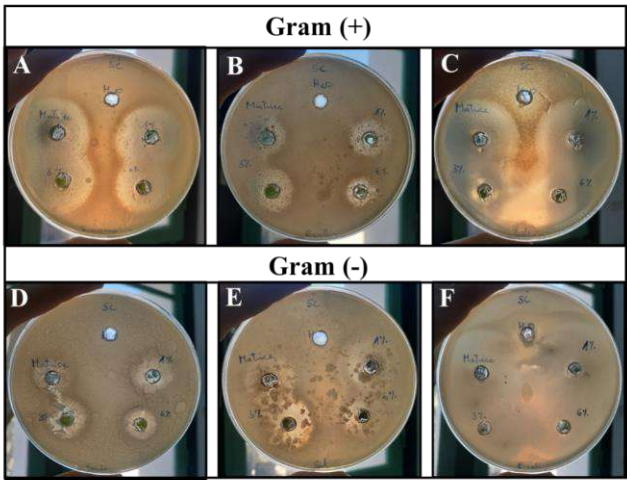
Keywords: nanoparticles, bactéria, antibacterial, material

The use of nanotechnology in medical research is growing quickly in recent years. Not long ago, the development of microbiology have obtained importance in the field of chemotherapy. Bacterial strains that are resistant to current antibiotics have become serious public health problems that raise the need to develop new bactericidal materials.

The aim of this research was to prepare the compound $CuTe_2O_5$;1,3 and 6% Er_2O_3 by the solid state reaction technique. The cristal structure was detailed by X-ray diffraction data refinements. The structure of this material was related in monoclinic system through the $P2_1/c$ space group. The structure can be described as a three dimensional network made of layers parallel to the (010) which hold two kinds of polyhedra TeO_4 and TeO_5 connected through a corner. These sheets are interconnected by Cu_2O_{10} dimers. The value of particle size range between 930 nm and 97 nm. This work is concentrated on the properties of nanoparticles and their mechanism of action as antibacterial agents.



Antibacterial powers of $CuTe_2O_5$ nanoparticles and the various doped compounds (x = 1;3 and 6%) against Staphylococcus aureus (A), Bacillus subtillis (B), Listeria monocytogenes (C), Pseudomonas aeruginosa(D), salmonella enteritidis (E), et Escherichia Coli (F).

Garden cress (Lepidium sativum Linn.) seed oil as a potential feedstock for biodiesel production

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Lepidium sativum L. (garden cress) is a fast-growing annual herb, native to Egypt and west Asia but widely cultivated in temperate climates throughout the world. *L. sativum* seed oil (LSO) extracted from plants grown in Tunisia was analyzed to determine whether it has potential as a raw material for biodiesel production. The oil content of the seeds was 26.77%, mainly composed of polyunsaturated (42.23%) and monounsaturated (39.62%) fatty acids. Methyl esters (LSOMEs) were prepared by base-catalyzed transesterification with a conversion rate of 96.8%. The kinematic viscosity (1.92 mm^2 /s), cetane number (49.23), gross heat value (40.45), and other fuel properties were within the limits for biodiesel specified by the ASTM (American Standard for Testing and Materials). This study showed that LSOMEs have the potential to supplement petroleum-based diesel.

Keywords: *Lepidium sativum* L., Biofuel, Vegetable oil, Fatty acid methyl ester, Transesterification

Detection of inulin, a Prebiotic Polysaccharide, in Tunisian truffle

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Terfez are edible mycorrhizal, hypogeal (Ascomycetes) mushrooms that grow mainly in arid and semi-arid areas of the Maghreb and the Middle East. Their healing properties such as antidiabetic and antitumoral activities have been recounted for several centuries by the Arabs and by certain religious hadiths.

Inulin as a representative of fructans has hypoglycemic activity due to its ability to increase glucagon-like peptide-1 (GLP-1), which increases the secretion of insulin, inhibits the secretion of glucagon and somatostatin, causes the proliferation and neogenesis of β-cells and increases the response of β-cells to glucose (Kietsiriroje et al. 2018; Paternoster and Falasca 2018).

The objective of this study is to extract the inulin from *Terfezia Boudieri*, a specie of truffle collected from Tunisian desert. A hot aqueous extraction was carried out to isolate inulin, followed by a purification and structural characterization using appropriate spectroscopic methods such as FTIR and NMR. Thereafter, the optimization of the operating conditions was determined using a Box-Behnken experimental design.

Following this study, we can deduce for the first time the presence of inulin in *terfezia boudieri*. This was confirmed by a structural analysis based on FT-IR and NMR spectra. The extracted inulin sample was tested for its antidiabetic activity using alpha-amylase method.

A Combined Theoretical and Experimental Study on the Synthesis of Novel Series of (Thio)Amide: Molecular Docking was a Powerful Approach for Structure-Based Drug Discovery

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A novel series of (thio)amide was synthesized and characterized by NMR spectra, IR and elemental analysis. DFT calculations were performed using the B3LYP hybrid functional combined with the extended 6-311++G(d,p) basis set. In recent years, since the molecular docking technique can greatly improve the efficiency and reduce the research cost, it has become a key tool in computer-assisted drug design to predict the binding affinity and analyze the interactive mode. Molecular docking was studied ***to*** investigate the efficacy against selected drug targets into ***ligand-receptor interactions between different proteins.*** Molecular docking were performed to evaluate that the (thio)amide derivatives as an anti-inflammatory, anti-fibrotic and antioxidant against. (**Figure 1**) [1]

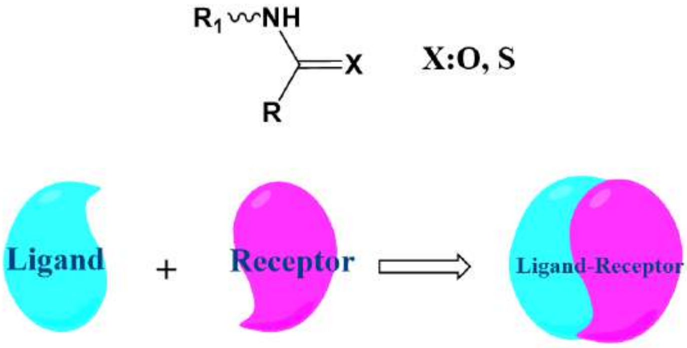

Figure 1

Key words: Thioamide, Amide, DFT calculations, Biological Activity, Molecular Docking

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Reference

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Batch and Continuous Fixed Bed Column Adsorption of Crystal Violet Dye from Water using Pomegranate Peels-Derived Biochar: Influencing factors and adsorption behavior

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Herein, potential biochar was prepared by the slow pyrolysis of pomegranate peels at 800 °C in absence of oxygen. The obtained pomegranate peels biochar (PP800) was characterized and used for aqueous crystal violet (CV) dye sorptive removal. A continuous mode fixed-bed up-flow column adsorption experiments were conducted to investigate the effect of influent CV concentration, flow rate, and column bed depth.

