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Book of Abstracts



The Hashemite University & Jordanian Chemical Society

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Conference Schedule

Day 1: Tuesday, 12th September 2023 @ Mövenpick Hotel Amman*

Time	Session	Presenter
9 ⁰⁰ -10 ⁰⁰	Registration	Organizers
10 ⁰⁰ -11 ⁰⁰	Conference Opening	Prof. Dr. Khaled Abu-Elteen/Conference Chair
		Prof. Dr. Abeer Al Bawab/JCC President
		Prof. Dr. Moza AlShamsi/Secretary General of the Union of Arab Chemists
		Prof. Dr. Fawwaz Al-Abed Al-Haq/HU President
11 ⁰⁰ -11 ³⁰	Coffee Break & Exhibition	
11 ³⁰ -12 ²⁰	Plenary lecture Chemical Structure-Property Relationships in Surfactant Monolayers	Prof. Dr. Matthew Paige University of Saskatchewan, Canada
12 ²⁰ -13 ¹⁰	Plenary lecture Catalysis for the Circular Economy: Upcycling of Polyethylene to Surfactant-Range Alkylaromatics	Prof. Dr. Mahdi Abu-Omar University of California Santa Barbara, US
13 ¹⁰ -13 ³⁰	Promotional Presentation	Hijaz Scientific Supplies Establishment
13 ³⁰ -14 ⁰⁰	Coffee Break & Exhibition	
14 ⁰⁰ -14 ⁵⁰	Plenary lecture Taking Advantage of the Analytical Footprint of Comprehensive 2D Gas Chromatography	Prof. Dr. Philip Marriott Monash University, Australia
14 ⁵⁰ -15 ¹⁰	OO The Global Greenchem Innovation and Network Inclusion Programme	Eng. Omar AlSaleh Royal Scientific Society, Amman, Jordan
15 ¹⁰ -15 ³⁰	Promotional Presentation	AnalyticaOne for Integrated Scientific Solutions
15 ³⁰ -16 ³⁰	Lunch	
16 ³⁰ -17 ³⁰	Panel Discussion The Chemical and Vocational Interaction and Intersection between the Outcomes of Chemistry Education in Universities and Industry, Innovation and Entrepreneurship Moderator: Prof. Dr. Abeer Al Bawab, JCC President Panellists: <ol style="list-style-type: none"> Prof. Dr. Sultan Abu-Orabi Former President of: Yarmouk University; Association of Arab Universities and JCC Dr. Nael AL-Husami CEO, Amman Chamber of Industry Eng. Mohamad Shaer Honorary President of Syrian Chemistry Society Dr. Mohammad Bitar General Manager, Alfa Chemicals Manufacturing Establishment Dr. Ashraf Bany Mohammed Board Member of Jordanian Innovative Startups and SMEs Fund (ISSF); Associate Professor of Technology Management Economics and Former Director of Innovation and Entrepreneurship Center at the University of Jordan Mr. Mohammad Abu Shanab Board of Directors Member, Al Shaker Company for Scientific and Medical Supplies Mr. Yousef Al-Qutt Technical Consultant at Giant for Chemical Industries Company 	

***Moderators of the first day are Dr. Lubna Alrawashdeh (HU) & Dr. Abdussalam Qaroush (UJ)**

Conference Schedule

Day 2: Wednesday, 13th September 2023 @ King Al-Hussein the Builder Complex, The Hashemite University

Time	Session	Presenter
8 ³⁰ -9 ⁰⁰	Registration	Organizers
9 ⁰⁰ -9 ⁵⁰	Plenary lecture CO ₂ -Switchable Materials for Separations Place: Ground Floor Theatre Moderator: Prof. Adnan Abu-Surrah (HU)	<i>Prof. Dr. Philip Jessop</i> Queen's University, Canada
	Session 1 @ Ground Floor Theatre	Session 2 @ 1st Floor Theatre
	Moderators Prof. Kayed Abu Safieh & Dr. Bassem Al-Maythalyon (RSS)	Moderators Dr. Hazem Amarne (UJ) & Dr. Hassan Abul-Futouh (HU)
10 ⁰⁰ -10 ²⁰	01 Hussam Almassad <i>Royal Scientific Society, Jordan</i> Environmentally Adaptive MOF-based Atmospheric Water Harvesting	05 Ayman Hammoudeh <i>Yarmouk University, Jordan</i> Synthesis, Characterization, and Luminescence Properties of Rare Earth Doped BaGd-Silicate Phosphors for Solid-State Lighting Applications
10 ²⁰ -10 ⁴⁰	02 Youssef Naimi <i>Hassan II University of Casablanca, Morocco</i> Green Hydrogen Production and Consumption: State of the Art and Perspectives	06 Mothana Al-Omari <i>Jordan University of Science and Technology, Jordan</i> Palladium-Catalyzed Highly Regioselective Mono and Double Sonogashira Cross-Coupling Reactions of 5-Substituted-1,2,3-Triodobenzene Under Ambient Conditions
10 ⁴⁰ -11 ⁰⁰	03 Abdussalam Qaroush <i>The University of Jordan, Jordan</i> New Pathways for CO ₂ Sequestration/Utilization from a Green Perspective	07 Amin Thawabteh <i>Birzeit University, Palestine</i> Masking the Bitter Taste of Guaifenesin-Design, Synthesis, Characterization and in vitro Kinetics-Prodrug Approach
11 ⁰⁰ -11 ²⁰	04 Hana Alhanash <i>Advanced Libyan Centre for Chemical Analysis, Libya</i> Green Synthesis and Characterisation of Zinc Oxide Nanoparticles using Olea Europaea and Citrus Aurantifolia Aqueous Leaf Extracts	08 Feda'a Al-Qaisi <i>The Hashemite University, Jordan</i> CO ₂ Utilization using Biorenewable Zinc Catalysts
11 ²⁰ -12 ⁰⁰	Coffee Break & Poster Session	
	Session 3 @ Ground Floor Theatre	Session 4 @ 1st Floor Theatre
	Moderators Prof. Amjad El-Sheikh (HU) & Dr. Mohammad Amer (UJ)	Moderators Prof. Fadwa Odeh (UJ) & Dr. Khaleel Assaf (BAU)
12 ⁰⁰ -12 ²⁰	09 Khaldun Al Azzam <i>Al-Ahliyya Amman University, Jordan</i> A Novel and Simple Dynamic Coating Capillary Electrophoresis Method for the Chiral Separation and Quantification of Mitiglinide Enantiomers using Hydroxyethyl Cellulose as a Dynamic Coating Agent	015 Lubna Tahtamouni <i>The Hashemite University, Jordan</i> Synthesis, Molecular Docking Studies, and in Vitro Anti-Tumor Effects of Novel Compounds Targeting EGFR and VEGFR
12 ²⁰ -12 ⁴⁰	010 Jafar Abdelghani <i>The Hashemite University, Jordan</i> Magnetic Solid Phase Extraction of Phthalate Products from Bottled, Injectable and Tap Waters using Graphene Oxide: Effect of Oxidation Method of Graphene	016 Lina Dahabiyeh <i>The University of Jordan, Jordan</i> Mass Spectrometry-Based Metabolomics Approach for Biomarker and Therapeutic Target Discovery: Examples from Parkinson's Disease and Colorectal Cancer
12 ⁴⁰ -13 ⁰⁰	011 Hiba Al Amayreh <i>Al-Balqa Applied University, Jordan</i> The Recovery of Vanadium Pentoxide from Spent Catalyst Utilized in Sulfuric acid Production Plant in Jordan	017 Frezah Muhana <i>Al-Ahliyya Amman University, Jordan</i> Mebendazole Loaded Nanoparticles for Lung Cancer Therapy



13 ⁰⁰ -13 ²⁰	O12 Mohammed Meetani <i>UAE University, UAE</i> Analysis of Synthetic Cathinones in Plasma and Urine using NCI GC-MS/MS	O18 Rawan Khalaf <i>An-Najah National University, Palestine</i> Design of Patchy DNA Particles by Colloidal Stamping
13 ²⁰ -13 ⁴⁰	O13 Hanan Alchaghouri <i>Damascus University, Syria</i> Can Solution Phase Synthesized Ultrafine Ferromagnetic Ni/NiO Nanocrystals with Strong Exchange Bias?	O19 Amneh Shtaiwi <i>Middle East University, Jordan</i> Kinetic, Thermodynamic and Modeling Studies of Spiroquinazoline Derivatives as Potential Acetylcholinesterase (AChE) Inhibitors for Alzheimer's Disease
13 ⁴⁰ -14 ⁰⁰	O14 Lamia Mamoly <i>Damascus University, Syria</i> Reduction of Oxalic Acid to Glyoxylic Acid Electrochemically Using a Selective Non-Crosslinked Sulfonated Polystyrene Membrane	O20 Mansour Nawasreh <i>Al-Balqa Applied University, Jordan</i> Efficient and Green Desymmetrization Methods toward anti-Cancer Cephalostatin Analogues
14 ⁰⁰ -15 ⁰⁰	<i>Lunch @ Employee Club Hall, Deanship of Student Affairs Building</i>	
	Session 5 @ Ground Floor Theatre	Session 6 @ 1st Floor Theatre
	Moderators Prof. Bader Salameh (HU) & Prof. Ayman Hammoudeh (YU)	Moderators Prof. Raed Ghanem (AABU) & Dr. Feda'a Al-Qaisi (HU)
15 ⁰⁰ -15 ²⁰	O21 Mousa Al-Smadi <i>Jordan University of Science and Technology, Jordan</i> Multiple 1,2,3-Thiadiazole Aromatic Derivatives: Synthesis, Characterization and Gas-Phase Pyrolysis	O25 Khaleel Assaf <i>Al-Balqa Applied University, Jordan</i> The Supramolecular Chemistry of Boron Clusters
15 ²⁰ -15 ⁴⁰	O22 Fuad Al-Rimawi <i>Al-Quds University, Palestine</i> Low Density Polyethylene/Zinc Peroxide Composite and Nanocomposite Prepared by Cast Solution: Thermal, Mechanical and Morphological Characterization	O26 Faisal Mustafa <i>Eastern Mediterranean University, Turkey</i> Mg-doped Mixed Metal Ferrite for Remediation of Trichlorophenol and Bacteria Strains: Experimental and Computational Mechanism Approach
15 ⁴⁰ -16 ⁰⁰	O23 Bassem Al-Maythaly <i>Royal Scientific Society, Jordan</i> Three-Ring Motifs in Zeolite Imidazole Frameworks for Enhanced Properties and Applications	O27 Osama Abuhasan <i>The Hashemite University, Jordan</i> Molecular Recognition of Amino Acids and Peptides by Cucurbit[8]uril. A Computational Study
16 ⁰⁰ -16 ²⁰	O24 Ayat Bozeya <i>Jordan University of Science and Technology, Jordan</i> UHMWPE/MWCNTs Nanocomposite Prepared by Wet Ball Milling and Hot Press	
16 ²⁰ -16 ⁴⁰	<i>Poster Session</i>	
	Closing Session @ Ground Floor Theatre	
16 ⁴⁰ -17 ⁰⁰	1. Announcing Poster Award Recipients 2. Presenting Shields to Keynote Speakers 3. Group Photo	

Chemical Structure-Property Relationships in Surfactant Monolayers

Matthew F. Paige

University of Saskatchewan, Saskatoon, Canada

Email: matthew.paige@usask.ca

Surfactant monolayers have been studied for over a century, with pioneering work in this field described by Langmuir and Blodgett culminating in the Nobel Prize in Chemistry in 1932 [1]. Despite this being a mature field of research, there is still an enormous amount of activity and interest in surfactant monolayers, both for applied film fabrication, for biological and nanomaterials science research as well as for probing fundamental properties of matter.

My research program explores the relationship between chemical structures of small-molecule surfactants and the resulting physical-chemical properties of the monolayers that form at both the air-water and solid-air interfaces. In this seminar, I will discuss several different systems in which intriguing chemical effects have been discovered, including phase-separated mixed hydrocarbon-perfluorocarbon monolayers [2], excited-state energy transfer in polydiacetylene-based films [3] and efficient metal chelation at the air-water interface. I will also discuss recent discoveries with a new class of synthetic gemini (dimeric) surfactants, referred to as a “gemini with a minimal-length spacer” [4], in which we observe dramatic differences in monolayer behaviour with very small changes in molecular structure; latest results indicate these molecules can act like a fatty acid, a phospholipid or an amorphous liquid-former with only minimal changes in molecular structure of the surfactant. I will also discuss future applications and directions of the field if time allows.

[1] <https://www.nobelprize.org/prizes/chemistry/1932/langmuir/facts/>

[2] Yan, C; Paige, M.F. Pattern Formation in Phase-Separated Langmuir and Langmuir Monolayer Films, *Langmuir*, **2021**, 37, 28, 8357-8369.

[3] Yeboah, A; Sowah-Kuma, D; Bu, W; Paige, M.F. Single-Molecule Fluorescence Spectroscopy of Phase-Separated 10, 12-Pentacosadiynoic Acid Films, *J. Phys. Chem. B*, **2021**, 125, 15, 3953-3962.

[4] Singh, S; Yeboah, A; Bu, W; Sun, P; Paige, M.C. Physicochemical Properties of Monolayers of a Gemini Surfactant with a Minimal-length Spacer, *Langmuir*, **2022**, 38, 51, 16004-16013.

Catalysis for the Circular Economy: Upcycling of Polyethylene to Surfactant-Range Alkylaromatics

Mahdi M. Abu-Omar

University of California Santa Barbara (UCSB), Santa Barbara, United States

Email: mabuomar@ucsb.edu

Dealing with the global plastic waste problem will require new and more effective waste management strategies. Conversion of waste polyolefins to commodity chemicals could divert plastic waste from landfills and incinerators, replace fossil feedstocks, and incentivize recycling. Strong Brønsted acid sites and Pt nanoparticles, present together in a bifunctional catalyst, efficiently convert polyethylene to surfactant-range aromatic chemicals with quantitative and predictive relationships between rates and acidity. This finding enhances the viability of chemical upcycling as an alternative to mechanical recycling. In this presentation, the UCSB process for making alkylaromatics from waste polyethylene using bifunctional catalysts and its mechanistic features will be discussed.

Taking Advantage of the Analytical Footprint of Comprehensive 2D Gas Chromatography

Philip J. Marriott

Monash University, Clayton, Australia

Email: philip.marriott@monash.edu

The high resolution afforded by multidimensional GC (MDGC) and comprehensive 2D GC (GC×GC) techniques is a paradigm shift in capabilities for volatile chemical analysis. Although we might be comfortable with our use of 1DGC, which has an extremely broad acceptance and utility across all manner of applications, we must be aware of the advantages that new operating modes offer.

The basic premise of the dual-separation column method – implemented by use of unique ‘modulation’ technologies – is that we achieve much greater overall separation, by virtue of the significant expansion of peak capacity, combined with independent elution of analytes on the two separation stages. With GC×GC we can summarise the advantages as:

One. Profile the total sample. This hallmark of ‘super-high resolution’ GC×GC means we see everything in a sample.

Two. Have a better-informed GC–MS method. Knowing potential interferences improves our understanding of GC–MS. Now pure mass spectra can be assured, that improves MS searching.

Three. Potentially reduce reliance on MS, with FID sufficing in many cases. It is all about separation!

Four. Remove ‘chemical noise’ and improve sensitivity for a true trace analysis method. Hence much lower abundance analytes can be reliably measured.

Five. Use the GC×GC picture to ‘tell a thousand words’ for facile sample-to-sample comparison and ‘chemical discovery’!

Six. Base decisions on the best method to be used for subsequent analyses for given sample types – the ‘Unilever strategy’.

Seven. Assess flavour and aroma using GC×GC and MDGC with FID/O/MS.

Best separation is fundamental to chemical measurement of volatile chemical compound applications. We have recently posed the question: “If you are not using GC×GC, you will not know what you are missing”.

CO₂-Switchable Materials for Separations

Philip G. Jessop

Queen's University, Kingston, Canada

Email: jessop@queensu.ca

Stimuli-responsive materials can switch back and forth between two forms, upon application or removal of a trigger. This flexibility makes it possible to reduce energy and materials consumption in industrial processes. While it's now well known that CO₂ can act as an inexpensive trigger for stimuli-responsive materials,¹ the extent of the utility of this concept is only now being realized. CO₂-switchable materials have applications in catalysis,² adhesives, particle formation, paints, and many other products and processes. This presentation will focus on new ways in which CO₂-switchable materials can contribute to industrial separations and potentially lower their economic and environmental costs. Example separations may include:

- industrial scale recovery of fresh water from highly polluted wastewater,
- isolation of organic products from fermentation broths,³
- removal of trace organic pollutants from water,
- extraction of organic products from biomass,⁴
- separation of components of mixtures for recycling⁵ (e.g., motor oil, plastics, waste Li batteries, etc.), and

If time permits, other recent discoveries will also be described, including switchable homogeneous and heterogeneous catalysts and new coatings.

Keywords: carbon dioxide, separations, stimuli-responsive materials, green chemistry

[1] Jessop, P. G.; Cunningham, M. F., *CO₂-Switchable Materials: Solvents, Surfactants, Solutes and Solids*, Royal Society of Chemistry, Cambridge, UK, 2021.

[2] Bordet, A.; El Sayed, S.; Sanger, M.; Boniface, K. J.; Kalsi, D.; Luska, K. L.; Jessop, P. G.; Leitner, W. *Nature Chemistry*, **2021**, 13, 916-922.

[3] Cunha, I. T.; Yang, H.; Jessop, P. G., *Green Chemistry*, **2021**, 21, 3996-4007.

[4] Sapone, V.; Iannone, A.; Alivernini, A.; Cicci, A.; Jessop, P. G.; Bravi, M., *Sep. Purif. Technol.*, **2023**, 308, 122843.

[5] Cunha, I. T.; McKeeman, M.; Ramezani, M.; Hayashi-Mehedy, K.; Lloyd-Smith, A.; Bravi, M.; Jessop, P. G.; *Green Chemistry*, **2022**, 24, 3704-371.

The Global Greenchem Innovation and Network Inclusion Programme

Omar AlSaleh

Royal Scientific Society, Amman, Jordan

Email: omar.alsaleh@rss.jo

The Royal Scientific Society (RSS) had the honor and pleasure to be the technical executer and main facilitator of This Major National project funded by the Global Environment facility (GEF), titled: “The Global Greenchem Innovation and Network Programme”. The project is implemented by Yale university and executed by UNIDO in partnership with Jordan’s National Cleaner Production Center (NCPC)/Environmental Studies Department (ESD) at the Water & Environment Center (WEC/RSS).

The Green Chemistry Programme focuses on the inherent properties of chemicals to ensure they are benign and beneficial throughout their life cycles. Its purpose is not simply to reduce pollution at the source by eliminating the hazards of chemical feedstock, reagents, solvents, and products, but also to ensure that the broad spectrum of sustainability concerns is built into the design framework through innovation and invention.