Results showed that PP800 exhibits highly porous structure because of its large BET specific surface area (S_{BET}=570.3 m^2/g) and important total pore volume (V_T=0.28 cm^3/g). The pH_{PZC} value of the prepared biochar was 6.42. According to the column study, the highest efficiency of CV dye removal was obtained in the case of column bed depth of 4 cm. The efficiency of discoloration decreased with increasing the flow rate and with the initial concentration of dye.

Experimental data for bed were interpreted by two kinetic models (Thomas and Yoon–Nelson) with error analysis. It was found that the two models were comparable for the entire break-through curve depiction. It could be computed that the PP-biochar can be used efficiently as an alternative option for textile wastewater treatment

Keywords: biochar; crystal violet; fixed-bed; flow rate, kinetic models.

Growth, crystal structure, Hirshfeld surface analysis, DFT studies, physicochemical characterization, and cytotoxicity assays of novel organic triphosphate

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A novel organic–inorganic hybrid compound, named (1-phenylpiperazinium) trihydrogen triphosphate, with the formula $(C_{10}H_{15}N_2)_2H_3P_3O_{10}$ has been obtained by low speed of evaporation of a mixture of an alcoholic solution of 1-phenylpiperazine and triphosphoric acid $H_5P_3O_{10}$ at room temperature after using the ion exchange chemical procedure. To carry out a detailed crystallographic structure analysis, single-crystal X-ray diffraction has been reported. In the molecular arrangement, the different entities are held together through N–H…O, O–H…O, and C-H…O hydrogen bonds, building up a three dimensional packing. Powder X-ray diffraction analysis is acquired to confirm the purity of the product. The nature and the proportion of intermolecular interactions were investigated by Hirshfeld surface analysis. In order to support the experimental results, a density functional theory (DFT) calculation was performed, using the Becke-3-parameter-Lee–Yang–Parr (B3LYP) function with LANL2DZ basis set, and the data indicate much agreement between the experimental and the theoretical results. Thus, the physicochemical properties were studied employing a variety of techniques (FTIR, NMR, UV–visible, and photoluminescence). To get an insight of the possible employment of the present material in biology, cell viability assays were performed.

Key words: Triphosphate, Density functional theory, Hirshfeld surface, Cytotoxicity assay

SYNTHESIS, STRUCTURE AND NONLINEAR OPTICAL PROPERTIES OF NEW ORGANO-LANTHANUM CRYSTAL

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In recent years, nonlinear optics has been recognized as a promising field with important application in the domain of opto-electronics and photonics. Thus, the combination of an inorganic compound with another organic molecule contributes to obtain a new semi-organic nonlinear material. In this contribution, nonlinear optical (NLO) single crystals of Lanthanum (La^{3+}) doped 4-aminobenzenesulfonic acid crystals was grown from aqueous solution by slow solvent evaporation method at ambient temperature.

In the first step, the structure of a new crystal is determined by X-ray diffraction analysis. The thermal stability was established by thermogravimetric analysis TGA. Then, its analysis of the ultraviolet-visible (UV–Vis) spectroscopic and the Energy dispersive X-ray analysis (EDAX) were recorded.

In the second step, the nonlinear optical properties as well as the second harmonic generation (SHG) behavior of a novel crystal was analyzed by Kurtz-Perry powder technique. Therefore, this nonlinear optical behavior was determined through the calculations of polarizability and first hyperpolarizability values.

Keywords: crystal growth; X-ray diffraction, optical properties; second harmonic generation, thermal analyses.

Influence of the anode materials on the electrochemical oxidation efficiency: Application to oxidative degradation of the pesticides chlorobenzene

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Electrochemical oxidation (EO) constitutes a powerful emergent technology for the treatment of organic pollutants in waters. It is based on the production of oxidant hydroxyl radical (•OH) on the surface of a high O2-overvoltage anode by water oxidation. In this contribution, the electrochemical oxidative removal of the chlorobenzene (CB) compound was studied in a batch reactor using a Boron-doped diamond (BDD), PbO_2 or platine (Pt) as anode and graphite bar as cathode. It was found that BDD anode was more efficient than PbO_2 and Pt to oxidize and mineralize totally CB in water. Then, the influence of several experiments parameters, such as applied current density, supporting electrolyte and initial pH value, was investigated. The total mineralization with 98% TOC removal of 225 mg/L CB aqueous solution was found after 360 min treatment. The mineralization current efficiency and specific energy consumption were also determined. CB was quickly oxidized by in-situ generated hydroxyl radicals formed from oxidation of water on the BDD surface following pseudo first-order reaction kinetics. The results obtained highlight the great efficiency of electrochemical oxidation process in effective destruction of a persistent pesticide such as CB that can be extrapolated to other toxic/persistent organic pollutants.

Keywords: Water treatment, Chlorobenzene, TOC removal, BDD, anodic oxidation.

Ag-Based Catalysts in Different Supports: Activity for BPA Oxidation

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Bisphenol A (BPA) is an industrial chemical and widespread used in many consumer products. It is manufactured in very high quantities and is used amongst others for the production of polycarbonate (PC), polyvinyl chloride (PVC) and epoxy resins, and is able to leach into food, beverages and air. Thus, humans are exposed to BPA through different routes of exposure. BPA is identified as an endocrine disrupting chemical and is able to lead to various adverse health effects. Experiments on catalytic-degradation of Bisphenol A (BPA) were carried out with water samples by catalytic-oxidation method in the presence of 5% Ag supported on TiO_2, Al_2O_3 and TiO_2-Al_2O_3 catalysts. The objective of this study was to develop an improved technique that can be used as a remediation procedure for a BPA contaminated water. The catalyst used were prepared by Sol-gel and impregnation method. XRD, TEM, FT-IR, BET, H2-TPR were used to characterize the materials. he XRD analysis showed the existence of different peaks of the silver on the surface of Al_2O_3 in the contrast with TiO_2 were no specific peaks exist. The Physicochemical and catalytic properties of the samples vary according to the support used. The intervention of the advanced catalytic oxidation (ACO) reduces the time of degradation to less than 1 h to reach a degradation rate of 100% for BPA in water. The catalyst Ag/TiO_2, provide the most effective treatment of contaminated water with phenolic products. TEM images for the catalysts Ag/TiO_2, Ag/Al_2O_3 and Ag/TiO_2-Al_2O_3 showed that silver particles were identified and very well dispersed on the support. The catalytic oxidation of organic pollutants represents a promising avenue for the treatment of wastewater in addition to biological treatment in order to obtain clean water that can be reused in agriculture and industry.

Key words: BPA oxidation, Silver (Ag), TiO_2, Al_2O_3, TiO_2-Al_2O_3.

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IMPACT OF TiO_2 QUANTUM DOTS ON THE PERFORMANCES OF TiO_2 CATALYSTS: APPLICATION IN PHOTOCATALYSIS

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Heterogeneous photocatalysis is an alternative method used frequently for the removal of various pollutants in water treatment. The reduction and oxidation sites on the photocatalyst surface are spatially close at the nanoscale [1]. Among the semi-conductors frequently used in photocatalysis, those based on TiO_2 are attractive candidates due to their photochemical stability and low cost. However, The large energy band gap (3.2 eV) and electron-hole recombination limit o TiO_2 photo-absorption ability and the lifetime of photoelectron-hole pairs [2,3]. Several approaches have been employed to formulate structures and electronic properties of TiO_2 at the nanocrystal level, including controlling band structure, doping and heterojunction interaction [4-6]. In this work, the effect of the preparation method (hydrothermal, solvothermal, sol-gel and precipitation method) on a successful synthesis of quantum dots (QDs) and their properties was investigated. In a second step, an alternative approach for constructing TiO_2 homojunctions between QDs and the support is developed. The synthesized catalysts were characterized by X-ray diffraction (DRX), Nitrogen physisorption, photoluminescence excitation spectroscopy (PL) and UV-Visible spectroscopy. Strong interfacial interactions between supports and QDs reducing efficiently the recombination of photogenerated electron-hole pairs [7] and decreasing the gap energy were observed on our catalysts. Regarding the catalytic application, QDs-TiO_2 catalysts demonstrated high photocatalytic activity for the degradation of methylene blue in aqueous solution (up to 70% methylene blue degrade after 140 min) these photocatalysts show better activities when compared to other TiO_2-based catalysts. This work could give a new vision of homojunction based on quantum dots and opens new paths for practical applications of photocatalysis in the field of water treatment.

Keywords: Heterogeneous photocatalysis, TiO_2, quantum dots, homojunction, semiconductor, water treatment.

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Optimization of ultrasound-assisted extraction of phenolic compounds from *verbana officinalis* L. leaves using response surface methodology and evaluation of its antioxidant activities.

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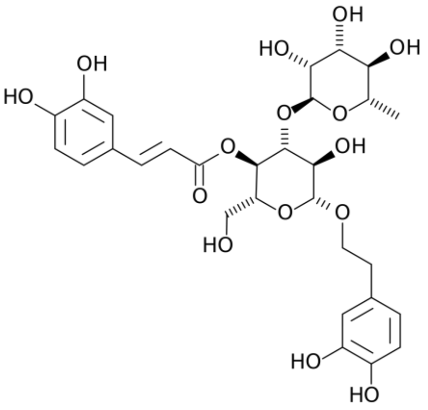
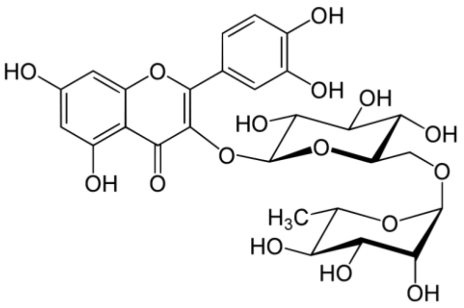
The ultrasound-assisted extraction of phenolic compounds from *Verbena officinalis* L. leaves parts was modeled using response surface methodology. Central Composite Design has been used to optimize four extraction parameters: extraction time (t), ultrasonic temperature (T), liquid-to-solid ratio (R) and pH (pH) in order to get a phenolic rich extract. The optimized conditions are t = 30.64 min, T = 52.70 °C, R = 28.71 ml/g and pH = 5.22. Under these conditions, the experimental TPC= 87.089 mg GAE/g DW, TFC= 52.706 mg QE/g DW, IC$_{50}$= 27.975 µg/ml and FRAP assay= 992.566 µM BHT/g DW. Consequently, this optimized UAE method has demonstrated a potential application for efficient extraction of phenolic compounds from *Verbena officinalis* L. leaves in the nutraceutical industries.



Verbascoside



Quercetin-3-*O*-rutinoside

Key words: Verbena officinalis, Ultrasound Assisted Extraction, antioxydant activities, Response Surface Methodology

Ultrasonic Activation of Sonogashira Coupling Reaction of aryl halides with Terminal Alkynes

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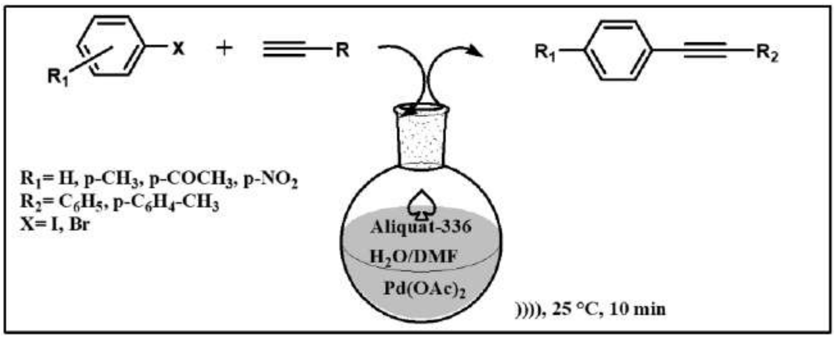
A convenient methodology has been developed for palladium catalyzed Sonogashira cross-coupling reaction under mild and green reaction conditions. The reaction is catalyzed by an in situ generated catalytic system based on $Pd(OAc)_2$ and Aliquat-336 in the absence of copper salt with excellent yield of cross coupled product. The reaction condition is compatible with electronically diversified aryl halides and electronically diversified aryl or aliphatic alkyne. The present method developed for the Sonogashira reaction offers many advantages including high conversion, high economy, the involvement of non-toxic green substrates, etc. This is an excellent catalyst system for the Sonogashira coupling under ultrasonic irradiation in optimized conditions at room temperature [1,2]. Yields increased with the sonochemical activation for a very short duration. The isolated products are of high purity. In this regard, we propose reaction mechanisms that could explain the results.

Key words: Sonogashira coupling, Ultrasound irradiation, green reaction, phase transfer catalysis.



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Iron-Catalyzed α-arylation of Acetone with Aryl Halides the presence of ultrasound

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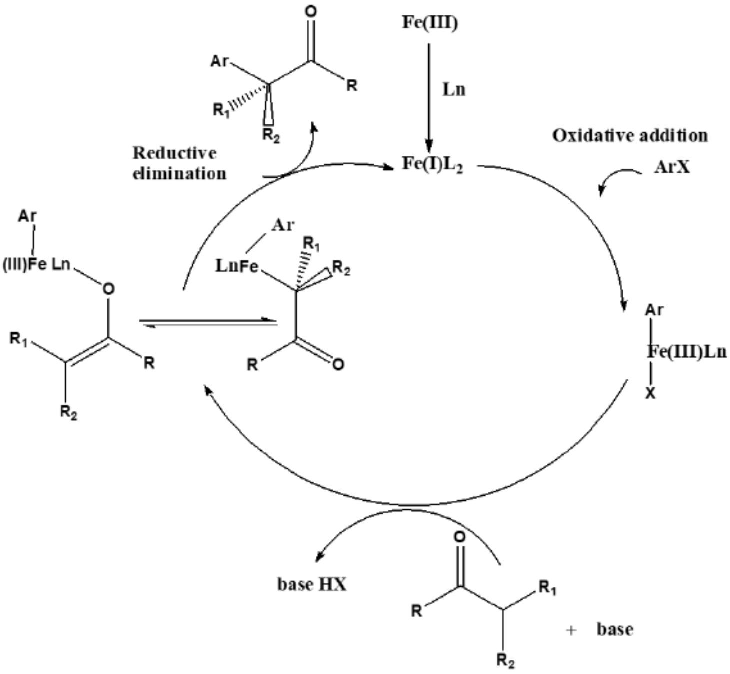
A versatile iron-catalyzed synthesis of highly substituted α,β-unsaturated carbonyl compounds has been developed. In contrast to the known Heck-type coupling reaction of unsaturated carbonyl compounds with aryl halides [1], the present methodology allows the use of stable and readily available saturated carbonyl compounds as the alkene source. In addition, the reaction proceeds well with low catalyst loadings A variety of saturated aldehydes, ketones, and esters are compatible for the reaction with aryl halides under the developed reaction conditions to afford α,β-unsaturated carbonyl compounds in good to excellent yields. it was found that ultrasound radiation [2] and improve the reaction efficiency. This method could be a clean, economical, efficient and safe technology in organic synthesis. This regard, we propose reaction mechanisms that could explain the results obtained.