The project concept is set as a complete national package encompassing: capacity building and networking (with national, regional and international experts), nurturing green entrepreneurs & researchers, nourishing and excelling the universities curricula by integrating the great insights of Green chemistry principles and its practice towards green economy, enhance and incentivize the industrial market to go green via piloting of Green Chemistry alternatives/solutions to reduce & potentially eliminate POPs, and last but not least complying with the decisions concluded at the Stockholm convention binding Jordan to its commitment of reducing and eliminating the Persistent Organic Pollutants (POPs).

A huge take-away will be excelling professional standards through capacity building and optimize sustainable production performance without compromising the financial or environmental aspect.

This Major national project serves both the Jordanian industries and society via innovation and by enhancing pollution prevention, reducing adverse environmental and health impacts, and capitalizing on the available resources for the betterment of the economy A full incentive-based project driving towards sustainability and circular green economy. RSS commitments towards sustainability will be further translated into the collective and integrated national approach that will be adopted throughout the project timeline and beyond. Jordan's tremendous capacity and resources will be vital to the success of this project nationally and regionally. Jordan and RSS in specific will benefit from this project for 6 years to go.

Together towards safer green planet.

Environmentally Adaptive MOF-based Atmospheric Water Harvesting

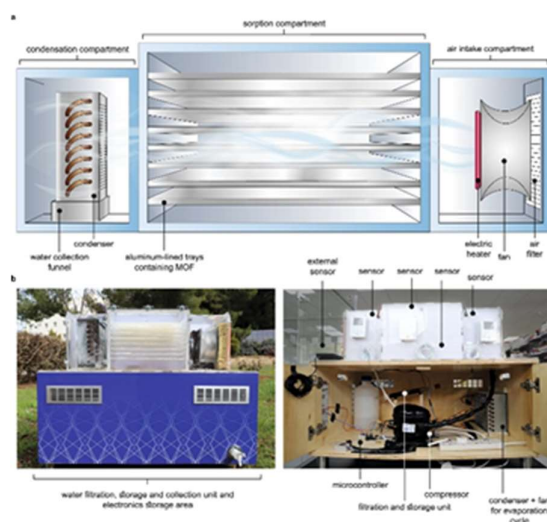
Hussam Almassad & Kyle Cordova

Royal Scientific Society, Amman, Jordan

Presenting author email: husam.massad@rss.jo

The process of water vapor harvesting from dry atmospheric air using MOFs is dependent on environmental climate conditions (i.e., temperature and humidity), which are continuously changing during a given day, week, month, and year. Reported MOF-based water harvesters are not able to adjust their water harvesting cycle (adsorption-desorption cycle) in real-time to these environmental condition fluctuations, which adversely affects water production and energy consumption and, therefore, lowers the efficiency of the water harvesting process.

In this presentation, I will detail our discovery of a MOF-based water harvesting device that functions via a new operational mode of water harvesting that we term ‘adaptive water harvesting’. The adaptive water harvester was proven to adapt its water harvesting cycle based on real-time environmental condition fluctuations to continuously optimize the water harvesting efficiency using temperature and relative humidity sensors located around the device. The optimization process results in a 169% increment in water production ($3.5 \text{ L}_{\text{H}_2\text{O}} \text{ kg}_{\text{MOF}}^{-1} \text{ d}^{-1}$), when compared to the best-performing, reported active device ($0.7\text{--}1.3 \text{ L}_{\text{H}_2\text{O}} \text{ kg}_{\text{MOF}}^{-1} \text{ d}^{-1}$) in an arid environment ($< 32\%$ relative humidity), a lower power consumption ($1.67\text{--}5.25 \text{ kWh L}_{\text{H}_2\text{O}}^{-1}$), and can perform 1.5 cycles more than the counterpart active device ^[1]. The daily production of 3.5 L of clean drinkable water tested based on the national drinking water standards is enough for human daily consumption.



Keywords: MOFs, water harvesting, water.

Almassad, H.A.; Abaza, R.I.; Siwwan, L.; Al-Maythaly, B. and Cordova, K.E., Environmentally adaptive MOF-based device enables continuous self-optimizing atmospheric water harvesting, **2022**, *Nature communications*, 13(1), p.4873

Green Hydrogen Production and Consumption: State of the Art and Perspectives

Youssef Naimi & Hassan Mabrak

Hassan II University of Casablanca, Casablanca, Morocco

Presenting author email: youssef.naimi@univh2c.ma; youssefnaimi@outlook.com

Global energy demand that is still growing as well as environmental problems due to greenhouse gas emissions taking combustion of fossil energy sources has propelled research and development of new renewable energy technologies. In this context, hydrogen could be an alternative carrier of energy to store and transport renewable energies. Green hydrogen, therefore, emerges as a massive energy support and an economic growth engine. Indeed, hydrogen is used as fuel in Fuel cell systems to produce. Thus, the transition to hydrogen energy can help to solve the problems of greenhouse gas emissions, cushion global warming and tensions over the supply and price of fossil fuels. The production of solar hydrogen via the thermochemical cycle in two stages with water is an attractive and completely durable "green" process [1]. Hydrogen can also be produced and consumed in situ in a system of microbial fuel cells (MFC) which converts spontaneously biomass to electricity through the metabolism of bacteria [2]. Consequently, decision-makers, energy analysts, industry leaders, and public opinion are persuaded that hydrogen is the fuel for the future. The technologies of hydrogen production are varied such as natural gas reform, carbon, and biomass gasification, water splitting via electrolysis [3], and high-temperature decomposition. These processes need improvements in their performance (efficiency, price, dependability, liveness, security). Hydrogen has a high energy density (a higher calorific value of 40Wh/g), but it is very difficult to store and transport it in the gaseous state. The development of the hydrogen economy will pass necessarily through the development of transport via pipelines for the gas form and the equipment of distribution stations. Hydrogen can also be transported in tanks on trailers (compressed gases, liquefied hydrogen, metal hydrides, etc.). The chemical energy of hydrogen (along with oxygen) can be converted to direct current electricity by powering a fuel cell system with hydrogen on the anode side and oxygen (air) on the anode side. The efficiency of the electrochemical reactions taking place at the electrodes, the management of the flows of the gases introduced and of the outgoing products (water and nitrogen in the case of air), and the heat produced are parameters to be improved. Furthermore, the development of a hydrogen economy requires the involvement of governments through the adoption of encouraging policies by granting aid or tax reductions that will facilitate the emergence of this sector.

Keywords: green hydrogen, renewable energies, electrolyzers, fuel cells.

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- [1] Lan Xiao, Shuang-Ying Wu, You-Rong Li, Advances in solar hydrogen production via two-step water-splitting thermochemical cycles based on metal redox reactions, *Renewable Energy*, Vol. 41, **2012**, Pages 1-12, ISSN 0960-1481, <https://doi.org/10.1016/j.renene.2011.11.023>.
 [2] S. Elmazouzi, Y. Naimi and I. Zerdani, "Microbial Fuel Cells for Depollution of Stagnant Water and Production of Electrical Energy", 11th International Conference on Renewable Energy Research and Application (ICRERA), Istanbul, Turkey, **2022**, pp. 441-445, doi: 10.1109/ICRERA55966.2022.9922813
 [3] Naimi Y. & Antar A., Hydrogen Generation by Water Electrolysis, *Advances in Hydrogen Generation Technologies*, **2018**, InTech, UK

New Pathways for CO₂ Sequestration/Utilization from a Green Perspective

Abdussalam K. Qaroush^a, Ala'a F. Eftaiha^b, Feda'a M. Al-Qaisi^b, Khaleel I. Assaf^c & Suhad B. Hammad^a

a) The University of Jordan, Amman, Jordan; b) The Hashemite University, Zarqa, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan

Presenting author email: a.qaroush@ju.edu.jo

The mitigation of CO₂ via carbon capture and sequestration, utilization, recycling, and direct air capture is considered as a plausible means to reduce the severe impacts of global warming and its enormous effects over the inhabitants of the planet. Herein, we have introduced several eco-friendly approaches for the synthesis and utilization of green materials for CO₂ the titled purposes. These methods offer collaborative solutions towards addressing the challenges associated with CO₂ emissions.

Since the early days of using scrubbing agents, like monoethanolamine, and its well-known associated problems, *e.g.*, degradation, evaporation losses, cross linking, it kept us motivated to address these issues. As a success story, [n]-oligoureas-based sorbents (dry scrubbing) have served as a primary model to ultimately optimize effective sorbents.^[1–5] Our research is focused on optimization and understanding the basic principles that made us comprehend CO₂ chemistry upon dealing with new phenomena and exploring mechanistic approaches to verify the catalysts activity relationship.

In this context, we have reported on the synthesis and exploiting of several families of monomeric, oligomeric, or polymeric catalysts that can incorporate CO₂ into cyclic carbonates under ambient conditions. Currently, new generation and models are still in the pipeline of R&D searching for materials that can effectively sequester and utilize CO₂, paving the way into a new type of task-specific materials.

Keywords: CO₂ mitigation, global warming, catalysis, new bonds.

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- [1] Qaroush, A. K.; Castillo-Molina, D. A.; Troll, C.; Abu-Daibes, M. A.; Alsyouri, H. M.; Abu-Surrah, A. S.; Rieger, B. *ChemSusChem* **2015**, *8*, 1618–1626.
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Green Synthesis and Characterisation of Zinc Oxide Nanoparticles using Olea Europaea and Citrus Aurantifolia Aqueous Leaf Extracts

H. B. Alhanash ^a, F. B. Alhanash ^b, S. Adela ^c & K. Algazla ^c

a) Advanced Libyan Centre for Chemical Analysis, Libya; b) Industrial Research Centre, Libya; c) Libyan Authority for Scientific Research, Libya

Presenting author E-mail: hanahanash@aal.ly

In this study, green synthesis of zinc oxide nanoparticles (ZnO NPs) was implemented using aqueous leaf extract of *Olea europaea* and *Citrus aurantifolia* as reducing agents. The use of different parts of the plants is novel, leading to true green chemistry with no need for toxic chemicals. The characterization using XRD, SEM, FTIR and UV-vis spectrophotometer reveals the preparation of ZnO NPs. The mean size of ZnO nanoparticle synthesized from *olea eurpaea* was approximately 17.9402nm whilst that of the citrus 22.383. Further, the SEM images of zinc nanoparticles show a porous structure. Further, zinc oxide nanoparticles were evaluated for free radical scavenging activity by capacity of total antioxidant assay.

Keywords: green synthesis, zinc oxide nanoparticles, *Olea europaea*, *citrus aurantifolia*, characterization.

Synthesis, Characterization, and Luminescence Properties of Rare Earth Doped BaGd-Silicate Phosphors for Solid-State Lighting Applications

Abdulla Abu-Qartuma, Joman AlDhirat, Yaser Yousef & Ayman Hammoudeh

Yarmouk University, Irbid, Jordan

Presenting author email: ayman@yu.edu.jo

High-efficiency, cheap, durable, environmentally friendly white light sources with high thermal and chromatic stability are required to minimize global electricity consumption. This work is a contribution to the search for new white light-emitting phosphors. It investigates the incorporation of Dy^{3+} and Sm^{3+} into a BaGd-silicate (BGSO) host material at various doping levels (0.5–7% of Gd^{3+}). System preparation was undertaken by a sol-gel method, followed by thermal treatment at 1200–1350 °C. X-ray diffraction revealed that the host material consists of three silicate phases: $\text{BaGd}_2\text{Si}_3\text{O}_{10}$, $\text{Ba}_2\text{Gd}_2\text{Si}_4\text{O}_{13}$ and $\text{Gd}_{4.67}\text{Si}_3\text{O}_{13}$. Under excitation at 275 nm, four bands rise in the case of Sm^{3+} -doped systems (green-yellow at 545-580 nm, orange at 585-625 nm, orange-reddish at 630-680 nm, and red at 695-745 nm), while in the case of doping with Dy^{3+} , three bands appear (blue at 460-505 nm, yellow at 555-610, and red at 640-695 nm). In both series, maximum intensity was obtained at a doping level of 0.5%. At higher doping levels, the intensity decreased with increased dopant concentrations because of the so-called concentration quenching resulting from the electric dipole-dipole interaction between the dopant ions. Regarding eye perception, the BGSO:0.5% Sm^{3+} yielded an almost monochromatic orange light just below 600 nm with a correlated colour temperature of 1300 K, while BGSO:0.5 Dy^{3+} resulted in yellowish emission and is thus promising to produce warm white light.

Keywords: LED, white light-emitting LED, phosphors, photoluminescence, rare earth metals, host material, barium gadolinium silicate.

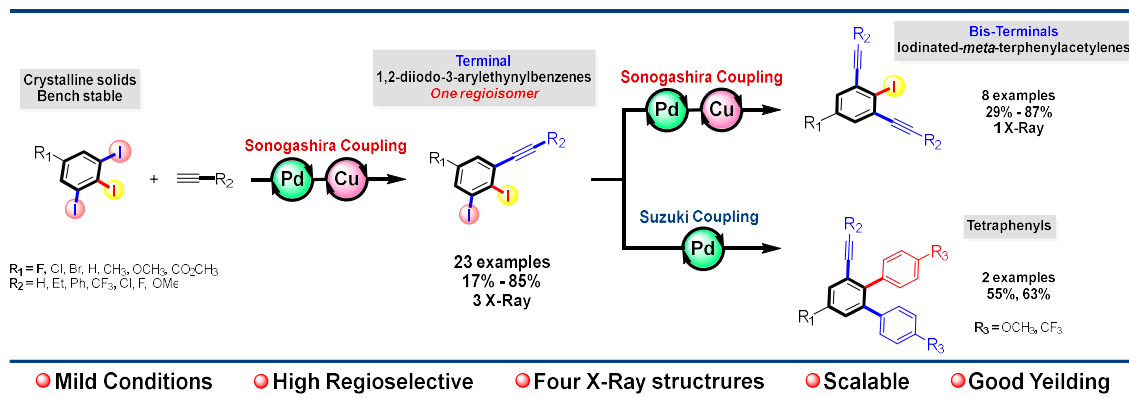
Palladium-Catalyzed Highly Regioselective Mono and Double Sonogashira Cross-Coupling Reactions of 5-Substituted-1,2,3-Triiodobenzene Under Ambient Conditions†

Mothana K. Al-Omari ^a, Raed M. Al-Zoubi ^a, Walid K. Al-Jammal ^a & Michael J. Ferguson ^b

a) Jordan University of Science and Technology, Irbid, Jordan; b) University of Alberta, Edmonton, Canada

Presenting author email: mkalomari16@sci.just.edu.jo

An efficient synthesis of 2,3-diiodinated diphenylacetylene and iodinated *meta*-terphenylacetylene derivatives through highly regioselective mono and double Sonogashira cross-coupling reactions of 5-substituted-1,2,3-triiodobenzene is reported. Significantly, the regioselectivity of coupling reactions is exclusively performed at the terminal C–I bonds, the less sterically hindered and the most regioactive positions. The highest isolated yields were achieved from reactions of electron-poor/neutral 1,2,3-triiodoarene and electron rich arylacetylene derivatives. The use of 2.0 equiv. of arylacetylenes in one pot fashion afforded the iodinated *meta*-terphenylacetylenes in excellent site selectivity and in good, isolated yields. Different functional groups were found to be suitable under optimized conditions. This report discloses the first method to synthesize hitherto unknown 2,3-diiodinated diphenylacetylenes and iodinated *meta*-terphenylacetylenes that is facile, highly regioselective, general in scope and produces remarkable building blocks for other chemical transformations.



Keywords: organic chemistry, catalytic coupling, synthetic methodology.

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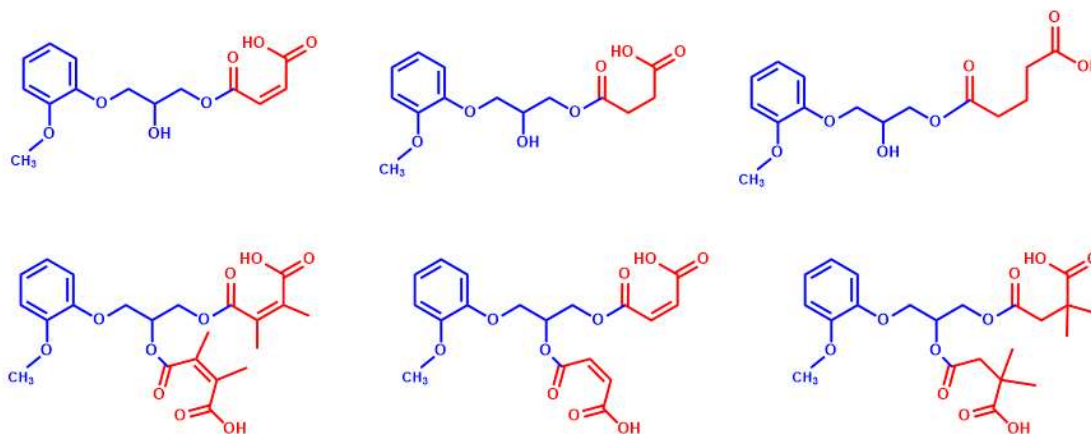
Masking the Bitter Taste of Guaifenesin-Design, Synthesis, Characterization and in vitro Kinetics-Prodrug Approach

Amin Mahmood Thawabteh ^a & Rafik Karaman ^b

a) Birzeit University, Ramallah, Palestine; b) Al-Quds University, Jerusalem, Palestine

Presenting author email: athawabtah@birzeit.edu

A respected number of drugs suffer from bitter taste which results in patient incompliance. With the aim of solving the bitterness of guaifenesin, dimethyl maleate, maleate, glutarate, succinate, and dimethyl succinate prodrugs were designed and synthesized. Molecular orbital methods were utilized for the design of the ester prodrugs. The density functional theory (DFT) calculations revealed that the hydrolysis efficiency of the synthesized prodrugs is significantly sensitive to the pattern of substitution on C=C bond and distance between the nucleophile and the electrophile. The hydrolysis of the prodrugs was largely affected by the pH of the medium. The experimental $t_{1/2}$ for the hydrolysis of guaifenesin dimaleate ester prodrugs in 1N HCl was the least and for guaifenesin dimethyl succinate was the highest. Functional heterologous expression of TAS2R14, a broadly tuned bitter taste receptor responding to guaifenesin, and experiments using these prodrugs revealed that, while some of the prodrugs still activated the receptor similarly or even stronger than the parent substance, succinate derivatization resulted in the complete loss of receptor responses. The predicted binding modes of guaifenesin and its prodrugs to the TAS2R14 homology model suggest that the decreased activity of the succinate derivatives may be caused by a clash with Phe247.



Keywords: bitter taste, prodrugs, guaifenesin, DFT calculations, acid-catalyzed ester hydrolysis, molecular modeling.