Key words: Iron, ultrasound radiation, carbonyl compounds, aryl halide.

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Seawater brines evaporation: Potential and kinetics of magnesium hydroxide crystallization

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As seawater desalination becomes the answer to the global water scarcity, the disposal of the brines emerged as a new challenge. In most cases, the simple alternative given to handle saline water was returning it back to the sea, which could have, in the long term, harmful effects on the marine environment and the quality of the seawater. This waste stream can be classified as a co-product and could constitute a secondary resource for extracting valuable minerals, such as magnesium, with environmentally friendly processes. Owing to its numerous uses, Magnesium is a strategic compound [1]. It can be produced from different raw material sources, among which we are focusing on Mg precipitation as magnesium hydroxide or Brucite ($Mg(OH)_2$) from highly concentrated bitterns leaving saltworks [2].

The magnesium content in the generated bitterns can reach values up to 50-55 kg/m^3. In fact, 80,000 to 115,000 estimated tons per year of magnesium are rejected by the Tunisian Saltworks. This work focuses on recovering magnesium hydroxide by reactive crystallization from highly concentrated bitterns using a neutralizing agent, for a wide range of supersaturations. Ions depletion were tracked by monitoring solution pH. Supersaturations were calculated using PhreeQC allowing obtaining species activities through the full Pitzer model. Brucite precipitation rates versus supersaturation showed a clear two trend curves.

Key words: Brines, saltworks bitterns, magnesium recovery, reactive crystallization, PhreeQC, supersaturation.

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Direct Functionalization of Lithium Phosphine Oxides bearing an Alkyne chain

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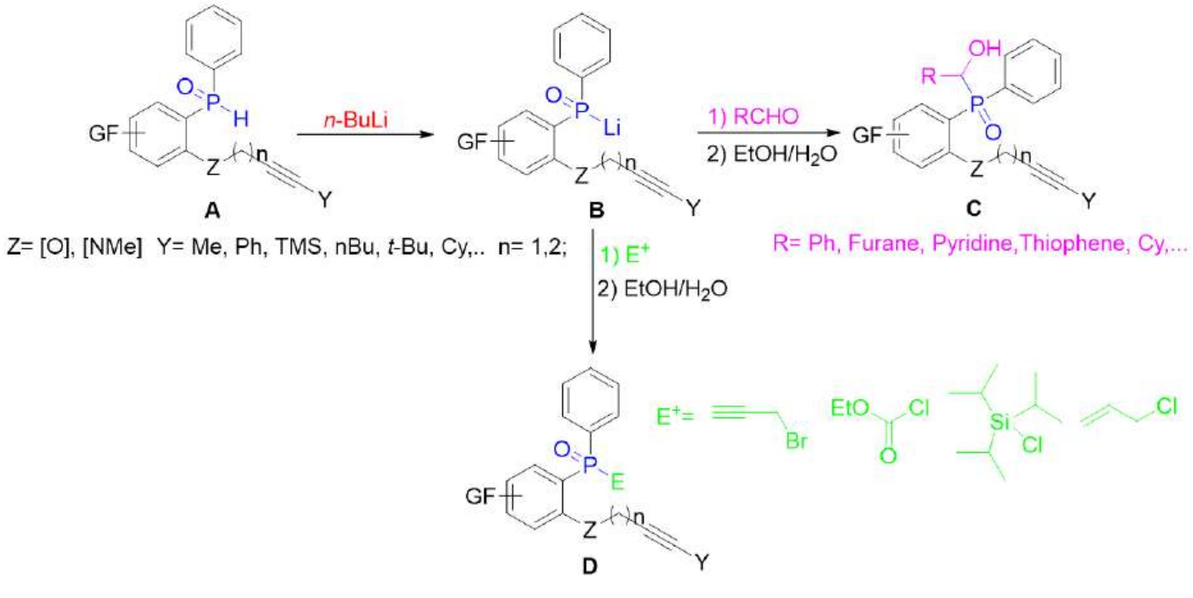
Lithium phosphide nucleophile is one of the most efficient approaches for the construction of new carbon–phosphorus bonds.[1]. Here we report the synthesis of a novel family of propargyl phosphorus alcohols starting from a propargyl phosphorus oxide as substrate. The present approach is based on phosphorus-hydrogen bond (P-H) activation using butyl lithium, followed by a subsequent condensation with a wide variety of electrophiles. Products **C** and **D** are obtained in ~~a~~ moderate to good yields by functionalization of the precursor propargyl lithium phosphide intermediate **B** (Scheme 1).



Scheme 1

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Study of oxidative stability and cold flow properties of *Citrillus colocynthis* oil and *Camelus dromedaries* fat biodiesel blends

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Recently, biodiesel has been gaining market share against fossil-origin diesel due to its ecological benefits and because it can be directly substituted for traditional diesel oils. However, the high cost of the raw materials required to produce biodiesel make it more expensive than fossil diesel. Therefore, low-priced raw materials, such as waste cooking oil and animal fats, are of interest because they can be used to drive down the cost of biodiesel. We have produced biodiesel from camel fat using a transesterification reaction with methanol in the presence of NaOH.

Biodiesel prepared from animal fat has been gaining increasing interest in the last few years. The main drawback of biodiesel prepared from animal fat is its poor low-temperature performance, which limits its use in cold climates. This study proposes a method of improving the low-temperature properties of young *Camelus dromedaries* (Hachi) fat biodiesel (HB) and improving select fuel properties [e.g., the cetane number and oxidative stability] of *Citrullus colocynthis* biodiesel (CCB), which has a high iodine value. HB and CCB were blended in different volume ratios and the fatty acid methyl ester composition and fuel properties of the biodiesel blends were evaluated according to the American Society for Testing and Materials (ASTM) methods.

The results of our study demonstrate that blending the biodiesel from Hachi fat and *C. colocynthis* seed oil provides a suitable alternative to biodiesel prepared using food crops.

Key words: Hachi fat, *Citrullus colocynthis* seed oil, Transesterification, Alkali catalyst, Fuel properties, Biodiesel blend

Physicochemical characterization of polysaccharides from apricot by-products: Antioxidant and antidiabetic activities

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The use of agricultural and food by-products is an economical solution to industrial biotechnology. Apricot is commonly used for medicinal purposes and the formation of food ingredients; it is also known to be used as a household remedies since antiquity [1]. In this work, polysaccharides from apricot by-products were extracted with water in a thermostated cell [2]. The obtained polysaccharide was characterized by Fourier Transform Infrared Spectroscopy analysis, Size Exclusion Chromatography (SEC/MALS/VD/DRI) and NMR spectroscopy. Then, the physicochemical and antioxidant of extract polysaccharide was studied, and the total sugar and galacturonic acid contents were 52.2% and 29.8%, respectively. In addition, FTIR analysis confirmed the presence of uronic acids. Finally, the results indicated that apricot polysaccharide presents a strong antioxidant activity *in vitro* in DPPH and FRAP and an interesting antidiabetic effect

Key words: Apricot, Polysaccharides, antioxidant activity, antidiabetic property.

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Determination of antibiotics substances in surface water using solid phase extraction and liquid chromatography

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Pharmaceuticals in water have been an environmental issue since the 1990s [1]. An important but often ignored aspect is the fate of antibiotic residues that reach the environment by different pathways. Because antibiotics are typically present in environmental water in low concentrations from µg L^{-1} to ng L^{-1}, the analytical methods require efficient sample preparation for their detection. A high-performance liquid chromatography method is reported for the determination of fluoroquinolones and nitroimidazoles antibiotics in water. The antibiotics were simultaneously preconcentrated by solid-phase extraction on carbon nanotubes. High-performance liquid chromatography was performed on a C-18 column with isocratic elution in 5 min. The separation was performed using isocratic elution with 24:76 acetonitrile: acidified water (pH = 4) and 0.4 % triethylamine. The antibiotics were identified by diode array detection. Recovery, linear range, limit of detection (LOD), and limit of quantification were calculated. Surface water samples from were analysed and recovery ranged between 69,88 et 90,12% with % RSD < 9,5.

Keywords: solid phase extraction (SPE), carbon nanotubes, antibiotics, HPLC-UV, surface water.

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Comparison of emulsifying properties of two biopolymers extracted from Prickly Pear: Contribution of the protein fraction

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Opuntia ficus indica (OFI) belongs to the Cactaceae family, it occupies extended areas throughout Tunisia estimated at 6,00,000 ha. Its cladodes are rich in mucilage which is a slimy fluid found in the parenchyma composed of a complex carbohydrate, proteins, and minerals. [1] Moreover, pectin extracted from OFI cladodes have shown interesting emulsifying properties. [2] The objective of this study is to compare the emulsifying capacity of the parenchyma's mucilage and the extracted pectin, to highlight the contribution of proteins in the formation, stability and particle size of the obtained emulsions. Stable oil-in-water emulsions were obtained. Very slow creaming was observed for emulsions stabilized with low concentrations of pectin. An in-depth investigation of the emulsion properties and stability was performed. The formulation parameters, oil content and pectin concentration were systematically varied.

Key words: *Opuntia ficus indica*; mucilage; pectin; emulsions

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Study of the effect of the combination with Abacavir and Lamivudine on the dissolution profile of the recently approved HIV inhibitor; Dolutegravir

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Dolutegravir (DTG) is the most recently approved human immunodeficiency virus (HIV) integrase inhibitor. It has demonstrated to be safe and highly effective in reducing the HIV-1 RNA viral load. DTG is indicated in combination with other antiretroviral agents for the treatment of HIV-1 infection in adults and in children ≥12 years. Quality assurance of DTG medicines is, hence, a major global health concern. Dissolution test is commonly used by the pharmaceutical industry to guide formulation design and control product quality. This test is a required performance analysis for solid dosage forms and it is the only test that measures the rate of in vitro drug release as a function of time, which can predict in vivo drug release. A comparative study of the dissolution profile of DTG (alone and in association) in two pharmaceutical specialties; «Tivicay» and «Triumeq», was carried out. Indeed, DTG is poorly soluble in water. This study aimed to evaluate the effect of the combination with Abacavir and Lamivudine on the rate of dissolution of DTG in an aqueous medium.

The dissolution study was conducted using 900 ml HCl 0.1N media maintained at 37°C using the paddle apparatus and stirring rate of 75rpm. Samples were taken at 15, 30, 60, 90 and 120 minutes. The quantification was carried out by reversed phase high performance liquid chromatography using a Thermo phenyl Hexyl column (l50 mm × 4.6 mm DI, 5µm) maintained at 40°C. Mobile phase consists of sodium perchlorate buffer 50 mM, pH=3.0 and acetonitrile (70:30 v/v) debited at a flow rate of 1.3 ml/min. The results of the study show that the DTG in the combined form has a relatively faster dissolution profile than in Tivicay tablets. This study led us to show the importance given to the kinetic of dissolution in combined form and leads to deepen the study of the interaction between these molecules.

Key words: Dolutegravir, Abacavir, Lamivudine, Dissolution test, RP-HPLC.

Effects of synthetic routes on structural, dielectric and electrical properties of $CaCu_3Ti_4O_{12}$ ceramics

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$CaCu_3Ti_4O_{12}$ (CCTO) ceramics was fabricated by solid, citrate, urea and glycine methods. The major goal is to assess the effects of synthesis techniques on the structural and electrical properties of the material. Independently of the synthesis method, X-ray diffraction XRD results confirmed presence of the cubic structure main phase with space group $\boldsymbol{Im}\bar{3}$. The average grain size of the sample CCTO varied according to the synthesis process. The surface morphology of the composite sintered at 1100 °C for 12 h obtained by scanning electron microscopy analysis indicates the evolution of large and small grains with a bimodal distribution. A high dielectric constants ($\varepsilon' \sim 10^4$) accompanied fortunately by a lowering loss tangent ($\tan\delta < 0.1$) was measured at room temperature in the 10^2 Hz- 10^7 Hz frequency range in all ceramics. Ceramics elaborated by the citrate method show a very interesting dielectric response, namely a relatively high dielectric constant ε' (6.735×10^4 at 1 kHz) and a low dielectric loss tanδ (0.07 at 1 kHz). In addition, the temperature stability of the dielectric constant also improved by solid, urea and glycine methods. The fits of impedance complex spectroscopy data, shows that the resistance of grain is lower than resistance of grain boundaries confirming the internal barrier layer capacitor model. This mechanism corresponds to the heterogeneous dielectric with semiconductor grains and insulating grain boundaries.

Key words: Dielectric constant, Microstructure, CCTO ceramic, Grain boundary, dielectric loss tanδ.