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CO₂ Utilization using Biorenewable Zinc Catalysts

Feda'a M. Al-Qaisi ^a, Abdussalam K. Qaroush ^b, Ala'a F. Eftaiha ^a & Khaleel I. Assaf ^c

a) The Hashemite University, Zarqa, Jordan; b) The University of Jordan, Amman, Jordan; c) Al-Balqa' Applied University, Al Salt, Jordan

Presenting author email: fedaam@hu.edu.jo

Global warming phenomenon is a result of increased greenhouse gases (GHGs) emissions, affecting humanity in a non-reversible fashion. One catastrophic effect locally, regionally, or even globally lies in rainwater scarcity, droughts, or even floods. To decrease the drastic effects of the phenomenon, several strategies can be used to mitigate those emissions such as "carbon capture and recycling", "sequestration" together with "utilization" (CCRSU). One important GHG contributing to the phenomenon is carbon dioxide, which is an abundant, renewable, C1-feedstock that might be implemented in value-added products such as cyclic urea, cyclic urethane and cyclic carbonates (CCs). The latter is of great interest for both academic and industrial sectors. They serve as green solvents with outstanding properties such as a high boiling point and low toxicity. From a green chemistry point of view, sustainable metals/materials would be exploited as catalysts which act as benign and efficient alternatives for CC production. In this context, and as an augmentation to the efforts of the scientific community to develop efficient sustainable catalysts for CO₂ utilization under ambient conditions, the Jordanian CO₂ Team (JCO₂T) have reported on CO₂ capturing and utilization using of modified biorenewables compounds based Zn^{II} catalysts such as ascorbic acid [1], curcumin [2], and adenine [3]. Furthermore, in this presentation, the mechanism of CO₂ capturing and its conversion into CC experimentally and theoretically under atmospheric CO₂ pressure will be presented.

Keywords: CO₂ utilization, cyclic carbonate, zinc catalyst.

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A Novel and Simple Dynamic Coating Capillary Electrophoresis Method for the Chiral Separation and Quantification of Mitiglinide Enantiomers using Hydroxyethyl Cellulose as a Dynamic Coating Agent

Khaldun M. Al Azzam

Al-Ahliyya Amman University, Amman, Jordan

Email: azzamkha@yahoo.com; k.azzam@ammanu.edu.jo

A capillary electrophoretic method for the chiral separation and quantification of mitiglinide (MTG) enantiomers is described (less than 9.5 min) with resolution value $R_s = 5.25$ and with excellent peak shapes after performing the dynamically coating for the bare fused capillary. The study aims to develop and validate a novel and simple method for the separation and quantification of MTG enantiomers using CE after dynamic coating the capillary wall using the hydroxyethyl cellulose (HEC) coating agent. Dynamic coating procedure of the capillary inner surface is conducted via rapid flushes using 0.1 M sodium hydroxide, water, and aqueous solution containing HEC, and hydroxypropyl- γ -cyclodextrin (HP- γ -CD). Besides buffer was used for the dynamic coating process in addition to its use as the separation medium. When the dynamic coating was used, peak symmetry was improved. A bare fused-silica capillary was used throughout the separation after being coated using HEC dissolved in the background electrolyte (BGE) of 50 mM Na_2HPO_4 – 1 M H_3PO_4 solution; pH 8.5; containing 25 mg mL^{-1} of each HP- γ -CD and HEC. The dynamic coating procedure achieved an improvement in migration time as well as peak area precision. The adsorbed coating agent showed slight interactions with MTG, providing efficient separation with outstanding durability and reproducibility at slightly alkaline conditions (pH 8.5). Acceptable validation criteria for selectivity, linearity, precision, and accuracy were also studied. The newly developed method was effectively applied to the assay of enantiomers of MTG in pharmaceutical formulations. Additionally, it was proven to have the advantages of being simple, rapid, and accurate.

Keywords: coating, hydroxyethyl cellulose, enantiomers, mitiglinide.

Magnetic Solid Phase Extraction of Phthalate Products from Bottled, Injectable and Tap Waters using Graphene Oxide: Effect of Oxidation Method of Graphene

Jafar I. Abdelghani, Rami Freehat & Amjad El-Sheikh

The Hashemite University, Zarqa, Jordan

Presenting author email: j.abdelghani@hu.edu.jo; jaf.chem@yahoo.com

Phthalate esters (PAEs) are considered as an endocrine disrupting chemical which cause harm on human and environment. Therefore, PAEs concentration should be determined and evaluated. In the present work, graphene (G) was oxidized with either nitric acid, ammonium persulfate or hummer method, to produce the corresponding graphene oxides (GO): GO-NA, GO-APS and GO-HUM, respectively. Magnetite was deposited on graphene and oxidized graphene to produce the magnetic sorbents: MG, MGO-NA, MGO-APS and MGO-HUM. These were used for optimization of simultaneous magnetic solid -phase extraction (MPSE) method of five phthalate products (DMP, DEP, BBP, DIBP, and DBP) from bottled, injectable and tap water. The highest recoveries were achieved using 40mg of MGO-APS at pH5, sample volume 50ml, elution with 5ml ethyl acetate, shaking time 45min, and elution time 15min. The following figures of merits were achieved: detection limits range (0.004-0.013 mg.L⁻¹), %RSD range(0.62-6.02)%, %bias range ((-16.6)-(-7.0))%, and sensitivity range (79-149)L⁻¹.mg. Application of the optimum MSPE on bottled, injectable, and tap water showed that DEP, BBP, DIBP, and DBP were present in bottled and injectable water. The adsorption tests of the phthalate ester were better fitting to Langmuir model with R² bounce between 0.9957-0.9997.

Keywords: graphene oxide; adsorption; phthalate; magnetic solid phase extraction.

The Recovery of Vanadium Pentoxide from Spent Catalyst Utilized in Sulfuric acid Production Plant in Jordan

Hiba Al Amayreh ^a, Aya Khalaf ^b, Majd I. Hawari ^c, Mohammed K Hourani ^d & Abeer Al Bawab ^d

a) Al-Balqa Applied University, Amman, Jordan; b) Al-Ahliyya Amman University, Amman, Jordan; c) Jordan Atomic Energy Commission, Jordan; d) The University of Jordan, Amman, Jordan

Presenting author email: hiba.alamayreh@bau.edu.jo

Vanadium is a significant metal, and its derivatives are widely employed in industry. One of the essential vanadium compounds is vanadium pentoxide (V_2O_5), which is mostly recovered from titanomagnetite, uranium-vanadium deposits and phosphate rocks, spent catalysts. A smart method for characterization and recovery of V_2O_5 was investigated and implemented as a benchtop small scale-model. Several nondestructive analytical techniques such as X-ray fluorescence (XRF), Inductively Coupled Plasma technique (ICP) and X-ray diffraction (XRD) have been used to determine the physical and chemical properties such as particle size and composition of the samples before and after the recovery process V_2O_5 . After sample preparation, several acid and alkali leaching techniques were investigated. Noncorrosive, environmentally friendly extraction method based on using less harmful acids was applied in batch and column experiments for extraction of V_2O_5 as vanadium-ions from spent vanadium catalyst. In batching experiments, different acids and bases were examined as leaching solutions agents; oxalic acid shows the best percent recovery for vanadium ion compared with the other acids used. The effects of contact time, acid concentration, and solid -to-liquid ratio, stirring rate, and temperature were studied to optimize the leaching conditions. Oxalic acid of 6% (w/w) to 1/10 solid-to-liquid ratio at 300 rpm and 50 °C were the optimal conditions for extraction (67.43 % recovery). On the other hand, the column experiment with a 150 cm long and 5 cm i.d. and 144 h. contact time using the same leaching reagent, 6% oxalic acid showed a 94.42% recovery. The results of the present work have indicated the possibility of recovery of vanadium pentoxide from the spent vanadium catalyst used in sulfuric acid industry in Jordan.



Keywords: vanadium pentoxide; leaching process; recovery of V_2O_5 ; recycling, extraction.

Analysis of Synthetic Cathinones in Plasma and Urine using NCI GC-MS/MS

**Mohammed A. Meetani^a, Rashed H Alremeithi^{a,b}, Anas A. Alaidros^a, Adnan Lengawi^b, Kalid Alsumaiti^b
& Jasim Alzaabi^{a,c}**

a) UAE University, Al-Ain, UAE; b) Dubai police, Dubai, UAE; c) Abu Dhabi police, Abu Dhabi, UAE

Presenting author email: mmeetani@uaeu.ac.ae

The latest version of new designer substances (NDS) is called “bath salts” and they spread in the drug abuse market. Bath salts are a group of central nervous system stimulants that consists mainly of synthetic cathinone derivatives. They are chiral substances that exist as a racemic mixture. Objectives: Development and validation of sensitive and selective method for enantioseparation and quantitation of synthetic cathinones “bath salts” has been done by using GC-MS and GC-MS/MS with chemical ionization source in negative mode (NCI). In addition, a comparison between two derivatizing agent is conducted. Methodology: Indirect chiral separation of thirty-six synthetic cathinone compounds has been conducted by using optically pure chiral derivatizing agent (CDA) called (S)-(-)-N-(trifluoroacetyl)pyrrolidine-2-carbonyl chloride (L-TPC) and Menthylchloroformate which converts cathinone enantiomers into diastereoisomers that can be separated on achiral GC-MS columns. Ultra inert 60 m column was used. Slow heating rate (2 °C/min) on the GC oven has resulted in an observed enhancement in enantiomer peak resolution. An internal standard, (+)-cathinone, was used for quantitation of synthetic cathinone. Conclusion & Significance: Method validation in terms of linearities, limits of detection (LOD), limits of quantitation (LOQ), recoveries and reproducibilities have been obtained for fourteen selected compounds that ran simultaneously as a mixture after being spiked in urine and plasma. Unlike the Electron Impact ion source (EI), NCI showed higher sensitivity by three orders of magnitude by comparing with the previous results. Moreover, signal intensity improvement observation after changing the CI reagent gas from methane to isobutane, argon or methane/ammonia (95:5) will be discussed.

Keywords: synthetic cathinones, chiral separation, derivatization, GC-MS/MS.

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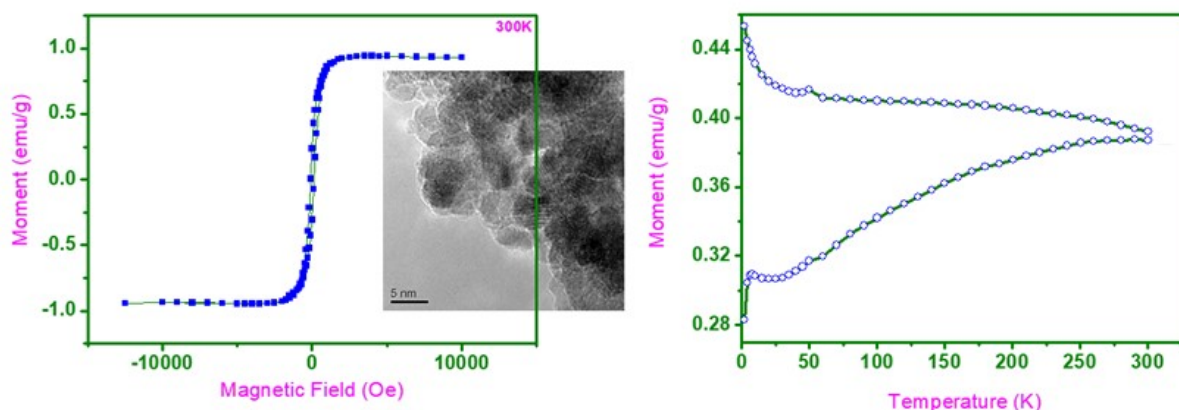
Can Solution Phase Synthesised Ultrafine Ferromagnetic Ni/NiO Nanocrystals with Strong Exchange Bias?

Hanan Alchaghouri^{a,b} & P. John Thomas^c

a) Damascus University, Damascus, Syria; b) The University of Manchester, Manchester, UK; c) Bangor University, Bangor, UK

Presenting author email: halchaghouri@gmail.com

It has been considerable interest in producing ultrafine particles in the last several years due to wide range of their potential applications, including magnetic recording media, ferrofluids, catalysts, medical diagnostics, drug-delivery system, and pigments in paints and ceramics. However, it remains challenging to devise solution phase routes to nanoparticles with strong exchange bias. Poor structural order and amorphous nature of the oxide shell are often thought to be responsible for weak or non-existent exchange bias. We have been able to identify a chemical route to Ni-NiO nanoparticles with a thin amorphous shell that appears to show strong exchange bias. Ni/NiO nanocrystals with size (5-7 nm) were synthesised by reducing nickel acetate with propanol and the seeds of Pd followed by controlled oxidation. Upon calcination, ferromagnetic particulates with freely dispersible in water and notable enhancement of moment were obtained. The effect of different deposition parameters on the size, structure and magnetic properties were studied. The structure of the nanocrystals was characterized by X-ray diffraction, scanning and transmission electron microscopy as well as energy-dispersive X-ray spectroscopy. We are in the process of carrying out detailed studies of these particulates and their films for some important applications. The talk will describe the structure, properties, and applications of these nanocrystals and their thin film.



Reduction of Oxalic Acid to Glyoxylic Acid Electrochemically Using a Selective Non-Crosslinked Sulfonated Polystyrene Membrane

Wael Bosnali, Mazhar Abdulwahed & Lamia Mamoly

Damascus University, Damascus, Syria

Presenting author email: dmamoly44@gmail.com

The electrochemical reduction of oxalic acid to glyoxylic acid has been studied using a selective membrane made of non-crosslinked sulfonated polystyrene in a cell equipped with lead cathode and lead dioxide anode. A chemical yield of $80.04\% \pm 2.34$ is obtained with $99.42\% \pm 4.87$ selectivity after 150 minutes of reaction under optimum conditions. Increased current density resulted in a significant improvement in conversion ratio and rate has been observed. It is found that the rate of the electrochemical transformation follows first order law with a rate constant of $4.76 \times 10^{-5} \text{ s}^{-1}$. The byproduct, glycolic acid, forms after more than 120 minutes in conjunction with decreasing selectivity of glyoxalic acid. Its formation is supported by current density and temperature. IR, EDX, and SEM techniques characterize the prepared film, it is assigned by degree of sulfonation, the ion exchange capacity, the water absorption ratio, the swelling ratio, and the ratio of water to sulfonic groups' molecules has been considered. The results indicate the success of sulfonation process, and it is found that the transport of the proton through the membrane in the form of hydronium. Prepared SPS membrane exhibited comparable performance to its analogue, the industrial Nafion117 membrane exhibits enduring product selectivity, while SPS membrane shows higher electrical yield due to a greater ion exchange capacity.

Keywords: oxalic acid, glyoxylic acid, glyoxalic acid, glycolic acid, electrochemical reduction, sulfonated polystyrene membrane, electro synthesis.

Synthesis, Molecular Docking Studies, and in Vitro Anti-Tumor Effects of Novel Compounds Targeting EGFR and VEGFR

Lubna Tahtamouni^{a,b} & Ammar A. Razzak Mahmood^c

a) The Hashemite University, Zarqa, Jordan; b) Colorado State University, Fort Collins, USA; c) University of Baghdad, Bagdad, Iraq

Presenting author email: lubnatahtamouni@hu.edu.jo; lubna.tahtamouni@colostate.edu

Cancer is the second leading cause of death in the world, and despite significant advances in cancer treatment, cancer drug resistance remains a major challenge. Chemotherapeutics that targets the EGFR and VEGFR-2 tyrosine kinase receptors, both of which are upregulated in solid tumors, are promising anti-tumor agents. Our research focuses on the development of novel biomolecules to target these receptors discovered through molecular docking studies. The docking results are validated in vitro, and the mechanism(s) by which these novel compounds induce apoptosis and cell cycle arrest are studied using cytotoxicity assays, qRT-PCR, immunoblotting, flow cytometry, and enzyme inhibition assays. Several biomolecules with potent anti-tumor activities that target either EGFR or VEGFR-2 have been successfully synthesized.

Keywords: cytotoxicity, apoptosis, tyrosine kinase, in silico.

Mass Spectrometry-Based Metabolomics Approach for Biomarker and Therapeutic Target Discovery: Examples from Parkinson's Disease and Colorectal Cancer

Lina A. Dahabiyeh

The University of Jordan, Amman, Jordan

Email: l.dahabiyeh@ju.edu.jo

Metabolomics is an advanced analytical approach that couples' state-of-the-art instruments, such as mass spectrometry (MS), with bioinformatics tools to identify unique biomarkers and obtain valuable insights into the underlying pathophysiological mechanisms of diseases and mechanisms of actions and/or toxicity of drug therapies. Herein, two different examples of the use of global MS-based metabolomics will be presented. The first one used metabolomics to identify potential diagnostic biomarkers and highlight promising therapeutic targets in the serum of patients with idiopathic Parkinson's disease (PD), while in the second metabolic profiling was used to evaluate the biochemical pathways altered in HCT116 cells upon exposure to dihydroquinazolin derivatives.

A total of 57 metabolites including cysteine-S-sulfate and N-acetyl tryptophan were significantly higher in patients with PD compared to controls. Xanthines, including caffeine and its downstream metabolites, were lower in PD patients relative to controls. Seven metabolites yielded a ROC curve with a high classification accuracy (AUC 0.977). Cysteine-S-sulfate levels were significantly increasing with the advancement of PD stages while LPI 20:4 was significantly decreasing with disease progression. For 2-(4-(Dimethylamino)phenyl)-2,3-dihydroquinazolin-4(1H)-one treated HCT116 cells, metabolomics revealed that the compound (IC₅₀ 1.4 µM against HCT116) induced significant perturbations in the level of several metabolites including spermine, polyamines, glutamine, creatine and carnitine, and altered biochemical processes essential for cell proliferation and progression such as amino acids biosynthesis and metabolism, redox homeostasis, energy-related processes (e.g., fatty acid oxidation, second Warburg like effect) and one-carbon metabolism.

The findings shed light on the promising role of metabolomics in identifying new therapeutic targets, discovering new biomarker candidates to assist in the diagnosis of PD and monitoring its progression and providing a better understanding of the pathways altered in treated cancer cells.

Keywords: mass spectrometry, metabolomics, parkinson's disease, quinazoline, biomarker.

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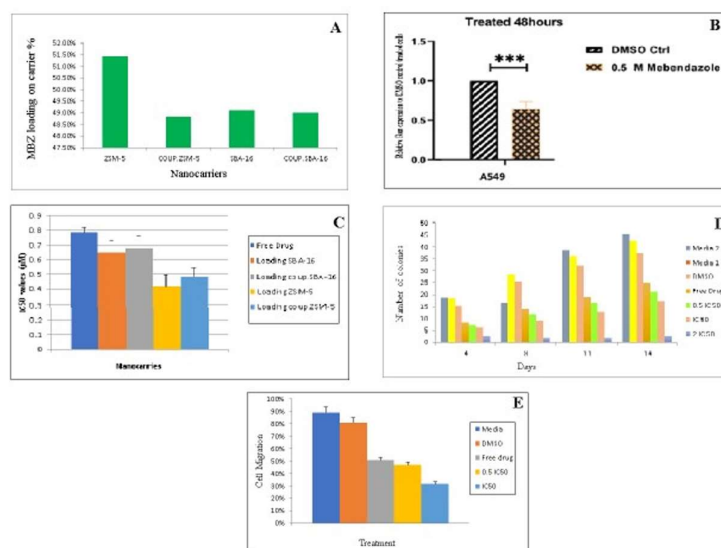
Mebendazole Loaded Nanoparticles for Lung Cancer Therapy

Frezah Muhana & Mohamed El-Tanani

Al-Ahliyya Amman University, Salt, Jordan

Presenting author email: F.muhana@ammanu.edu.jo

Lung cancer is the leading cause of cancer mortality. Lung cancers are classified into two types based on their microscopic appearance: small cell lung cancer (SCLC) and non-small cell lung cancer (NSCLC). Many individuals are first diagnosed at stage III or IV, when their prognosis is bleak. Non-small cell lung cancer is a lethal and incurable illness that can be treated with surgery, chemotherapy, radiation therapy, targeted therapy, or a combination of therapies. Targeted treatment focuses on particular abnormalities seen in cancer cells, such as the EGFR mutation. The T 790M mutation in the EGFR's tyrosine kinase domain causes acquired resistance to first-generation EGFR TKIs, mebendazole. As a result, combining diverse targeted therapeutic drugs not only improves treatment outcomes but can also be a more effective preventer of acquired resistance improvement. Loaded drug Nanoparticles ZSM-5 and SBA-16 were utilized as targeted treatment, and their stability and loading % were determined using multiple methods, including infrared, X-Ray Diffraction, TGA, and HPLC. The therapy was used in in-vitro cell culture investigations such as the MMT assay, colony assay, and migration assay. The results showed that the loaded drug nanoparticles had a lower IC50 than the free drug mebendazole we utilized, indicating that the nanoparticles improved therapy and reduced medication dosage.