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Evaluation of the antioxidant activity of cinnamon essential oil loaded into sodium and copper-exchanged clays

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Essential oils (EOs) are well known to have therapeutic potential as they have various potent biological activities including antimicrobial, antifungal, anti-inflammatory, and antioxidant activities. However, their use showed some limits like high volatility, low water solubility and chemical instability when exposed to heat, oxygen…. In order to avoid these problems, nanoencapsulation has been suggested as an innovative mean to overcome these limitations. In recent years, the interest for clay nanoparticles as nanoencapsulation materials of EOs is increasing owing to their abundance in nature, low cost, inertness and special structure.

The main objective of this study was to develop new organic-inorganic nanohybrid materials based on sodium (H-Na) and copper exchanged Tunisian clays (H-Cu) and Cinnamon essential oil (CEO) for therapeutic purposes.

The CEO extraction was performed by steam distillation in a Clevenger type apparatus and its chemical composition was determined by Gas chromatography-mass spectroscopy (GC-MS).

The clay sample, from the South of Tunisia, was saturated with NaCl and $CuCl_2$ solutions to obtain respectively sodium (H-Na) and copper (H-Cu) exchanged clays. The resulting modified clays were characterized by X-ray fluorescence (XRF) and X-ray diffraction (XRD). In addition, the cation exchange capacity was evaluated.

The hybrid materials were prepared by simple adsorption of CEO onto H-Na and H-Cu. The antioxidant activity of the prepared materials and free CEO was evaluated by the DPPH (2,2-diphenyl-1-picrylhydrazyl) method.

The GC-MS analysis of CEO revealed the presence of six components accounting for 100% of the total amount. Cinnamaldehyde was found as the major component along with endobornyl acetate (1.134%) δ-cadinene (0.603%). The highest inhibitory activity (85%) was observed at a CEO concentration of 50 $mg.mL^{-1}$. The results obtained by chromatography (GC-FID) showed that a maximum CEO adsorption is about 45 and 95 mg/g on H-Na and H-Cu, respectively. CEO/H-Na and CEO/H-Cu hybrids exposed similar antioxidant activities compared to free CEO, suggesting their great potential application in the pharmaceutical field.

Fabrication of amorphous solid dispersions of ketroprofen by spin-coating and assessment of their stability with relative humidity

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Utilizing surfaces for nucleation and growth is often adopted as a means to enhance crystallization. Certain surfaces can accelerate crystallization while other prevents it. On the other hand, constrains induced by the surface can trigger crystal growth on well-defined contact planes and thus along specific crystallographic directions i.e. texture or epitaxial growth can result.[1]It has also been shown that surfaces can increase the crystallization rate when compared to the bulk.[2] Furthermore, it has been shown for several organic semiconductors (organic molecules deposited on flat solid substrates as thin films a hundred of nm thick) that new polymorphs could be stabilized only close to the substrate (called "substrate induced polymorphs or SSPs).[3,4]The use of thin film deposition by spin-coating on glass substrates to fabricate amorphous solid dispersions of ketoprofen (KTP, an non-steroidal anti-inflammatory) with polyethylene glycol (PEG) an inert polymer is reported. Namely, KTP and PEG are solubilized in dichloromethane at different PEG mass content (from 0% to 100%) and different concentration of the mixture (10 mg/mL, 20 mg/mL and 40 mg/mL) and the solution is cast on a pre-cleaned glass substrates which is subsequently rotated at a given speed during a given time. All the films have been characterized by X-ray powder diffraction (XRPD) and atomic force microscopy (AFM). Furthermore, the different films were submitted to atmosphere with different relative humidity (0%, 57%, 84% and 98% RH) during several months and subsequently characterized by XRPD and AFM to assess their stability and find the sample parameters which influence this stability. In particular, solution concentration which is related to film thickness and so the nucleation rate of ketoprofen appears to significantly influence the stability of the amorphous dispersions.

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Physical and chemical stability of amorphous Candesartan

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The use of amorphous solid form remains an attractive method to improve the solubility and biopharmaceutical performance of poorly soluble drugs. However, this metastable form may undergo physical and chemical transformations that impair drug therapeutic efficiency. Therefore, an ability to control these transformations would be highly valuable.

This work aims to study the chemical and physical stability of amorphous candesartan, which belongs to a class of drugs called angiotensin receptor blockers (ARBs). Samples with disordered form were formulated using, milling and melt quenching and were characterized by spectroscopic, thermal and chromatographic techniques.

Upon milling samples at moderate condition, DSC, XRD and FTIR measurements showed a drastic decrease of crystallinity, even though HPLC and 1H NMR profiles display no significant degradation. However, a higher level of milling energy leads to an important change in chemical stability but does not generate a profound physical and structural change.

Under humidity, CDS exhibits a highly crystallizing feature, more intense XRD peaks and more intense melting event without any shift indicating the maintain of the same polymorph.

Compared to Melt-quenched samples that revealed a good stability, milled ones exhibit a lower stability resulting in an easier tendency toward crystallization.

By adding PVP while milling, disappearance of cold crystallization is observed upon first DSC heating and enhancement of Tg values is reached for samples obtained by quench cooling.

Based on the obtained results, it can be considered that introduction of the polymer promotes the ability of CDS amorphisation without chemical nor physical interaction.

Aldiminium and 1,2,3-Triazolium Dithiocarboxylate Zwitterions Derived from Cyclic (Alkyl)(Amino) and Mesoionic Carbenes

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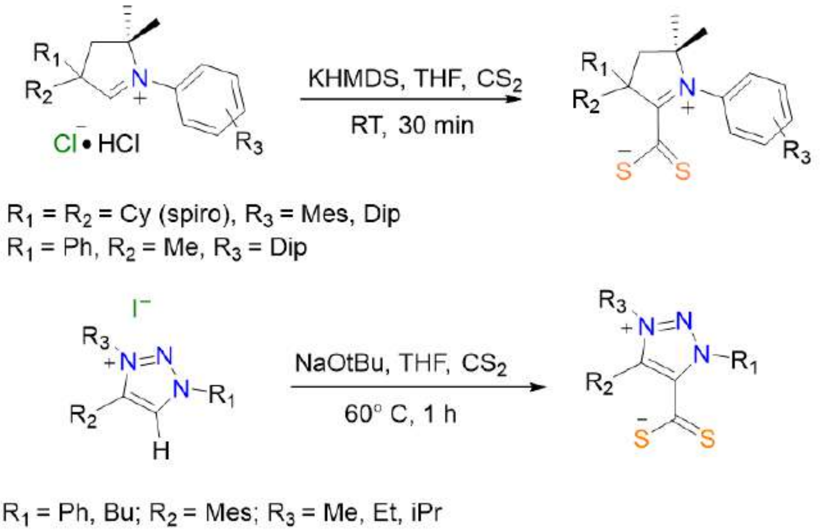
Following previous investigations from our laboratory on imidazol(in)ium-2-dithiocarboxylates betaines derived from N-heterocyclic carbenes [1], a series of three aldiminium and six 1,2,3-triazolium dithiocarboxylates zwitterions derived, respectively, from cyclic(alkyl)(amino) and mesoionic carbenes were synthesized and fully characterized by various analytical techniques, including X-ray diffraction analysis (**Scheme 1**) [2].

Scheme 1.