Keywords: medication; mebendazole; anticancer; ZSM 5 nanoparticle; SBA 16 nanoparticle.

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Design of Patchy DNA Particles by Colloidal Stamping

Rawan Khalaf ^{a,b}, Rémi Mérimindol ^b, Etienne Ducrot ^b & Serge Ravaine ^b

a) An-Najah National University, Nablus, Palestine; b) Univ. Bordeaux, Pessac, France

Presenting author email: r.khalaf@najah.edu

For years scientists have been exploring the design of particles that can self-assemble into complex superstructures. Such colloidal assemblies can serve as photonic sensors or model systems to understand molecular processes [1]. Taking inspiration from atoms, where valence directs the assembly of well-defined molecules, we expect that anisotropic colloids that can interact directionally will broaden the diversity of colloidal assemblies accessible. This concept is known as patchy particles [2]. Unlike isotropic colloids which mostly yield compact assemblies, patchy particles can direct the formation of new architectures controlled by the physical and chemical interactions between their patches. Several studies validated this concept showing that patchy particles yield new colloidal assemblies [3]. Despite considerable work on the synthesis of patchy colloids, the rational design of particles with multiple addressable patches remains elusive.

We present here a new route to design complex particles with multiple addressable patches, using DNA coated colloids and strand displacement reaction [4]. The synthesis of colloidal particles and their grafting using different single-stranded DNA sequences will be first presented. We will then describe their subsequent functionalization using fluorescent oligomers and their assembly using DNA linkers complementary to the grafted DNA sequences (Fig. 1 A, B). The key process relies on strand displacement reactions to transfer information only at the contact point between two particles. Strand displacement reaction consists in the replacement of one strand of a duplex by an “eject” strand of higher stability at room temperature. This process is highly specific and can be programmed independently to create multiple addressable patches. Proof-of-concept experiments showing the formation of particles with one patch (Fig. 1 C) as well as dissimilar patches will be described (Fig.1 D). These results open the way to the synthesis of custom patchy particles in bulk [5].

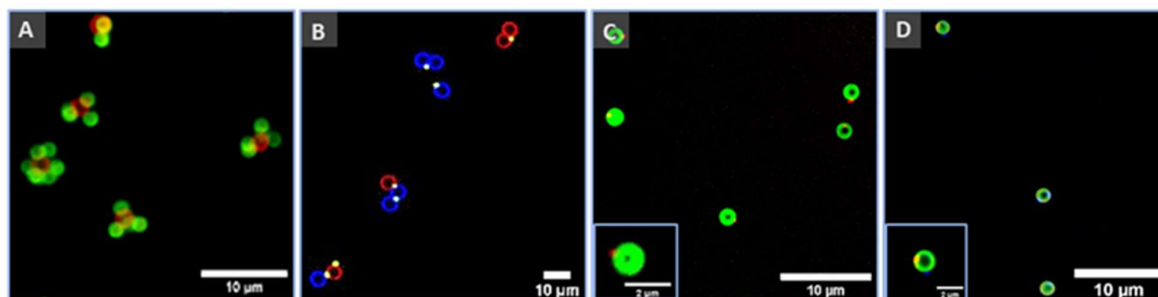


Figure 1. Confocal fluorescence microscopy images of clusters of (A) two and (B) three types of DNA-coated particles and of the obtained particles with (C) one patch and (D) two patches after strand displacement.

Keywords: DNA, programmable assembly, stamping, patchy.

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Kinetic, Thermodynamic and Modeling Studies of Spiroquinazoline Derivatives as Potential Acetylcholinesterase (AChE) Inhibitors for Alzheimer's Disease

Amneh Shtaiwi

Middle East University, Amman, Jordan

Email: ashtaiwi@meu.edu.jo

Acetylcholinesterase (AChE) plays an essential role in the hydrolysis of the neurotransmitter acetylcholine (ACh). Indeed, the rapid degradation of ACh by AChE lowered its concentration levels in the brain, which is responsible for Alzheimer's disease (AD). Hence, AChE has been studied as a promising drug target. The present study combines binding kinetics experimental using surface plasmon resonance (SPR), isothermal titration calorimetry (ITC), and in silico approach to evaluate the molecular interactions of spiroquinazolines with AChE. Residence times results (τ) of the physical approach SPR assays confirmed the potential binding of spiroquinazoline inhibitors with the AChE target, with compound 3d showing a residence time of 4.52 minutes which was comparable with the original drug galanthamine (GNT). In addition, isothermal titration calorimetry (ITC) measurements showed good binding interaction of the compounds with the active site of AChE, with compounds 2b and 3d showing average free energies of -10.09 and -10.93 , respectively. The analysis of the long-scale 9- μ s MD simulations of the two spiroquinazolinone derivatives (2a-2d and 3a-3d) and GNT demonstrates stable interactions, and the complexes undergo low conformational fluctuations. Furthermore, the flexibility and conformational change analysis based on the RMSD, Rg, RMSF, torsion profiles, and principal component analysis revealed stable interactions with fewer conformational fluctuations for 2b and 3d ligand-binding interactions. Finally, the identified spiroquinazoline compounds might be worth exploring in the evolution of promising compounds such as AChE inhibitors for Alzheimer's disease.

Keywords: molecular interactions, thermodynamics, residence times, MD simulations.

Efficient and Green Desymmetrization Methods toward anti-Cancer Cephalostatin Analogues

Mansour Nawasreh ^a & Lubna Tahtamouni ^{b,c}

a) Al-Balqa Applied University, Amman, Jordan; b) The Hashemite University, Zarqa, Jordan; c) Colorado State University, Fort Collins, Colorado, USA

Presenting author email: nawasreh@bau.edu.jo

The discovery of cephalostatins (*e.g.*, cephalostatin **1**, Fig. **1**), which have shown remarkable activity against human cancer cells, attracted us as some groups abroad to target the synthesis of such impressive and complicated molecules. In this review, we summarize the progress in desymmetrization of symmetrical bis-steroidal pyrazines (BSPs) (*e.g.*, diketone **2**, Fig. **2**). This will be an approach toward potentially active anti-cancer agents, namely cephalostatins/ ritterazines. Synthesizing a gram-scaled prodrug with potential activity using green methods is our primary target. Scaling up of these methods based on the symmetrical coupling (SC) of two identical steroidal units. The discovery of new green pathways that help in structural reconstruction programming toward the total synthesis of at least one potentially active family member is our secondary target. Our strategy is based on functional group interconversions with high flexibility and brevity using green selective methods. The backbone of our work is based on introducing controlling groups using nontrivial reconstruction methodologies. The resulting analogues after certain modifications underwent several chemo-selective transformations through three main routes in rings F, D, and C (Fig. **2**). These routes including chemo-selective spiroketal opening (ring-F), the functionalization of $\Delta^{14,15}$ bond (ring-D), including chlorination/dechlorination in addition to epoxidation/ oxygenation processes. Introduction of the C-11 methoxy group on ring-C led to several chemo-selective transformations. Also, a potentially active analogue was obtained after functionalization of C-12 on ring-C after methylenation followed by hydroboration-oxidation. The alignment of these results paves the way toward the targets. The culmination of our efforts was the effective preparation of an anti-cancer prodrug which overcomes cancer-drug resistance (chemoresistance) and has almost no toxicity to the normal cells. The mechanistic drug action was by inducing the atypical endoplasmic reticulum-mediated apoptosis pathway which works through the release of Smac/Diablo and the activation of caspase-4.

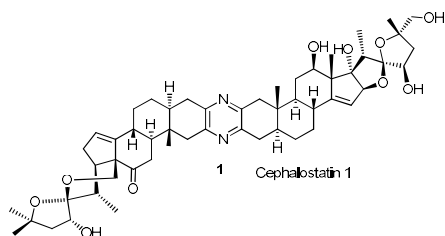


Figure 1. Structure of cephalostatin 1

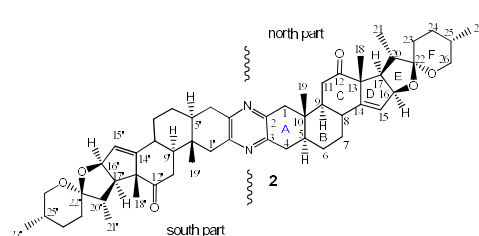


Figure 2. Structure of the starting material diketone 2

Keywords: cephalostatin, desymmetrization, bis-steroidal pyrazine, symmetrical coupling, chemoselectivity, ER-mediated apoptosis, chemoresistance.

Multiple 1,2,3-Thiadiazole Aromatic Derivatives: Synthesis, Characterization and Gas-Phase Pyrolysis

Mousa Al-Smadi ^a, Nouria Al-Awadi ^b, Mohammad El-khateeb ^a

a) Jordan University of Science and Technology, Irbid, Jordan; b) Kuwait University, Safat, Kuwait

Presenting author email: mariam10@just.edu.jo

1,2,3-Thiadiazole is a heterocyclic organic compound having a 5-member ring with one sulphur and two nitrogen atoms. It has several isomers that are 1,2,3-thiadiazole, 1,2,5-thiadiazole, 1,2,4-thiadiazole and 1,3,4-thiadiazole. This study focuses on the 1,2,3-thiadiazoles which can be prepared from the corresponding hydrazones by applying the Hurd and Mori method. Thiadiazoles and derivatives have interesting pharmacological and biological applications. They have been used in applications such as chromogenic reagents in the spectrophotometric determination of transition metal ions. Therefore, many multiple 1,2,3-Thiadiazole benzene derivatives were prepared and fully characterized.

The thermal stability of the synthesized derivatives was tested through pyrolysis. is a chemical degradation reaction that is caused by thermal energy alone at a temperature higher than ambient. Chemical degradation refers to the decomposition and elimination, which occurs during pyrolysis with the formation of molecules smaller than the starting material. Analytical pyrolysis is the technique of studying molecules either by observing their behavior during pyrolysis or by studying the resulting molecular fragments with the purpose of obtaining analytical information on a given sample. The type of analytical information sought can be qualitative, Pyrolysis is routinely coupled with analytical techniques, mostly chromatographic or spectroscopic, in order to analyze the pyrolysis products. Flash vacuum pyrolysis was developed as a relatively new technique in the 1960s, but pyrolysis reactions are as old as chemistry. In the 1960s many organic chemists started performing FVP experiments with the purpose of isolating new and interesting compounds and understanding pyrolysis processes. 1,2,3-Thiadiazoles and derivatives can undergo extrusion of nitrogen under thermal conditions and generate 1,3-diradical intermediates that could undergo a Wolff rearrangement to the corresponding thioketene. The current study discusses an effective and easy method of synthesizing thioketene, dithioketene and trithioketene compounds as they are very useful because they have a potential wide application.

Keywords: pyrolysis, heterocycle, 1,2,3-thiadiazole, characterization.

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Low Density Polyethylene/Zinc Peroxide Composite and Nanocomposite Prepared by Cast Solution: Thermal, Mechanical and Morphological Characterization

Ahmad Jabarin, Hannibal Mansour & Fuad Al-Rimawi

Al-Quds University, Abu Dis-Jerusalem, Palestine

Presenting author email: falrimawi@staff.alquds.edu

The present study deals with the influence of different concentrations of zinc peroxide (ZnO_2) nanoparticles on thermal, mechanical, morphological, and antibacterial properties of low-density polyethylene/ ZnO_2 composite and nanocomposite. Different compositions of LDPE/ ZnO_2 and LDPE/nano ZnO_2 composites were prepared by solution cast technique with ZnO_2 concentration of (1 %, 3 % and 5%) for composite and (0.5%, 1%, 1.5%, 3% and 5 %) for nanocomposite. Zinc peroxide nanoparticles were prepared using three different methods: reflux reaction method with polyethyleneimine (PEI) as capping agent, reflux method without capping agent, and sol gel method. The reflux method without capping agent was used for preparation of nanocomposite as it gave highest percentage yield. ZnO_2 nanoparticles were characterized by X-Ray Diffraction (XRD), Scanning electron microscope (SEM), FTIR and Differential scanning calorimetry (DSC).

Highly crystalline cubic- ZnO_2 nanoparticles grown in a near- spherical shape were obtained with an average size of about 82 nm ,48 nm and 55 nm for reflux without PEI, reflux with PEI and sol-gel respectively, based on SEM and XRD analysis. It was found by DSC that the synthesized ZnO_2 samples decompose into zinc oxide (ZnO) at about 230-238 °C. Results showed that zinc peroxide particles were dispersed and embedded in the matrices of the composite. The addition of ZnO_2 filler in the composite and nanocomposite imparted slight variations in melting temperature of composite and nanocomposite and gave significant improvements in the degree of crystallinity. Results showed that tensile properties of LDPE/ ZnO_2 nanocomposites are higher than those of LDPE/ ZnO_2 composites, while the composite can withstand high stress without permanent plastic deformation. It was found that LDPE without any filler achieved a tensile strength of 4.94 MPa and for ZnO_2 /LDPE nanocomposites increased with increasing amounts of zinc peroxide nanoparticles. The elastic modulus of composite and nanocomposite was found to increase progressively with ZnO_2 concentration.

Keywords: low density polyethylene, zinc peroxide, composite, nanocomposite, thermal, mechanical, morphology.

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Three-Ring Motifs in Zeolite Imidazole Frameworks for Enhanced Properties and Applications

Bassem Al-Maythality^a, Ala'a Al-Ghourani^a, Xiangyi Zha^b, Xinhao Li^b, Shan Liu^b, Cong-Cong Liang^b, Jingjing Yang^b, Zhaolin Shi^b, Yue-Biao Zhang^b & Kyle E. Cordova^a

a) Royal Scientific Society, Amman, Jordan; b) ShanghaiTech University, Shanghai, China

Presenting author email: bassem.maythality@rss.jo

Limited information has been disclosed regarding the occurrence and characteristics of the three-ring (3-ring) motif within zeolite imidazole frameworks (ZIFs), often arising serendipitously. The main challenge in constructing structures based on the 3-ring motif is the considerable strain resulting from the narrow bond angles involved. In my presentation, I will shed light on our data-supported theories that enabled the successful incorporation of the 3-ring motif in ZIFs, drawing comparisons with inorganic zeolites. The underlying concept revolves around incorporating a benzimidazolate linker (L), a benzotriazolate linker (L'), and a tetrahedral metal center (T) into ZIF structures. By introducing both L-T and L'-T bonds, the structure can self-adjust, relieving strain and facilitating the formation of the 3-ring motif. This self-adjustment strategy allowed for the synthesis of four isostructural ZIFs, named ZIF-1001, 2, 3, and 4, all possessing the NPO topology. These synthesized ZIFs exhibited intriguing characteristics such as ultra-microporosity, inherent hydrophobicity, and notable chemical and thermal stability. Consequently, they displayed attractive properties, including selective capture of CO₂ from simulated flue gas containing humidity, SO_x, and NO_x. Furthermore, the synthesized ZIFs demonstrated the ability to trap ethane at ambient temperature and pressure, which is a crucial feature for shale gas extraction.

Zha, X.; Li, X.; Al-Omari, A. A.; Liu, S.; Liang, C. C.; Al-Ghourani, A. a.; Abdellatif, M.; Yang, J.; Nguyen, H. L.; Al-Maythality, B., Zeolite NPO-Type Azolate Frameworks. *Angewandte Chemie* **2022**, 134 (39), e202207467.

UHMWPE/MWCNTs Nanocomposite Prepared by Wet Ball Milling and Hot Press

Ayat Bozeya^a, Yahia F. Makableh^a, Laith A. Al-Mezead^a & Rund Abu-Zurayk^b

a) Jordan University of Science and Technology, Irbid, Jordan; b) The University of Jordan, Amman, Jordan

Presenting author email: aabouzieh@just.edu.jo

In this study, wet ball milling and hot press methods were used for the preparation of nanocomposite from ultra-high molecular weight polyethylene (UHMWPE) as a matrix, and modified multi wall carbon nanotubes (MWCNTs) as reinforcement nano-additives. First, the MWCNTs were oxidized (oxide-MWCNTs) by wet chemistry using strong acids, then further functionalized with amide group (A-MWCNTs). Fourier-transform infrared spectroscopy (FTIR), and Thermal gravimetric analysis (TGA) results confirm the functionalization of the MWCNT with Amide group. Scanning electron microscopy (SEM) and X-ray diffraction (XRD) were used to examine the surface morphology and crystalline behavior of MWCNT after functionalization. Ball milling was used to mix the UHMWPE with pristine MWCNT (1.5 % wt.), Oxide-MWCNT (1.5 % wt.), and A-MWCNTs (0.5 – 2 % wt.). Then, hot press melding was used to prepare the nanocomposite sheets. Fourier transform infrared spectroscopy (FTIR) confirmed the impact of the balls milling process with time factor on UHMWPE crystallinity and the interaction of the functionalization MWCNT with the UHMWPE matrix. The structure (crystallinity, crystal size) was validated using X-ray diffraction (XRD) patterns. Thermal gravimetric analysis (TGA), differential scanning calorimeter (DSC), and universal testing machine (UTM) were utilized to analyse the structural, thermal, and mechanical properties of the nanocomposites respectively. The results showed that after 2 hours of ball milling, UHMWPE crystallinity increased, while crystallinity decreased when pristine-MWCNT, oxide-MWCNTs, and A-MWCNTs (0.5 - 2 wt. %) were added without affecting the crystal structure of UHMWPE. The results showed that adding 1.5 wt. % A-MWCNTs/UHMWPE increased thermal stability by 16 °C and elongation at break by up to 74 %. This shows that the ball milling methods and amide group improved the dispersion and interface interaction between MWCNTs and UHMWPE matrix.

Keywords: MWCNTs; UHMWPE; nanocomposite; ball milling.

Bozeya A., Makableh Y. F., Al-Mezead L. A., Abu-Zurayk R. Wet Ball Milling and Hot Press for the Preparation of UHMWPE /Modified MWCNTs Nanocomposite with Enhanced Mechanical and Thermal Properties, *Polymer Bulletin*, **2023**. <https://doi.org/10.1007/s00289-023-04790-w>.

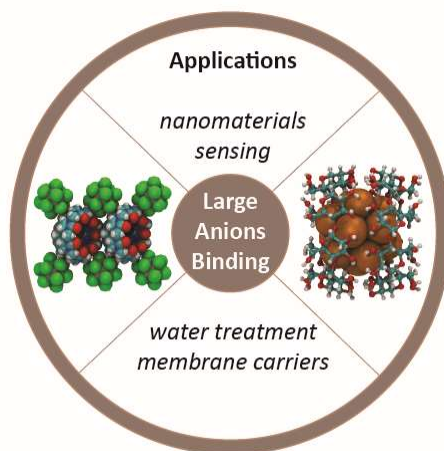
The Supramolecular Chemistry of Boron Clusters

Khaleel I. Assaf

Al-Balqa Applied University, Al-Salt, Jordan

Email: khaleel.assaf@bau.edu.jo

Boron clusters have recently emerged as unique recognition motifs in supramolecular chemistry.^[1] Among others, polyhedral *clos*o-dodecaborate^[2,3] and metallacarborane anions^[4] have received a great deal of attention due to their globular structure, delocalized charge, high stability. Recently, these large anions have been classified as a prototype of *superchaotropic anions* revealing surprisingly strong supramolecular interactions in water, for example with macrocyclic receptors, polymers, biomembranes, as well as other hydrophobic cavities and interfaces. The high affinity is traced back to a *hitherto* underestimated driving force, the *chaotropic effect*, which is orthogonal to the common hydrophobic effect.^[1] Herein, the binding of large anions with water-soluble macrocyclic hosts, including cyclodextrins and cucurbiturils will be described. The high affinity of large anions to molecular receptors has been implemented in several lines of new applications, which are also highlighted.^[5-7]



Keywords: superchaotropic, molecular recognition, large anions, macrocycles.

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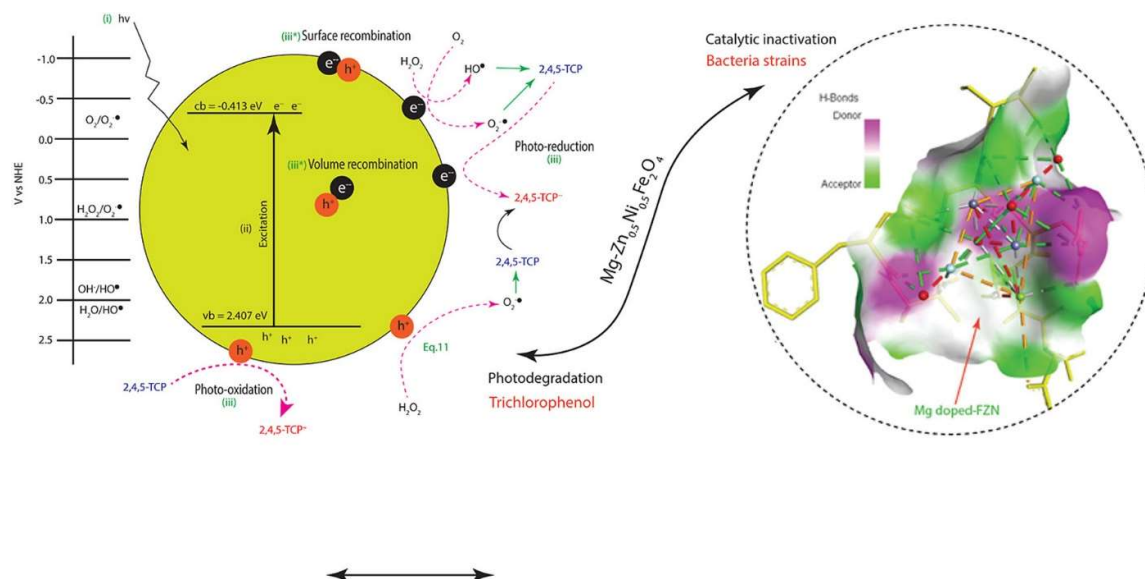
Mg-doped Mixed Metal Ferrite for Remediation of Trichlorophenol and Bacteria Strains: Experimental and Computational Mechanism Approach

Faisal Suleiman Mustafa & Akeem Adeyemi Oladipo

Eastern Mediterranean University, TR North Cyprus, Turkey

Presenting author email: Faisal.mustafa@emu.edu.tr

A facile co-precipitation-doping method was used to synthesize a dual-function Mg-doped $\text{Zn}_{0.5}\text{Ni}_{0.5}\text{Fe}_2\text{O}_4$ (Mg-FZN) nanocatalyst. Utilising a variety of physicochemical techniques, Mg-FZN was characterised and demonstrated a remarkable capacity to degrade refractory phenolic pollutants and inactivate bacterial strains. With a conduction band of -0.413 eV, an average pore width of 2.32 nm, and a crystal size of 31.45 nm, Mg-FZN is an *n*-type semiconductor, according to the results of the characterisation. Based on the degradation of 2,4,5-trichlorophenol, the photocatalytic activity of Mg-FZN was evaluated, and under optimized conditions, it demonstrated a degradation efficiency of 83.8%. According to the radical quenching data, h^+ made a major contribution to the photodegradation process, whereas $\bullet\text{OH}$, and $\bullet\text{O}_2^-$ contributed to the degradation process. Additionally, in both the presence and absence of UV light, 25 mg of Mg-FZN exerted bactericidal effects on the bacteria *E. coli* and *S. aureus* within 60 minutes. Mg-FZN demonstrated H-bonding, electrostatic, and metal-contact interactions with the amino acid residues of the bacterial protein with high binding scores (varying from -4.711 kcal/mol to -5.872 kcal/mol), according to computational molecular docking studies.



Keywords: photocatalysis, mixed metal ferrites, metal dopants, chlorophenols, bacteria time-kill.

Mustafa F.S.; Oladipo A.A. Dual function Mg-doped binary metal ferrite: Photocatalytic degradation of trichlorophenol, bactericidal activity and molecular docking analysis. *Chemosphere*, **2023**, 312, 137348.

Molecular Recognition of Amino Acids and Peptides by Cucurbit[8]uril. A Computational Study

Osama M. Abuhasan^a, Khaled Bodoor^b, Khaleel I. Assaf^c, Abdel Monem M. Rawashdeh^d, Baker Jawabrah Al Hourani^e & Musa I. El-Barghouthi^a

a) The Hashemite University, Zarqa, Jordan; b) The University of Jordan, Amman, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan; d) Embry Riddle Aeronautical University, Prescott, AZ, USA; e) Yarmouk University, Irbid, Jordan

Presenting author email: osama96abuhasan@gmail.com

We study ternary complexes formed by cucurbit[8]uril (CB8) with the aromatic AAs: tryptophan (W), phenylalanine (F), tyrosine (Y), and with tripeptides containing W, in the presence and absence of the auxiliary ligands (ALs), using molecular dynamics (MD) simulations and quantum mechanical calculations. All complexes were stable and generally showed encapsulation of the aromatic side chains of the AAs within the cavity of CB8. The visual analysis of the structures for the homoternary complexes indicated the presence of π - π stacking between the aromatic side chains of the AAs. Furthermore, the Molecular Mechanics-Poisson Boltzmann Surface Area (MM-PBSA) method revealed that the complexes were stabilized mainly through the van der Waal interaction with the CB8 cavity, and electrostatic interactions between the carbonyl portal of CB8 and the ammonium group of the AA. UV-Visible spectra of the heteroternary complexes were computed with time-dependent density functional theory (TD-DFT) calculations and revealed the appearance of new bands for some complexes corresponding to transitions corresponding to AA-AL charge transfer complexes formed within the CB8 cavity.

Keywords: cucurbit[8]uril, amino acid, tripeptides, molecular dynamics.

Association between Water Electrolytes and Bacterial Antibiotic Resistance Development in Drinking Water

Arwa Mujahed, Atef Zahdeh, Baraa Sakhdam, Falak Zatari & Leen Arafeh

Palestine Polytechnic University, Hebron, Palestine

Presenting author email: arwam@ppu.edu

Antibiotic resistance (AR) and its wider consequences are threatening the world with an increasing health problem. The latest literature refers to the environment as a core component of the spread of resistant bacteria and the development of resistant pathogens. However, there is also a lack of a deeper understanding of the developmental and ecological processes that lead to the clinical expression of resistance genes. One of the environmental causes of the AR ecosystem is electrolytes. When bacteria are subjected to large concentrations of electrolytes, they serve as a harmful agent for these organisms. Furthermore, Accumulation of reactive oxygen species (ROS) occurs as a response to electrolyte toxicity when the bacteria are under environmental stress. ROS has many effects on the bacterial genetic material and proteins, particularly these changes that occur in the genetic material leading to mutations, and protein biochemical and structure leading to changes in protein function and the structure of the genetic material, which play a crucial role in the production of AR. In this study different drinking water samples were collected, and their bacterial sensitivity was tested before exposure to electrolytes comparing those results with the sensitivity of those bacteria after exposing to different concentrations of electrolytes to interpret the effect of electrolytes on AR of drinking water bacteria. After exposing 4 types of isolated bacteria to Fe, Cu and K electrolytes for a month the results show a direct relationship between rising in Fe and Cu concentrations and *Shigella sp.*, *Pseudomonas aeruginosa*, *S.epidermidis*, bacteria resistance level for antibiotics. After specific high concentrations those bacteria started adapting the stress by moderating the resistance. The results of K electrolytes vary between mild to no effect with antibiotic resistance for bacteria in general. Otherwise, *S.aureus* had no change in antibiotic sensitivity level due to its own mechanism to adapt electrolytes stress.

Keywords: antibiotic resistance, antibiotic sensitivity, water electrolytes, drinking water, resistance genes.

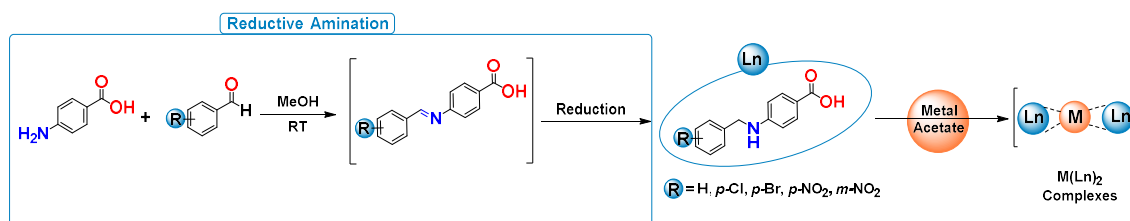
Novel Transition Metal Complexes Mediated by 4-(Benzylamino)benzoic Acid Derivatives: Synthesis, X-ray Crystallographic Analysis for Ligands, and Biological Activities

Qusai Sarayrah^a, Abdelrahman Malkawi^a, Ahmed K. Hijazi^a & Hassan Abul-Futouh^b

a) Jordan University of Science and Technology, Irbid, Jordan; b) The Hashemite University, Zarqa, Jordan

Presenting author email: gmsarayrah21@sci.just.edu.jo

New transition metal complexes have been synthesized from ligands obtained by reductive amination reaction to give (Ln). Various Benzaldehyde (R= H, 4-Cl, 4-Br, 3-NO₂, 4-NO₂, 2-OCH₃, 3-OCH₃, 4-OCH₃, 2,3-OCH₃) are mixed with 4-aminobenzoic acid, followed by reduction for the imine bond. After that, metal complexes [M(Ln)₂.solvent] were synthesized from transition metal acetates and ligands where (M= Cu^{II}, Zn^{II}). The structure of the ligands has been determined using single crystal X-ray diffraction (R= H, 4-Cl, 4-Br, 2-OCH₃, 3-OCH₃, 4-OCH₃, 2,3-OCH₃). All metal complexes have been characterized by a variety of spectroscopic techniques (FT-IR, ¹H and ¹³C NMR) and elemental analysis, The antibacterial activities of ligands (Ln) and their (M^{II}) complexes were tested against some gram-positive and gram-negative bacterial strains.



Keywords: transition metal complexes, reductive amination, X-ray structure, biological activities.

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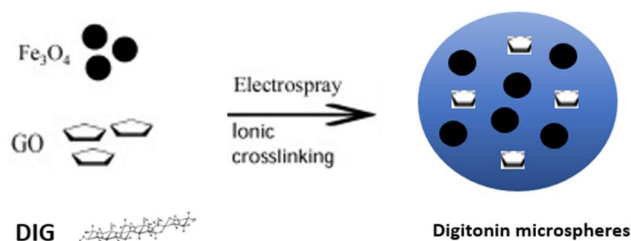
Encapsulation of DIG-GO and DIG-GO-Fe₃O₄ Composites into CDs

Batool M. Malkawi ^a, Khaled Q. Shawakfeh ^a, Nathir A. Alrawashdeh ^a & Bashar Aljawarneh ^b

a) Jordan University of Science & Technology, Irbid, Jordan; b) Al-Zaytoonah University of Jordan, Amman, Jordan

Presenting author email: bmmalkawi21@sci.just.edu.jo

Digitonin (DIG) is a steroidal, monodesmosidic saponin (saraponin) derived naturally from Lady's Glove, a kind of foxglove plant, and *Digitalis pupurea*. Graphene oxide (GO) usually acts as a starting material for the synthesis of graphene-based materials. Due to their unique qualities, magnetic nanoparticles (MNPs) have aroused a great deal of interest. A family of cyclic oligosaccharides having a lipophilic inner and a hydrophilic exterior is known as cyclodextrins (CDs). In this work, we have included nanocomposites containing Digitonin, Graphene oxide with and without Fe₃O₄ within several types of cyclodextrin for the first time, we started with β -cyclodextrin (β -CD) through a technique named co-precipitation. Magnetite nanoparticles Fe₃O₄ were dispersed on the prepared nanocomposite surface to produce magnetically modified nanocomposite (GO-DIG-Fe₃O₄). To study the effect of the encapsulation of nanocomposite on solubility and stability of several types of cyclodextrin. The prepared nanocomposites and encapsulation complex (DIG-GO/ β -CD, DIG-GO-Fe₃O₄/ β -CD) were characterized by Fourier transform infrared spectroscopy (FT-IR), the nanocomposites (DIG-GO, DIG-GO-Fe₃O₄) were characterized by X-ray diffraction (XRD). The morphology of the nanocomposites (DIG-GO, DIG-GO-Fe₃O₄) were characterized by scanning electron microscopy (SEM).



Keywords: encapsulation, digitonin, DIG-GO nanoparticles, drug delivery system

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The Synthesis and Interfacial Properties of Gemini Surfactants based on Nicotinic Acid

Ahmad Abo-shunnar^a, Ala'a F. Eftaiha^a, Abdussalam K. Qaroush^b, Suhad Hammad^b, Khaleel I. Assaf^c, Feda'a M. Al-Qaisi^a & Matthew F. Paige^d

a) The Hashemite University, Zarqa, Jordan; b) The University of Jordan, Amman, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan; d) University of Saskatchewan, Saskatoon, Canada

Presenting author email: ahmadaboshnnar@gmail.com

In this work, we have reported on the synthesis of pyridinium based Gemini surfactants (GSs) and investigate their Langmuir monolayer properties using π -A isotherm measurements. The morphology of the films at the air-water and air-solid interfaces was explored using Brewster Angle Microscopy (BAM) and the Atomic Force Microscopy (AFM).

The isotherms measurements indicated that GSs with ethylene, butylene and xylylene spacers formed stable monolayer with kinks, indicating the formation of highly packed film, at approximately $\pi = 45$ mN/m, with a collapse plateau ranging between 55-58 mN/m. The morphology was dependent on the spacer, transitioning from a three lobed structure in the case of the ethylene, to a more complex lobed structure for the xylylene. The Excess Gibbs free energy of mixing indicated that the mixed films comprised of nicotinate ester GS and palmitic acid were less stable than the pure monolayers, and the film morphology varied depending on the composition of the film.

Keywords: gemini surfactant, nicotinic acid, Langmuir-Blodgett film, Langmuir monolayer.

A. F. Eftaiha, A. K. Qaroush, A. S. Abo-shunnar, S. B. Hammad, K. I. Assaf, F. M. Al-Qaisi and M. F. Paige, *Langmuir*, **2022**, 38, 8524–8533.

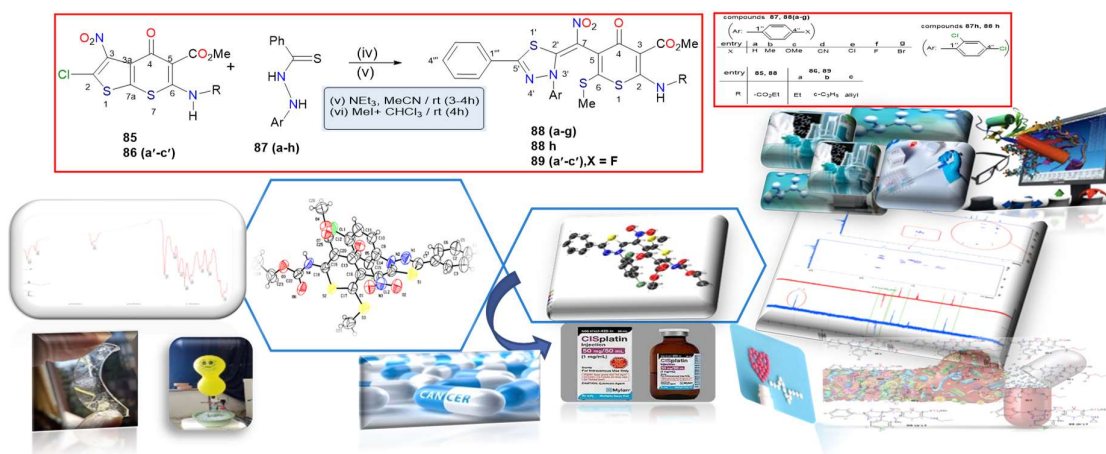
Thiophene Ring-Opening Reactions: Synthesis and Properties of 1,3,4-Thiadiazoline-6-Sulfanylthiopyran-4(1H)-One Hybrids

Shaimaa Alsawalha, Mustafa El Abadelah, Jalal Zahra & Salim Sabri

The University of Jordan, Amman, Jordan

Presenting author email: sheom964@gmail.com

A new series of 1,3,4-thiadiazoline-4-thiopyranone hybrids have been synthesized via the interaction of N'-(aryl)benzothiohydrazides, under basic conditions (NEt_3) in acetonitrile, with methyl 2-chloro-6-((substituted)amino)-3-nitro-4-oxo-4H-thieno[2,3-b] thiopyran-5-carboxylate; these hybrids incorporate ethylcarbamate, ethanamine, cyclopropanamine, 4-fluoro-2,6-dinitroaniline, or 2,3-dinitropropan-1-amine moiety at C-6. The formation of the 1,3,4-thiadiazoline ring led to the thiophene ring opening at the C2-S1 bond, together with the formation of the S-anions at C-7a and the nitromethylene bridge at C-3a. The thiolate anions were then alkylated with iodomethane to yield the respective thiadiazoline-6-sulfanylthiopyran-4 (1H)-one hybrids. The new compounds were characterized by HRMS and NMR spectral data and confirmed by single-crystal X-ray crystallography. The biological activity of most compounds was studied through computer modeling and found to be most effective against Aurora A, ALK, FLT3, PPAR-gamma, and ADORA enzymes as anti-cancer agents. The samples were sent to biology, where the compounds have anticancer efficacy. The cell line study shows that compounds containing the OMe group have higher activity compared to cisplatin.