Key words: cyclic(alkyl)(amino) carbenes, mesoionic carbenes, imidazol(in)ium-2-dithiocarboxylates zwitterions.

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Development and validation of a new method for simultaneous quantitative determination of six preservatives by high performance liquid chromatography

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The aim of this study is to develop a new method for simultaneous determination of six preservatives (ascorbic acid, sodium benzoate, methylparaben, ethylparaben, propylparaben et butylparaben) in bulk form and in cosmetic products. Reversed-phase High-Performance Liquid Chromatography (RP-HPLC) coupled to ultra-violet detection (UV) was employed in this study. The optimum separation was achieved on an X-TERRA® C18 (4.6 × 250 mm, 4 µm) column with a mobile phase consisting of methanol and phosphate buffer (pH 3.5; 10 mM) (48:52, v/v) pumped at a flow rate of 1 mL min^{-1}. The temperature was maintained at 25°C and an injection volume of 20 µL was used. The procedure was validated according to the International Conference on Harmonization (ICH) Q2 (R1) guideline. Good linear relationships were obtained ($r \geq 0.999$) for all analytes over their respective concentration ranges. Intra- and inter-day precision were less than 2 % and recoveries ranged from 98 to 102 %. The developed method was successfully applied for the analysis of cosmetic products. The method may also be used in food industry for the quantification of those conservatives.

Key words: HPLC, Cosmetics, Preservatives, Validation.

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Development and validation of a reversed phase high performance liquid chromatographic method for the determination of oseltamivir in presence of its degradation products

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A simple, selective, linear and accurate high-performance liquid chromatographic method for the determination of Oseltamivir in presence of its degradation products was developed. Isocratic elution at a flow rate of 1 mL/min was employed on a Supelcosil LC-18 column (250 mm × 4.6 mm; 5 µm) at 25°C. The mobile phase consisted of methanol and 50 mM formic acid pH 6 (50:50, v/v). The UV detection wavelength was 220 nm and the injection volume was 50 µL of sample. The developed method was further validated according to the International Conference on Harmonization guideline Q2 (R1). Our method is linear over the concentration range of 30 to 70 µg mL^{-1}. It was successfully applied for quality control of pharmaceutical products.

Keywords: Oseltamivir, HPLC, Pharmaceuticals, Validation

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SYNTHESIS OF NEW CHIRAL *N*-(DIPHENYLPHOSPHINYL)-1,3-OXAZOLIDIN-2-ONES DERIVED FROM NATURAL ENANTIOPURE L-AMINOACIDS

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Oxazolidin-2-ones are pentagonal heterocycles containing two heteroatoms (oxygen and nitrogen). This scaffold is present in the pharmacophore of some commercialized drugs: antibacterial, anti-depressive, anti-inflammatory, anti-mitotic, analgesic, anti-histaminic, anti-depressive agents. The pharmaceutical industry continues to explore new scaffolds that incorporate this moiety. Several compounds containing 4-substituted and 4,5-disubstituted oxazolidin-2-one rings are under development and some of them have shown promising pharmacological activities. Also, the use of enantiomerically pure oxazolidin-2-one derivatives as chiral auxiliaries in asymmetric synthesis (such as aldol condensations) has been amply demonstrated. We describe here the preparation of a series of chiral 1,3-oxazolidin-2-ones derivatives substituted with a diphenylphosphinyl group on the nitrogen of the ring. Synthesis was carried out according to a four step method using L-aminoacids as commercially available chiral starting material, $LiBH_4$ as hydride donor (generated *in situ* by reaction between LiBr and $NaBH_4$) and involving triphosgene as carbonyl donor for the cyclisation of the 1,2-aminoalcohols. Difficulties were encountered to achieve the last step of cyclisation and many attempts were realized in order to define appropriate experimental conditions (solvent, temperature, time and reagents). Yields were low to moderate (20 to 40%) and are probably due to the steric bulk caused by the *N*-diphenylphosphinyle substitution and the reduced nucleophily of the nitrogen.

Key words: 1,2-aminoalcohols, L-aminoacids, oxazolidin-2-ones, triphosgene, chiral

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Synthesis, characterization and biological properties of new nanostructured apatites

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This work is a part of the general framework of systematic studies of the physico-chemical and biological properties of apatites, in order to highlight their interest in the field of biomaterials.

Apatites $Ca_{9-x}NaZn_x(PO_4)_5(SO_4)(OH)_2$ (x= 0-0.5) were synthesized by the solid-state reaction method. The compounds were characterized using X-ray diffraction, Infrared spectroscopy and Raman scattering spectroscopy. Biological properties of the materials have been studied by testing of the antibacterial activity using human pathogenic bacteria.

X-ray diffraction patterns show that these materials crystallize in the hexagonal system with $P6_3/m$ as space group. Infrared and Raman spectra are reported and band assignments are made. The antibacterial activity indicates that the prepared samples can be considered as new prospective biomaterials with antibacterial potential.

Key words: Apatite, Zinc, Antibacterial activity, Biomaterial

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Oxidation of Triclosan by Fe/ZrO2 and Fe-Co/ZrO2 Catalysts

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The objective of this work was to study the catalyzed wet oxidation reaction with metal catalysts based on iron supported on Zirconia oxide and bimetallic catalysts based on cobalt and iron deposited on ZrO2, in order to degrade one of the endocrine disruptors: Triclosan.

In this study, we used the sol-gel route for the development of airgel supports. These supports are then used to prepare a series of catalysts based on iron alone or on iron and cobalt with fixed percentages by dry impregnation.

All these catalysts are reduced under hydrogen flow at 300°C.

The study of the textural and structural properties of the solids was carried out by measuring the specific surface by the BET method and by TPR. The N2 adsorption-desorption analysis of the different solids shows similar isotherms with the ZrO2 support, with varied hysteresis loops which reflects different textures and porous distributions.

The TPR-H2 profiles show the non-reducibility of ZrO2. The TPR analysis of the catalysts shows characteristic peaks of the reduction of iron and cobalt. The results of the catalytic tests show that the monometallic catalyst based on Iron supported on ZrO2 and the bimetallic catalyst impregnated simultaneously on the ZrO2 support exhibit significant catalytic activity in the degradation of Triclosan. This seems to be due to an increase in the average pore diameter and the pore volume, which results in a better iron-support interaction and therefore a good dispersion of the metallic phase at the ZrO2 surface.

Key words: Triclosan, Oxidation, Catalysts, Environment

Liposomal emulsion prepared by using Chitosan as antioxidant and emulsifier

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For its biocompatibility, bio-absorbability, and antibacterial activity 1, chitosan is used in various fields such as cosmetics, food and pharmacy [1-3]. With the possibility of establishing hydrogen bonds between H_2O, and the amine and hydroxyl groups of this polysaccharide, this biopolymer could constitute a promising active ingredient for the development of moisturizing, antibacterial, and antioxidant products [2]. It is in this context that we are interested in the formulation of stable emulsions based on chitosan.