Keywords: 1,3,4-thiadiazoline-4-thiopyranone, thiadiazoline-6-sulfanylthiopyran-4 (1H)-one hybrids, anticancer, Aurora A.

Promising Treatment for Late-Stage AD's Through Novel Dual-Acting BChE's Pseudo Irreversible Inhibitor and Antioxidant

Rayanah Amro^a, Nafisah AL Rifai^b, Jalal Zahra^a, Mutasem Taha^a & Fouad Darras^c

a) University of Jordan, Amman, Jordan; b) German Jordanian University, Madaba, Jordan; c) Resonance Research Lab, Amman, Jordan

Presenting author email: amroyana@gmail.com

Alzheimer's disease (AD) is the most common form of dementia. The exact causes of AD aren't fully understood, but it is accompanied by specific neuropathological changes, such as a reduction in levels of the neurotransmitter acetylcholine (ACh). Two enzymes responsible for ACh decomposition are acetyl cholinesterase (AChE) and butyryl cholinesterase (BChE). AD can be categorized into three stages: early, middle, and late. In the late stage, BChE activity rises, while AChE activity remains unchanged or declines. Thus, AChE inhibitors become clinically ineffective. In this work, where the inhibition of BChE at later stages will enhance the cholinergic transmission, three different moieties of carbamate compounds were synthesized to investigate their inhibitory activity. Carbamate-based compounds were found to possess selective inhibition to BChE over AChE. The basic moiety of heptyl carbamate compound (**C3**) Figure 1. was found to have an IC_{50} value of 6.70 ± 3.06 nM for BChE at a purity of 96.5% as determined by HPLC. The released compound after enzyme carbamoylation was also found to have antioxidant activity ranging from 70.2 to 85.3% at concentration ranges from 0.0136 to 0.1088 mM, which means that **C3** can be used as a dual-acting compound. Moreover, the docking study supported the biological activity data, and compound **C3** was found to have the highest interaction energy with a value of 54.293 kcal/mol.

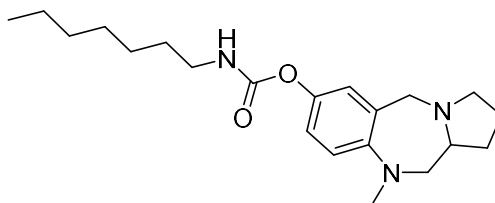


Figure 1: Compound C3

Keywords: alzheimer's disease, BuChE inhibitors, AChE inhibitors, carbamate-based compounds.

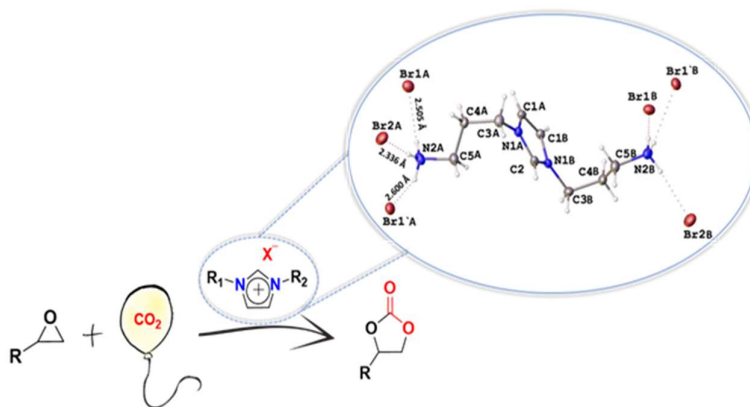
Exploring Aprotic and Protic Imidazolium Salts for CO₂ Capturing and Utilization

Suhad B. Hammad^a, Abdussalam K. Qaroush^a, Ala'a F. Eftaiha^b, Feda'a M. Al-Qaisi^b, Khaleel I. Assaf^c, Malak H. Al-Anati^a, Enas S. Radwan^d & Firas F. Awwadi^b

a) The University of Jordan, Amman, Jordan; b) The Hashemite University, Zarqa, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan, d) Zarqa University, Zarqa, Jordan

Presenting Author email: suhadhammad1@gmail.com

As a contribution of the Jordanian CO₂ team (JCO₂T) to CO₂ mitigation technology, specifically in the areas of utilization and sequestration, we synthesized a series of imidazolium-based precursors and the corresponding ionic liquids (ILs). This includes both protic and aprotic catalysts for facilitating the atmospheric cycloaddition reaction between CO₂ and epoxides. Quantitative conversion of cyclic carbonates (CCs) was achieved under mild reaction conditions using the protic amine-tethered IL (1,3-bis(3-aminopropyl)-1*H*-imidazol-3-ium bromide), while the overall activity of the other synthesized catalysts showed good conversions. Moreover, the isolated yields of CCs and a 5-run recyclability experiments for the aprotic catalyst 1,3-bis(3-(1,3-dioxoisindolin-2-yl)propyl)-1*H*-imidazol-3-ium bromide were accomplished with high purity. Furthermore, the reaction of protic amine IL with CO₂ in DMSO resulted in the formation of an ionic ammonium carbamate following a 1:2 reaction mechanism which was fortified using spectroscopic analyses and supported *via* density functional theory calculations. Experimental isolation of some intermediates was achieved. Single crystal X-ray diffraction verified the chemical structure of the ammonium-based protic precursor 1,3-bis(3-ammoniopropyl)-1*H*-imidazol-3-ium bromide.



Keywords: homogenous catalysis, CO₂ utilization and sequestration, cyclic carbonates, ionic liquids.

Qaroush A.K.; Eftaiha A.F.; Al-Qaisi F.M.; Assaf K.I.; Hammad S.B.; Al-Anati M.H.; Radwan M.H.; and Awwadi F.F., *Catal. Sci. Technol.*, **2023**, *13*, 3245–3257.

Adsorption of Cd(II) using Newly Prepared and Characterized Polymeric Material

Rahaf Ghadieh, Eyad Younes & Amjad El-Sheikh

The Hashemite University, Zarqa, Jordan

Presenting author email: rahafghodayya@gmail.com

Civilization resulted in great improvements in all aspects of life. This led to an increase in agricultural and industrial activities which resulted in the throwing of toxic and harmful substances into the water resources. [1] Heavy metals, such as cadmium, are one of these harmful substances where efficient water treatment is required. [1,2] Modern research strongly relied on using newly prepared and efficient adsorbents, where adsorption proved itself as a powerful treatment technology. [3] In the current study, two polymers were prepared using 5,7-dibromo-8-hydroxyquinoline derivatives (monomer) with benzene-1,4-diboronic acid (cross-linker). These were characterized by FT-IR and NMR. The polymers were used for adsorption of cadmium (II) where the following parameters were optimized: pH, mass of adsorbent, initial concentration (adsorption isotherm), effect of time and effect of temperature. The polymers exhibited the appropriate ability to remove cadmium (II) ions at pH 8.

Keywords: water pollution, cadmium, adsorption, polymers.

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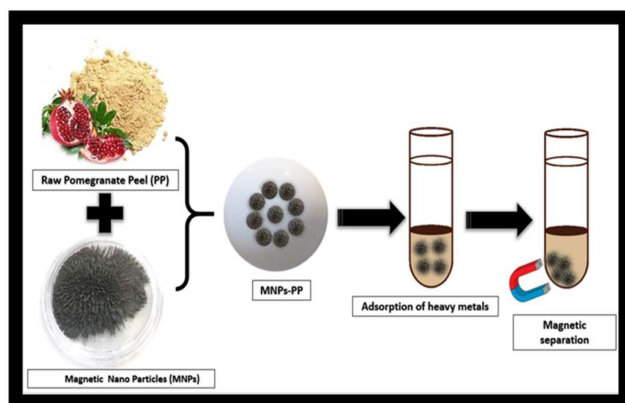
Synthesis, Characterization and Application of Nano Magnetic Adsorbent based on Pomegranate Peels for Multi Heavy Metal Ions Removal

Abdelmnim Altwaiq, Leen Ali & Muayad Esaifan

University of Petra, Amman, Jordan

Presenting author email: leen.ali@uop.edu.jo

Water pollution caused by heavy metals is a significant environmental problem that has detrimental effects on ecosystems and living organisms. One of the most effective technologies for removing heavy metals is adsorption, and there has been a growing focus on utilizing agricultural waste materials as low-cost adsorbents for these pollutants in aqueous solutions. The application of Nanotechnology has further enhanced the efficiency of adsorbents for heavy metal removal. Nanomaterials possess unique properties such as a large surface area, enhanced active sites, and functional groups on their surface, making them highly effective in adsorbing heavy metals from aqueous solutions. A new magnetic bio adsorbent, Nano magnetic particles based on pomegranate peel (NMPs-PP), was synthesized by coating powdered pomegranate peel with Nano particles of Fe_3O_4 , then characterized by Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), Zetasizer, Point of zero charge (pHPZC), PET, and Magnetization measurements. Then it was used for removing Pb (II), Cu (II), and Cd (II) from aqueous solutions. The influencing factors (Contact Time, Adsorbent Dose, pH, and initial concentration of Pb, Cu, and Cd adsorption) by NMPs-PP were investigated using batch assays and compared with the results with Raw pomegranate peel. Optimum Pb, Cu, and Cd adsorption by NMPs-PP was achieved using a contact time of 120, 100, and 10 min, respectively, and an optimum adsorbent dose of 40, 10, and 8 g/L. Efficiency was greater than 90% at 25 ppm, but it was less efficient at higher concentrations, and vice versa for the raw pomegranate peel, which was more efficient at high concentrations, and finally all solutions pH of 6.



Keywords: magnetic bioadsorbent, pomegranate peel, wastewater treatment, heavy metals.

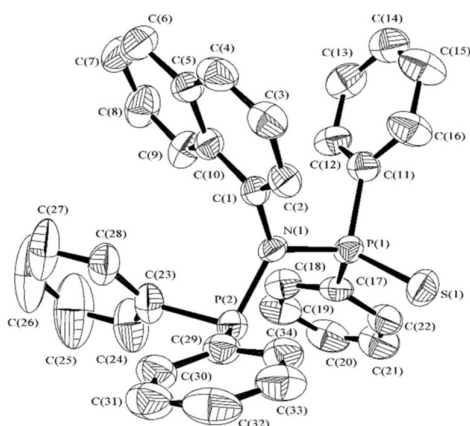
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Hg(II) and Ru(II) Complexes of Mono- and Dichalcogenides of Bis(diphenylphosphino)amine Chelating Ligands: Synthesis, Characterization and Catalytic activity in Transfer Hydrogenation of Acetophenone Derivatives

Akram Ali Almejled & Harbi Tomah Al-Masri

Al-Bayt University, Mafrqa, Jordan

Reactions of $C_{10}H_7-1-N(PPh_2)_2$ (1) and $C_{10}H_7-1-N(P(Se)Ph_2)_2$ (2) ligands with mercury (II)iodide in equimolar ratio gave $cis-[HgI_2\{1-j^2P,P\}]$ (3) and $cis-[HgI_2\{2-j^2Se,Se\}]$ (4). Also, refluxing of mono oxidized thioyl and selenoyl bis(phosphino)amine ligands $C_{10}H_7-1-N(P(E)Ph_2)(PPh_2)$ ($E=1/2S$ (5), Se (6)) with $[Ru(CO)_3Cl_2]_2$ dimer afforded $cis-[Ru(CO)_2Cl_2\{5-j^2P,S\}]$ (7) and $cis-[Ru(CO)_2Cl_2\{6-j^2P,Se\}]$ (8). Complexes 3, 4, 7 and 8 were identified and characterized by multinuclear NMR (1H , ^{13}C , ^{31}P and ^{77}Se) and IR spectroscopy. The molecular structure of 5 was determined by single X-ray crystallography. 5 is the first structurally characterized example of this kind of j^2P,S -bidentate ligand. The novel ruthenium (II) complexes 7 and 8 show high catalytic activity in the transfer hydrogenation of acetophenone derivatives to 1-phenylethanol derivatives in the presence of 2-propanol as the hydrogen source.



Keywords: bis(diphenylphosphino)amine, mercury, ruthenium catalysis, transfer hydrogenation.

Investigation of Solvent Effect and H-Bonding on Spectroscopic Properties of 1-(3-Amino-6-(2,5-dichlorothiophen-3-yl)-4-phenylfuro[2,3-b]pyridin-2-yl) ethenone: Experimental and Computational Study

Omar Almashaqbeh^a, Raed Ghanem^a, Rasha Abuflaha^a, Fakhri Yousef^b, Khaldoun Al-Sou'od^a, Ihsan Shahdi^c & Mahmoud Al-Refai^a

a) Al Al-Bayt University, Mafraq, Jordan; b) Al-Hussein Bin Talal University, Ma'an, Jordan; c) University of Sharjah, Sharjah, UAE

Presenting author email: omkarredt345@gmail.com

The furo[2,3-b]pyridine moiety is an important scaffold for many biologically active compounds, therefore, the spectral data of the derivative 1-(3-Amino-6-(2,5-dichlorothiophen-3-yl)-4-phenylfuro[2,3-b]pyridin-2-yl) ethenone (FP1) were investigated. Analysis of absorption-pH profile and Förster cycle of FP1 revealed that its excited state is more acidic than its ground state ($pK_a^* < pK_a$). The main fluorescence emission band of FP1 at 480 nm (in hexane) is shifted to longer wavelengths with increasing polarities of solvents. Linear Lippert's plot and linear correlation between bands maxima and Camlet-Taft parameter, α , of the protic solvents indicated efficient intramolecular charge transfer and noticeable H-bonding. Moreover, the disappearance of the absorption band of FP1 at 385 nm in water, along with the noticeable red shift and quenching of the emission band, and the lower lifetime, relative to nonaqueous solvents, indicate the interruption of the furo[2,3-b]pyridine aromatic moiety. In addition, results from the Time Dependent Density Functional Theory (TDDFT) and Molecular Mechanic (MM) calculations agreed with experimentally determined spectra of FP1. Stable structures of FP1 in A) vacuum and in B) water as minimized by MM calculations showing intra- and intermolecular H-bonding.

Keywords: furo[2,3-b]pyridine, fluorescence spectral analysis, förster cycle analysis, Lippert's plot, excited state H-bonding, TDDFT calculations.

Almashaqbeh O, Ghanem R, Abuflaha R, Yousef F, Al-Sou'od K, Shahdi I, Al-Refai M, *J Fluoresc*, **2023**, 10.1007/s10895-023-03243-x.

Kinetic Study of Degradation of Rosuvastatin Calcium to Rosuvastatin-Lactone under Different Solvents Conditions

Areej AL-Kayed ^a, Raed Ghanem ^a, Fatima Azzahra Delmani ^b, Fakhri O. Yousef ^c, Haitham Al-Sa'doni ^a, Khaldoun Al-Sou'od ^a, Omar K. Almashaqbeh ^a, Mahmoud Eqab Rabi ^a & Ahmad Abdo ^d

a) Al Al-Bayt University, Mafraq, Jordan; b) Jerash university, Jerash, Jordan; c) Al-Hussein Bin Talal University, Ma'an, Jordan; d) Vivid Separation and filtration, Amman, Jordan

Presenting author email: alkayedareej1993@yahoo.com

Rosuvastatin Calcium (RST) is a medication used to lower cholesterol levels by increasing the number of low-density lipoprotein receptors on the cell surface. RST undergoes different degradation processes under different conditions. leading to the formation of different degradation products; 5-oxo isomer, anti-isomer, and lactone form of RST. Lactone form of RST is the major degradation product. Chromatographic techniques were used to identify and quantitatively determine the concentration of RST and its degradation products, where the aqueous aprotic solvent mixture (acetonitrile (25): water (75)) is used as an extraction medium to release RST and its degradation product RST-Lactone from the dosage form. Unfortunately, the presence of water in the extraction mixture or mobile phase could enhance the acid hydrolysis of lactone (i.e., conversion of RST-Lactone into RST) during the analysis time giving an underestimated result of the actual content of the degradation product. The type of solvent matrix used in sample extraction was found to control the direction of $\text{RST} \rightleftharpoons \text{RST-lactone}$ equilibrium. It is found that: (a) In aprotic solvents, the forward reaction (i.e., the conversion of RST to its lactone form is the only reaction that occurs. (b) When RST extracted in the acidic aqueous mobile phase, the reverse reaction was observed, and RST-Lactone was converted into RST. (c) When organic protic solvents such as methanol was used for the extraction, both RST and RST-Lactone were stable, and no reaction was observed. Kinetics helps to distinguish and control the type of and sources of degradation impurities. The rates of both reactions were found to follow the first order kinetics with rate constants directly related to the ageing temperature, the rate constant for the reverse reaction ($\text{RST-Lactone} \rightarrow \text{RST}$) was 20 times greater than the forward reaction. The formation of RST-Lactone form from RST occurs via intramolecular esterification mechanisms followed by proton transfer to the solvent.

Keywords: rosuvastatin, statin, rosuvastatin-lactone, thermal stability, kinetic study.

Ghanem R, Delmani F, Yousef F et al, *Chem. Pap*, **2023**, 10.1007/s11696-023-02864-7

Photophysical and Spectral Characterization of Atenolol: Insights into Solvent Effects, Quenching Behavior, and Dissociation Constants

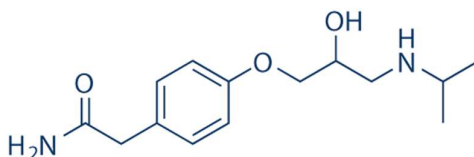
Sereen M. Abu Alkishik & Raed Ghanem

Al Al-Bayt University, Mafraq, Jordan

Presenting author email: sereenabualkishik@gmail.com

The absorption spectrum of atenolol exhibited two distinct bands at 226 nm and 280 nm, while the emission spectra ranged at 295 nm. Assessing the effect of solvents on the absorption spectra revealed negligible influence of polar protic solvents on the position of the absorbance bands. In polar aprotic and non-polar solvents. No significant effects on the absorption bands of atenolol were observed. However, in ethyl acetate, a red shift (bathochromic effect) was detected, indicating a lower energy absorption wavelength. Examining the excitation spectra under different solvent conditions revealed a red shift in polar aprotic solvents. Conversely, in non-polar solvents, a blue shift (hypsochromic effect) occurred, with maximum excitation wavelength shifting towards higher energy in cyclohexane and toluene. The solvent polarity index played a crucial role, as it influenced the excitation spectra behavior. In polar aprotic and polar protic solvents, the emission spectra of atenolol remained largely unaffected by solvent variations. However, in non-polar solvents such as cyclohexane and hexane, a blue shift in the maximum emission wavelength was observed as the solvent polarity decreased. Presence of HCl or NaOH resulted in increased absorbance intensity of atenolol, while the fluorescence intensity was significantly quenched.

Further investigation into the interaction between atenolol and semiconductors revealed their quenching effect, which reduced the absorbance and emission intensities. Additionally, the impact of different viologens on the absorbance and emission of atenolol was studied. The lifetime of atenolol varied with the polarity of the solvent, as well as in the presence of different viologens and semiconductors.