Key words: Liposomal, Chitosan, Emulsifier, Formulation

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

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Polyoxovanadates (POV), as a relevant subfamily of polyoxometalates (POM), have attracted increasing attention over the years due to the variable oxidation states that vanadium can adopt and the various spheres of coordination demonstrated by vanadium oxide polyhedra, which gives them the ability to form an exceptional variety of different architectures **[1]**.In contrast to molybdates and tungstates, which are typically based on [MoO_6]/[WO_6] octahedra as fundamental building units, POVs show more structural flexibility and feature tetrahedral [VO_4], square pyramidal [VO_5], and octahedral [VO_6] coordination modes **[2]**. In order to obtain new materials with news structures and interesting properties, we report in this work for the first time the synthesis, characterizations, crystal structure and stability of the novel bicapped Keggin phosphotetradecavanadates with organic cations $(C_7H_{10}N)_6[H_3PV_{14}O_{42}].7H_2O$ crystallized in a monoclinic system, $P2_1/n$ space group with the cell parameters : a = 18.7299 (3)Å, b= 11.30107 (15) Å, c = 35.8837 (5) Å, β = 95.5187 (14)°and Z = 4.

Key words: Synthesis, Characterization, X-ray diffraction, bicapped Keggin phosphotetradecavanadates.

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Theoretical investigation of the regio- and stereoselectivity of the [3+2] cycloaddition of nitrones with methyl-acetophenone

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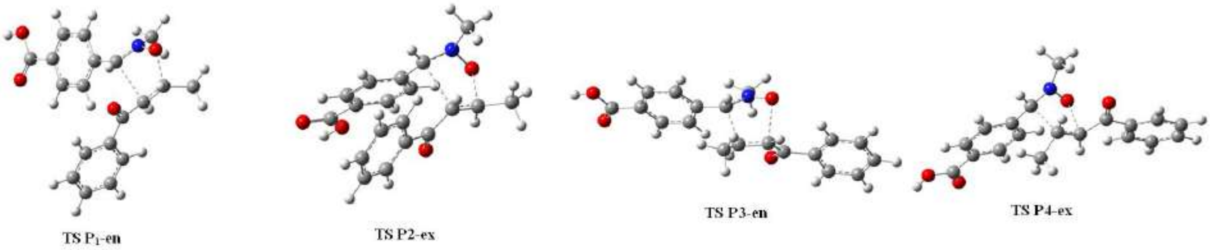
The regio- and stereoselectivity of [3+2] cycloaddition reactions [1] of nitrones with substituted alkenes (methyl acetophenone) was theoretically investigated using density functional theory (DFT) at the B3LYP/6-311+G(d, p) level [2]. The four possible pathways, fused and bridged regioisomeric modes, and the two stereoisomeric approaches, endo and exo, for the cycloaddition reactions were analyzed and discussed. Analysis of TS geometries and bond lengths demonstrates that these reactions follow a one-step mechanism with asynchronous transition states. The activation energy indicated a favored endo approach along the four reaction pathways.



TS P_1-en TS P2-ex TS P3-en TS P4-ex

Figure: Optimized geometries of transition states for the 1,3-DC reaction between the olefin (A) and nitrone (N4) at the B3LYP/6-311G+(d,p) level of theory

Keywords: Nitrones, Acetophenone, 1,3-DC reaction, DFT, GEDT

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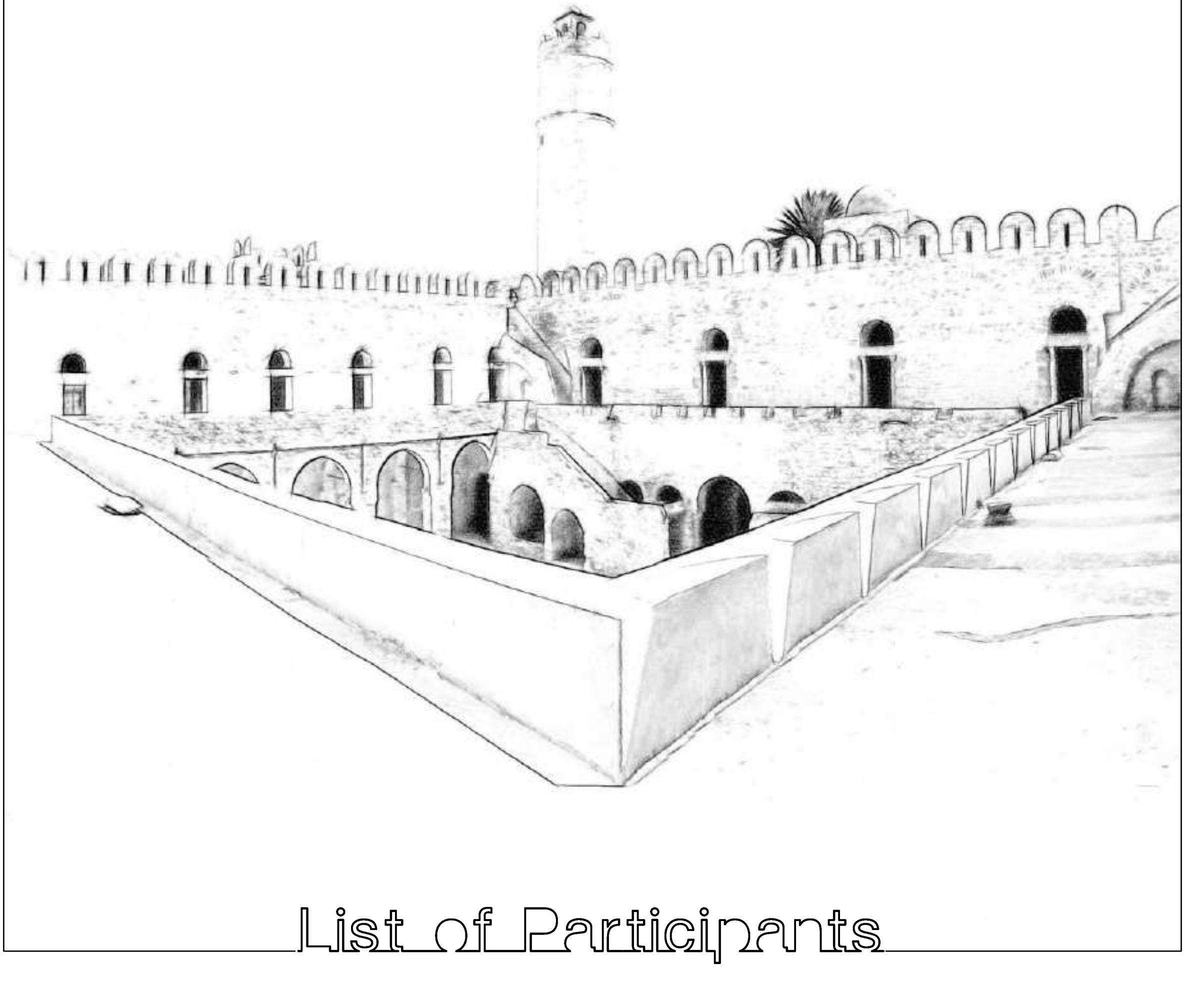

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