Chemical structure of Atenolol

Keywords: atenolol, n type semiconductor, p-type semiconductor, methyl viologen.

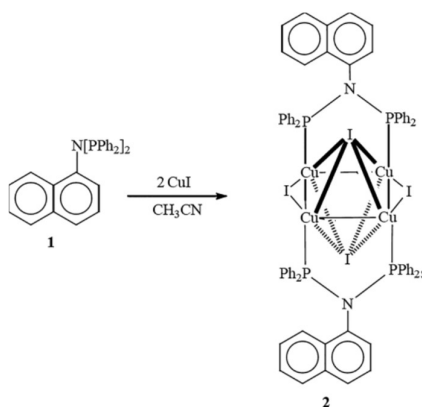
Synthesis, X-ray Structures, and Photoluminescence of the Octahedral Cu₄I₄ Cluster with Bulky Bidentate Bis(phosphanyl)amine Ligand

Suzan Alrawashdeh, Akram Almejled & Harbi Al-Masri

Al Al-Bayt University, Mafrq, Jordan

Presenting author email: suzan.rawashdeh99@gmail.com

The reaction of C₁₀H₇-1-N(PPh₂)₂ (**1**) with two equivalents of CuI in acetonitrile resulted in the formation of octahedron Cu₄I₄[**1**]₂ complex (**2**). The crystal structure of **2** showed it adopted a rare octahedral arrangement. The rectangular Cu₄ plane is μ_4 -capped by two of the iodides and is placed in axial positions above and below the Cu₄- plane form an octahedron, whereas the other two iodides are bonded to two copper atoms in a μ_2 -fashion. The luminescence of complex **2** arises from a triplet halide-to-ligand charge transfer (3XLCT) excited state and 3CC (Cu₄I₄ cluster-centered) excited state are not involved in the luminescence by the rigid bidentate ligand **1** in spite of the short CuI–CuI bond length. Complex **2** was identified and characterized by multinuclear NMR (¹H, ¹³C, ³¹P NMR) and IR spectroscopy. Crystal structure determinations of **1** and **2** were carried out.



Keywords: p-donor; luminescence; x-ray diffraction; copper cluster.

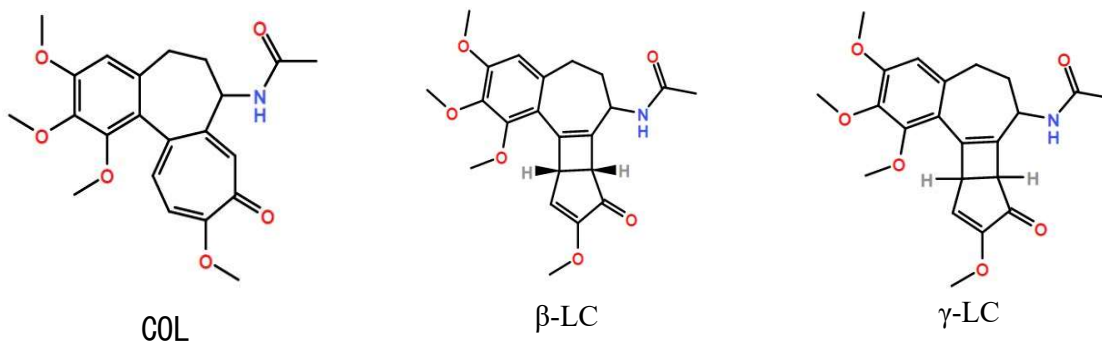
Al-Masri H, Almejled A, 2020, Z. Anorg. Allg. Chem, 10.1002/zaac.202000058.

The Effect of N-type and P-type Semiconductors on Photoconversion of Colchicine

Fakhri O. Yousef ^a, Omar K. Almashaqbeh ^b & Raed Ghanem ^b

a) Al-Hussein Bin Talal University, Ma'an, Jordan; b) Al Al-Bayt University, Mafraq, Jordan

The effect of p-type and n-types semiconductors on the photoconversion of colchicine (COL) is investigated. All investigated semiconductors caused quenching of the fluorescence emission of COL with comparable Stern-Volmer quenching constants k_{sv} . The effect of the n-type semiconductors on the photoconversion of COL is noticeable with the lowest values of the photoconversion rate constant and conversion percent yield were in the presence of 6×10^{-5} mol L⁻¹ of TiO₂ and SnO₂. However, the effect of the p-type semiconductors SnO and TiO on the rate of COL photoconversion was limited. Density functional methods (DFT and TDDFT) were used to provide a clear insight into the solvation effects on Frontier Molecular Orbitals (FMO). Also, DFT method was used to propose a reaction pathway of the photo-conversion of COL to γ - and β -lumicolchicine with a difference of 13.46 kcal/mole in favor of the beta structure.



Structures of colchicine (COL), β -lumicolchicine (β -LC) and γ -lumicolchicine(γ -LC)

Keywords: colchicine, photoconversion, lumicolchicine, fluorescence, DFT, TDDFT.

Ghanem, R., Hadi, A. *J Solution Chem*, **2009**, 10.1007/s10953-009-9403-6.

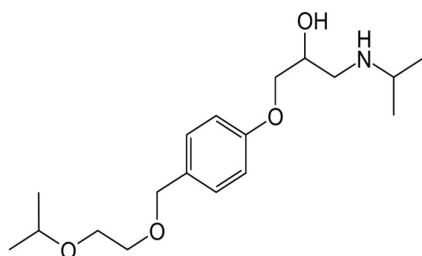
The Role of Electron Acceptor-Donor Materials on Photostability of Bisoprolol

Heba S. Alrefaei & Raed Ghanem

Al Al-Bayt University, Mafrq, Jordan

Presenting author email: Hebaref98@gmail.com

The photophysical properties of Bisoprolol at pH = 7.4 in different solvents and under different conditions have been studied. It was found that Bisoprolol exhibits a characteristic absorption band at 223 nm and 275 nm and emission band at 295 nm. The nature of solvent was found to significantly affect the position of these bands, especially the non-polar solvent. Different pH aqueous media was used to interact with Bisoprolol to measure pKa and pKa*. In this research the role of electron transfer and energy transfer was studied. Semiconductors are the best materials that are used as electron donor or electron acceptor, acid and base also used. Viologens are used to interact with Bisoprolol by energy transfer. The lifetime of Bisoprolol was also studied under different conditions and with different materials.



Chemical structure of Bisoprolol.

Keywords: bisoprolol, n type semiconductor, p-type semiconductor, methyl viologen.

Ghanem, R., Hadi, A. *J Solution Chem*, **2009**, 10.1007/s10953-009-9403-6.

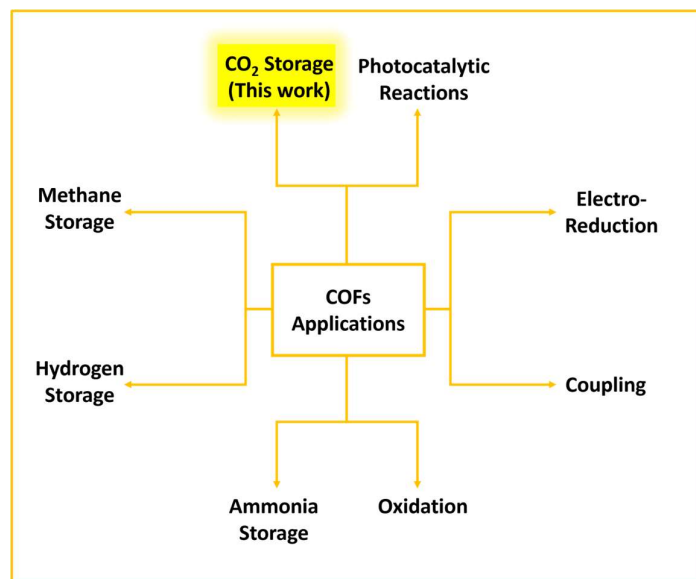
Synthesis of Post-Modified Schiff Base-based COFs for CO₂ Capture: Carbamation and Carbonation Pathways

Ayham A. Aladwan^a, Abdussalam K. Qaroush^a, Ala'a F. Eftaiha^b, Suhad B. Hammad^a, Feda Al-Qaisi^b, Khaleel I. Assaf^c & Timo Repo^d

a) The University of Jordan, Amman, Jordan; b) The Hashemite University, Zarqa, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan; d) University of Helsinki, Helsinki, Finland

Presenting author E-mail: ayhamadwan@yahoo.com

Covalent Organic Frameworks (COFs) are typically nano-porous assemblies that generate extended architectures for multiple applications, such as gas storage and many others (**Scheme 1**). The increased accumulation of CO₂ as a significant contributor to global warming has attracted serious attention to reduce its emission in the atmosphere through utilization, recycling and storage technologies. In this study, we report on the synthesis of novel post-modified Schiff base-based COFs for CO₂ capture through carbamation and carbonation pathways. Interestingly, upon activation with 1,8-diazabicyclo[5.4.0]undec-7-ene, a DMSO-soluble ionic organic carbonate adduct is obtained. Moreover, the ethylenediamine-functionalized COF derivative demonstrates unprecedented water-solubility and captures CO₂ *via* carbamation, as confirmed by colorimetric, conductivity and other spectroscopic analyses.



Scheme 1. Diverse applications of COFs (*CO₂ Storage is highlighted due to its importance in this work*).

Keywords: chemisorption, ionic organic carbonate, carbamate, covalent organic framework.

New Azolate Frameworks based on 3-Rings in a Rational Way

Ala'a Al-Ghourani, Bassem Al-Maythalony & Kyle Cordova

Royal Scientific Society, Amman, Jordan

Presenting author email: ala.ghourani@rss.jo

Designing three membered rings (3-rings) within the zeolitic imidazolate frameworks (ZIFs) have only been few discovered, and in most cases their occurrence was by chance. The challenge for building structures based on 3-rings is the significant strain created by the tight bond angles. In this research, a design principle for targeting new ZIFs based on 3-rings is demonstrated by linking tetrahedral (T) metal centers, with azolate linkers. The strategy used to achieve the 3-rings can be summarized in the inclusion of the benzotriazolate (bTZ) linker and functionalized benzimidazolate (RbIM) linker within the structures. The presence of bTZ increases the bond length of T-bTZ and reduces the T-bTZ-T angle to 120-130°, this gives more room for the angle T-RbIM-T angle and relieves the ring strain. In addition, RbIM guided the coordination chemistry of bTZ to bind preferentially in the imidazolate-type mode, linker-linker interaction orients the synthesis without needing of structure directing agent. This strategy led to the generation of four isorecticular ZIF structures with NPO topology. The synthesized ZIFs showed attractive properties in selectively capturing CO₂ from high-humidity and acidity flue gas; also, they have the potential to consistently separate ethane from tail gas at normal temperature and pressure during shale gas extraction.

Keywords: azolate, ZIFs, 3-ring, NPO topology.

Zha, X.; Li, X.; Al-Omari, A.; Liu, S.; Liang, C.; Al-Ghourani, A.; Abdellatif, M.; Yang, J.; Nguyen, H.; Al-Maythalony, B.; Shi, Z.; Cordova, K. and Zhang, Y. Zeolite NPO-Type azolate frameworks. *Angew. Chem., Int. Ed.* **2022**, 61 (39).

Systematic Identification and Characterization of Impurities in Pharmaceuticals Products

Anas Alshishani

Zarqa University, Zarqa, Jordan

Email: anasshishani@gmail.com

The safety, efficacy, and regulatory compliance of pharmaceuticals require the careful identification of unknown impurities. This presentation explores a systematic approach involving advanced analytical techniques for identifying these impurities that often arise during manufacturing or stability studies. Two case studies that highlight this approach will be discussed. First, we'll examine the synthesis, isolation, identification, and characterization of a drug-exipient interaction degradation impurity in Pramipexole. Techniques like high-performance liquid chromatography, liquid chromatography-mass spectrometry, and nuclear magnetic resonance were used to unravel the nature of this impurity. Next, we will explore the identification of an unknown degradation impurity in cefpodoxime proxetil tablets. By combining LCMS and NMR, the impurity was identified and characterized. These case studies underline the vital role of synthetic and analytical methodologies in impurity identification, thus enabling the development of effective quality control strategies. The knowledge acquired assists in enhancing pharmaceutical manufacturing processes and ensuring the production of safe, high-quality medications.

In conclusion, this talk highlights the role of advanced analytical techniques in decoding unknown impurities in pharmaceuticals. The insights gained support regulatory compliance, improve process efficiency, and elevate the quality of pharmaceutical products.

Keywords: impurities, identification, characterization, pharmaceutical analysis, HPLC, mass spectrometry, NMR spectroscopy, IR spectroscopy, synthetic approaches, quality control, regulatory compliance, pharmaceutical manufacturing.

Electrochemical Determination of Omeprazole

Salsabeel AlSawa'eer^a, Mohammad Khanfar^b, Eyad Abu-Nameh^a, Munib Saket^b, Ahlam Al Kselat^b, Amira Zidan^b & Sameer Hasan^b

a) Al-Balqa Applied University, Al-Salt, Jordan; b) German Jordanian University, Amman, Jordan

Presenting author email: salsabeel.ajarmah@gmail.com

Molybdenum disulfide, MoS₂, is commonly used as a substrate in supercapacitors and other energy production systems, but it is of limited utility in pharmaceutical analysis. In this article, molybdenum disulfide composite was prepared, and the electro-activity of MoS₂ toward the oxidation of omeprazole (OMZ) was investigated. The molybdenum disulfide content of the prepared material was quantified by thermal gravimetric analysis (TGA), its crystallinity revealed by X-ray diffraction (XRD), and its topographic features probed by scanning electron microscopy (SEM). Glassy carbon electrode was modified by MoS₂, and the electrochemical activity of the modified electrode toward omeprazole oxidation was investigated in a phosphate buffer solution (pH 7.00) using differential pulse voltammetry (DPV). Well resolved anodic peak at ca. 0.85 V vs. Ag/AgCl was reported at the modified and the bare glassy carbon electrodes. The impact of the modification with MoS₂ was noticed as a 2.3-fold enhancement of the OMZ oxidation current. Under the applied experimental conditions, and with the utilization of the modified electrode, linear response was obtained in the range 15.8–500. µM with a limit of detection equal to 4.74 µM and a correlation coefficient of 0.989. The modified electrode was also employed for the detection of omeprazole in its commercial pharmaceutical formulations, with percent recovery values of 84.0 to 100.%.

Keywords: omeprazole, voltammetry, molybdenum disulfide.

Determination of Some Rare Earth Elements in Oil Shale Ash

Merania Qawaqneh, Eyad Abu-Nameh & Omar Al-Ayed

Al-Balqa Applied University, Al-Salt, Jordan

Presenting author email: merania.qawaq@gmail.com

Oil shale ash is prepared from the regions of El-Lajjun and Sultani for rare earth elements quantification. The XRF analyses of samples indicated that calcium oxide, silica, sulfur trioxide and aluminum oxide are most abundantly compounds present in oil shale ash, and falls in the ranges, 26-40, 6-26, 1.5-5.8 and 1.9-3.8 wt.% respectively. All the known rare earth elements are detected in different oil shale ash samples with different proportions. The range of maximum-minimum total sum of rare earth elements traced by ICP-MS and LA-ICP-MS in the studied samples are 8-75 and 63-344 ppm respectively. Whereas the sum of the light and heavy rare earth elements is 24-183 and 26-161 ppm as found in the results of LA-ICP-MS findings. The calculated ppm ranges of these metals fluctuated between 12-22 ppm according to the findings of ICP-MS, whereas the range of these metals is 130-5 ppm calculated from the LA-ICP-MS results. Further investigation is performed on Sultani oil shale ash sample where Element Intensity Images obtained using LA-ICP-MS.

Keywords: rare earth elements, oil shale ash, ICP-MS, LA-ICP-MS.

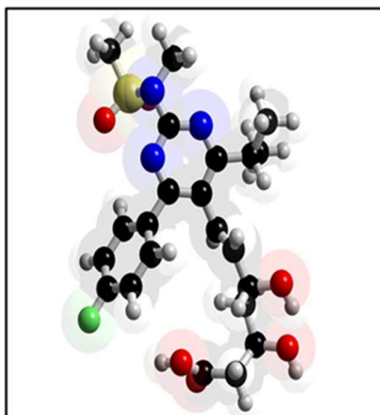
The Role of Electron Acceptor-Donor Materials on Photostability of Rosuvastatin

Bara'ah M. Mshagba ^a, Omar K. Almashaqbeh ^a, Fakhri O. Yousef ^b & Raed Ghanem ^a

a) Al Al-Bayt University, Mafrq, Jordan; b) Al-Hussein Bin Talal University, Ma'an, Jordan

Presenting author email: drbaraah1997@gmail.com

Rosuvastatin (RST) photophysical properties, lifetime, emission, and absorption spectra with various semiconductors were recorded. Rosuvastatin absorption spectra in water show two bands at 204 and 244 nm. There were two transitions shown: π - π^* and n - π^* . The Rosuvastatin emission spectrum shows sole band at 369 nm. The photostability of the Rosuvastatin was studied on the presence and absence of different type of semiconductors. It was found that presence of semiconductors influenced the rate constant for the photoconversion reaction (conversion of RST into its lactone form). Results reveled that presence of semiconductor strongly affect the conversion rate; Semiconductor found to slow down the reaction rate. The maximum effect was attributed to the addition of titanium dioxide. A significant decrease in the reaction rate constant's value from $(4.37 \pm 0.032) \times 10^{-3} \text{ s}^{-1}$ to $(1.35 \pm 0.021) \times 10^{-3} \text{ s}^{-1}$ was recorded due to presence of titanium dioxide.



Structures of RST

Keywords: rosuvastatin, photophysical properties, fluorescence, kinetic analysis.

Ghanem R, Delmani F, Yousef F *et al.*, *Chem. Pap*, **2023**, 10.1007/s11696-023-02864-7

Cucurbit[10]Uril With Iridium(III)Complexes: A Policy to Enhance the Photophysical Properties in Aqueous Media

Shrouq Almarabeh ^a, Lubna Alrawashdeh ^a, Khaleel I. Assaf ^b, Lynne Wallace ^c & Anthony Day ^c

a) The Hashemite University, Zarqa, Jordan; b) Al-Balqa Applied University, Al-Salt, Jordan; c) University of New South Wales, Canberra, Australia

Presenting author email: shorougawad97@gmail.com

The photophysical properties of luminescent iridium (III), Ir(III), cyclometalated complexes are especially interesting for diverse applications, such as in organic light emitting diodes (OLEDs) and as labelling reagents for biomolecules. In many cases, water is the preferred medium in which sensing will be applied, especially for biological systems. However many Ir(III) complexes have much weaker luminescence intensity in aqueous systems compared to organic solvent. In our previous work, we found that the weaker emission typically seen for Ir(III) cyclometalated complexes in aqueous medium can be enhanced via encapsulation in cucurbit[10]uril (Q[10]). As an extension of that effort, in this current work we introduced Q[10] to new iridium(III) cyclometalated complexes that have different substituent groups on bipyridine ligands. ¹H NMR study showed that the solubility of the encapsulated complexes was much lower than that of both of the free guest and host molecules, thus a precipitate was formed upon adding Q[0] to iridium sample. However, the solubility was enough to detect the encapsulation process using fluorescence spectroscopy. A significant enhancement in the luminescence properties of Ir(III) complexes was observed upon adding Q[10] in aqueous medium. The Q[10] cavity was shown to effectively maximize the life time and the quantum yields for of Ir(III) cyclometalated complexes, compared to any other medium. This may provide significant advantages for several sensor applications. The binding study showed that the formation of cavity-encapsulated 1:1 host–guest species dominate the emission, but 1:2 species are also indicated based on lifetime results, which also give some enhancement of intensity. Results demonstrate that the enhancement is due primarily to much lower rates of nonradiative decay. Temperature effect on the encapsulation process was also investigated in this study, it was found that the equilibrium of the encapsulation systems for both complexes was strongly affected by the temperature, as 1:1 cavity bound species was less favorable at a higher temperature.

Keywords: iridium cyclometalated, host-guest, cucurbituril[10], photophysical.

Supercritical CO₂ Extraction of Oil from Oil Shale: Green Extraction Methods and Structural Analysis

Eman M. Khdeir^a, Francesco Barzagli^b, Fawwaz I Khalili^b, Maurizio Peruzzini^b & Mohammad W. Amer^a

a) The University of Jordan, Amman, Jordan; b) ICCOM Institute, Florence, Italy

The supercritical CO₂ (SC-CO₂) extraction technique has recently become a reality in the unconventional oil industry, and its importance is rapidly increasing due to various advantages. These include non-toxicity, reasonable critical properties, the capability of dissolving the primary shale pores and fractures, among others. In this study, we performed oil extraction from Jordanian oil shale using supercritical CO₂ and 10 vol% H₂O as a polar modifier, with the assistance of 10 minutes of ultrasonic extraction. We conducted SC-CO₂ extraction at different operating conditions to investigate the effects of temperature (35-200 °C) and pressure (4-10 MPa) on the yield and organic composition of the extracted oil. The results showed a significant yield of extracted oil using green extraction methods at 75 °C and a pressure of 7.4 MPa. This yield was close to the oil yield obtained from conventional thermal pyrolysis methods. Notably, the subcritical pressure of CO₂ at various temperatures resulted in the minimum extracted oil yield from the shale. Furthermore, we analyzed the extracted oil using elemental analysis, ¹H NMR, and GC-MS. The different analytical methods used for oil characterization revealed a high proportion of saturated carbon compounds. Additionally, it was observed that as the reaction temperature increased, the aliphatic oil content decreased. Interestingly, changing pressure reactions had only a relatively slight effect on the ¹H NMR parameters. This suggests that the oils had almost the same distribution of aliphatic chains and aromatic compounds under different pressure conditions. Overall, these findings demonstrate the potential and efficiency of supercritical CO₂ extraction with water as a polar modifier in obtaining oil from Jordanian oil shale, offering a greener alternative compared to conventional thermal pyrolysis methods.

Keywords: supercritical fluid extraction, GC-MS, oil shale, NMR.

Syntheses and Optical Properties of 2-(anthracen-9-yl)-4,5-bis(4-bromophenyl)-1H-imidazole Derivatives as Chemosensors

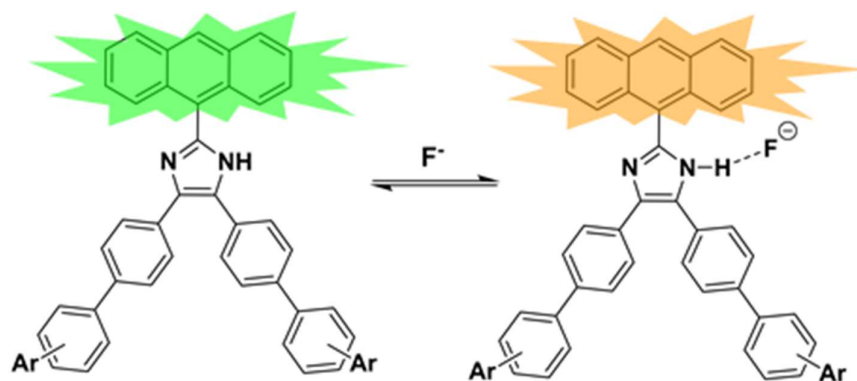
Amneh Snaid, Eyad Younes & Kayed A. Abu Safieh

The Hashemite University, Zarqa, Jordan

Presenting author email: amnahalsnead@gmail.com

Chemosensors play a crucial role in various scientific, industrial, and environmental applications due to their selectivity, sensitivity, real-time monitoring capabilities, non-destructive analysis, versatility, and potential for miniaturization. [1-2]

In this work, novel anthracene-based imidazole derivatives will be presented. The new derivatives were synthesized by the condensation of 4,4-dibromobenzil with 9-anthracene carboxaldehyde, followed by Suzuki coupling reaction with different boronic acids. The isolated compounds were characterized by single-crystal X-ray crystallography, NMR spectroscopy, UV-vis absorption spectroscopy and fluorescence spectroscopy to elucidate their structural, solid-state packing, and electronic properties. Most importantly, they were found to serve as selective chemosensors for fluoride and cyanide ions.



Keywords: chemosensors, anthracene, optical chemosensors, supramolecular chemosensor.

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Tunable Sulphur Doping on ZnO Nanostructures for the Selective Elimination of Dispersed Red 1 Dye from Water

Alaa Bani Omer^a, Qais Al-Bataineh^{b,c,d}, Ahmad Al-Omari^a & Ahmad Telfah^b

a) Jordan University of Science & Technology, Irbid, Jordan; b) The University of Jordan, Amman, Jordan; c) Leibniz Institut für Analytische Wissenschaften-ISAS-e.V., Dortmund, Germany; d) TU Dortmund University, Dortmund, Germany

Presenting author email: ambanyomer20@sci.just.edu.jo

Azo dyes are widely used in textile industries as well as a hazardous wastewater pollutant. Photocatalyst mechanism is one of the most effective methods for wastewater treatment. In this research, we will study the photocatalytic mechanism and degradation pathway of dispersed red 1 dye by zinc oxide nanoparticles (ZnO-NPs) and Sulphur-doped zinc oxide nanoparticles (S/ZnO-NPs) upon UV-irradiation. The size, shape, morphology, and crystallinity of ZnO-NPs and S-doped ZnO-NPs will be examined by Scanning Electron Microscope (SEM), X-ray diffraction (XRD), X-ray fluorescence (XRF), UV-vis spectrophotometer, 4-point prop, and Fourier transform infrared spectroscopy (FTIR). After that, the photocatalyst mechanism, degradation efficiency, and degradation pathway of dispersed red 1 solution by ZnO-NPs and S-doped ZnO-NPs using UV-light were studied by employing UV-vis spectrophotometer, FTIR, and high-performance liquid chromatography HPLC.

Keywords: treatment, azo-dyes, photocatalyst degradation, degradation efficiency.

Inclusion of Digitonin into Beta Cyclodextrin to increase its Stability and Solubility

Heba Haddad ^a, Khaled Shawakfeh ^a, Nathir Alrawashdeh ^a & Bashar Aljawarneh ^b

a) Jordan University of Science and Technology, Irbid, Jordan; b) Al-Zaytoonah University, Amman, Jordan

Presenting author email: hahaddad21@sci.just.edu.jo

Digitonin (DIG), is a steroidal saponin derived from the foxglove plant *Digitalis purpurea* (Plantaginaceae), exhibits potent lytic activity on several kinds of biological membranes as well as cytotoxic effects against a number of cancer cell lines. Because it is widely available and has a hole size that is appropriate for a variety of guest molecules, β -cyclodextrin is employed extensively. The capacity of cyclodextrins to form an inclusion complex with different organic compounds via host-guest interaction with the interior hole, which creates a hydrophobic condition to trap a polar pollutant, is generally considered to be their unique property. In this work, we have included Digitonin within several types of Cyclodextrin for the first time and we started with β -cyclodextrin (β -CD) through a technique named co-precipitation, one of the most popular techniques for obtaining CDs inclusion complexes is co-precipitation, which has the advantages of both ease and efficacy, the technique involves dissolving a particular amount of CDs in water before mixing in an ethanol solution holding the visitor. To study the effect of the encapsulation of Digitonin within β -cyclodextrin on the solubility and stability of several types of cyclodextrin. Digitonin, cyclodextrin, and the prepared complex (DIG/CD) were characterized by Fourier transform infrared spectroscopy (FT-IR), Digitonin and cyclodextrin were characterized by X-ray diffraction (XRD). The morphology of Digitonin and cyclodextrin were characterized by scanning electron microscopy (SEM).

Keywords: inclusion, cyclodextrin, digitonin, co-precipitation.

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Utilizing Natural Cyclodextrins to Improve the Solubility of Apixaban, an Anticoagulant Drug

Rania Atwa^a, Ali I. Ismail^a, Khaled Bodoor^b, Osama M. Abuhasan^a, Khaleel I. Assaf^c, Bayan F. Kulaib^a & Musa I. El-Barghouthi^a

a) The Hashemite University, Zarqa, Jordan; b) The University of Jordan, Amman, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan

Presenting author email: raniaatwa297@gmail.com

Apixaban (APX) is an anticoagulant drug with poor aqueous solubility, limiting its bioavailability. This work aims to investigate the enhancement of its solubility via complexation with the α -, β - and γ -cyclodextrins (CDs). Results from phase solubility studies demonstrate significant enhancement in the case of β -CD. Complex formation was studied using fluorescence, IR and NMR spectroscopy. Furthermore, molecular dynamics (MD) simulations were conducted to study the complexes of APX with the studied CDs and their dynamics, as well as the host-guest interactions.

Keywords: apixaban, cyclodextrin, inclusion complex, molecular dynamics.

Molecular Dynamics Simulations of Cucurbit[n]uril Recognition of Glucosamine Anomers

Dima F. Alhamed^a, Khaleel I. Assaf^b, Khaled Bodoor^c, Lubna Alrawashdeh^a & Musa I. El-Barghouthi^a

a) Hashemite University, Zarqa, Jordan; b) Al-Balqa Applied University, Al-Salt, Jordan; c) The University of Jordan, Amman, Jordan

Presenting author email: dima.fawwaz@outlook.com

Molecular dynamics (MD) simulations were used to study complexation between cucurbit[n]uril (CBn, n = 6, 7, 8) and the neutral (N) and protonated (P) forms of α - and β -anomers of glucosamine (G) in water, and all CBs formed stable inclusion complexes with both forms of each anomer. MM-PBSA revealed that CB6 and CB8 had lower affinities for glucosamine than CB7, with favorable contributions from to stability from electrostatic and van der Waals interactions. Furthermore, 2:1 G: CB8 complexes were found to dissociate to 1:1 complex and free G. The relative stabilities of the bound anomers within each CBn were estimated with thermodynamic integration (TI). The preferred binding by CB7 of GP over GN, as estimated by TI, resulted in a complexation-induced pKa shift of G.

Keywords: cucurbiturils, glucosamine, molecular dynamics, thermodynamic integration.

Preferential Binding of Cucurbit[7]uril toward a Toxic Impurity in Chlorzoxazone, a Muscle Relaxant Drug

Aya W. Bani Melhem^a, Ali I. Ismail^a, Khaled Bodoor^b, Osama M. Abuhasan^a, Khaleel I. Assaf^c, Bayan F. Kulaib^a, Raed Ghanem^d & Musa I. El-Barghouthi^a

a) The Hashemite University, Zarqa, Jordan; b) The University of Jordan, Amman, Jordan; c) Al-Balqa Applied University, Al-Salt, Jordan; d) Al Al-Bayt University, Mafraq, Jordan

Presenting author email: ayawbanimelhem@gmail.com

Chlorzoxazone (CZ) is an orally administered, centrally acting skeletal muscle relaxant. In the manufacturing process of CZ, 2-Amino-4-chlorophenol (ACP) could be formed as a major impurity. ACP is considered toxic material and its maximum allowed limit was set by the USP at 0.5%. Using NMR, isothermal calorimetry (ITC), and fluorescence titrations, we found that cucurbit[7]uril (CB7) preferentially binds ACP over CZ. This suggests that CB7 can be used in quantitative analysis of ACP in pharmaceutical dosage forms of CZ. Furthermore, molecular dynamics (MD) simulations were conducted to study the complexes of CZ and ACP with CB7 and their dynamics, as well as the host-guest interactions.

Keywords: cucurbit[7]uril, chlorzoxazone, inclusion complex, molecular dynamics.

Encapsulation of the Neurotransmitter Dopamine by Cucurbit[7]uril and β -Cyclodextrin

Abdallah H. Suleiman^a, Khaled Bodoor^b, Khaleel I. Assaf^c, Ali I. Ismail^a, Zaher Algharaibeh^a, Osama M. Abuhasan^a,
Bayan F. Kulaib^a, Raed Ghanem^d & Musa I. El-Barghouthi^a

a) The Hashemite University, Zarqa, Jordan; b) The University of Jordan, Amman, Jordan; c) Balqa Applied University, Al-Salt, Jordan; d) Al Al-Bayt University, Mafrq, Jordan

Presenting author email: Abdallahshrouf1999@gmail.com

Dopamine (DP) is a catecholamine neurotransmitter produced in the brain from the precursor tyrosine and is involved in a wide array of functions, including mood, movement, sleep, and cognition among others. The dysfunction of the DP system results in many diseases. In addition, DP is used as a medication in the treatment of Parkinson's disease (PD) and low blood pressure among others, but it suffers in the case of PD, for example, from delivery problems related to the brain blood barrier. Improved delivery can be achieved via its encapsulation within a suitable carrier. Our investigation of the encapsulation of protonated dopamine (DP) within cucurbit[7]uril (CB7) and β -cyclodextrin (β -CD), using fluorescence titrations, isothermal calorimetry (ITC) and NMR reveals higher affinity by the protonated DP for CB7. Furthermore, the effect of adding CD/CB7 on the oxidation potential of DP has been studied using cyclic voltammetry (CV). Molecular dynamics (MD) simulations reveal the formation of complexes by DP with CB7 and β -CD, with the former being more rigid than the latter. Results from the Molecular-Mechanics Poisson-Boltzmann Surface Area (MM-PBSA) method agree with experimental findings for affinity, revealing the importance of electrostatic and van der Waals interactions for the affinities of DP toward CB7 and β -CD, respectively.

Keywords: cucurbit[7]uril, cyclodextrin, dopamine, neurotransmitter, molecular dynamics.

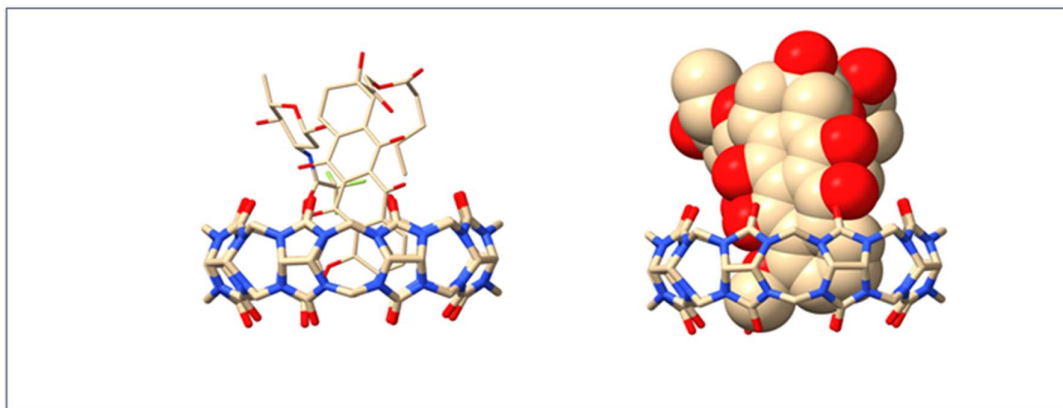
Host-Guest Complexes of Cucurbituril with the Neutral Guest Valrubicin: Synthesis and Characterization

Yara N. Al-Shdifat, Abdelmonem M. Rawashdeh & Yazan H. Ahmad Alakam

Yarmouk University, Irbid, Jordan

Presenting author email: 2020104027@ses.yu.edu.jo

Valrubicin is an anti-cancer drug which belongs to the anthracyclines family which is used for the treatment of bladder cancer. It has been solubilized with Cremophor EL, a solvent known for its systemic toxicity, and because of that its clinical use is currently restricted to intravesical route for bladder cancer treatment. In this work, the possibility of complexation, and to check the cytotoxicity, activity, solubility in water, drug release, and stability will be investigated. Molecular dynamics (MD) simulations were performed to study the binding of the (guest) valrubicin molecule with the (host) cucurbit[n]urils, and to confirm the possibility of the complexation. UV and H-NMR titration will be used to confirm the binding and HPLC for stability and release studies. The resulted MD trajectories show that the inclusion complexes between each CB and valrubicin in water are thermodynamically favorable. UV and H-NMR titration also confirm the complexation. Based on the experimental results from HPLC cucurbituril could be a suitable host for the delivery of Valrubicin and to enhance some of its properties.



Keywords: molecular dynamics, anti-cancer, solubility.

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Fabrication of Photostable Polyvinyl Chloride Films Doped with Tin(IV) Complexes

**Muna Bufaroosha ^a, Noor Emad ^b, Emad Yousif ^b, Dina S. Ahmed ^c, Gamal A. El-Hiti ^d, Amani Husain ^e,
Hassan Hashim ^b & Khalid Zainulabdeen ^b**

a) UAE University, Al-Ain, UAE; b) Al-Nahrain University, Baghdad, Iraq; c) Middle Technical University, Baghdad, Iraq; d) King Saud University, Riyadh, Saudi Arabia; e) Mustansiriyah University, Baghdad, Iraq

Presenting author email: muna.bufaroosha@uaeu.ac.ae

Polyvinyl chloride is used in the manufacturing of a wide range of products, but it is susceptible to degradation if exposed to high temperatures and sunlight. Therefore, a need to continuously explore the design, synthesis, and application of new and improved additives to reduce the photodegradation of polyvinyl chloride in harsh environments and for outdoor applications. New methyldopa–tin complexes as additives inhibit the photodegradation of polyvinyl chloride to make it last longer. Reactions between methyldopa and substituted tin chlorides gave the corresponding organotin complexes. The chemical structures of the synthesized complexes were established, and their effect on the photodegradation of polyvinyl chloride due to UV irradiation was investigated. The films were irradiated for a period of up to 300 h, and the damage that occurred was assessed using infrared spectroscopy, polymeric materials weight loss, depression in molecular weight, and surface inspection. The use of the additives leads to a reduction in photodegradation (e.g., a reduction in the formation of short-chain polymeric fragments, weight loss, and roughness factor) of irradiated PVC. The methyldopa–tin complexes contain aromatic moieties. Therefore, they act as efficient photostabilizers by absorbing ultraviolet radiation and scavenging hydrogen chloride, peroxides, and radical species.

Keywords: polyvinyl chloride films; methyldopa–tin complexes; polymers weight loss; photodegradation; average molecular weight; surface morphology.

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