



6th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

17 – 18 OCTOBER 2020

6th ICNTC BOOK OF ABSTRACTS



6th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

17 – 18 OCTOBER 2020

<http://www.icntcconference.com/>

ICNTC E- Conference 2020

6th International Conference on New Trends in Chemistry

Published by the ICNTC Secretariat

Editor:

Assoc. Prof. Dr. Dolunay ŞAKAR DAŞDAN

ICNTC Secretariat

Büyükdere Cad. Ecza sok. Pol Center 4/1 Levent-İstanbul

E-mail: icntcconference@gmail.com

<http://www.icntcconference.com>

Conference organised in collaboration with Monre Academy

ISBN:978-605-67476-5-6

Copyright @ 2020 ICNTC and Authors

All Rights Reserved

No part of the material protected by this copyright may be reproduced or utilized in any form or by any means electronic or mechanical, including photocopying , recording or by any storage or retrieval system, without written permission from the copyrights owners

SCIENTIFIC COMMITTEE

Prof. Dr. Janusz Stafiej,

Cardinal Stefan Wyszyński University, Warsaw, Poland

Assoc. Prof. Dr. Dolunay Sakar Dasdan,

Yıldız Technical University, Turkey

Conference Chair

PhD Dr. Habil. Agnieszka Kaczor,

Medical University of Lublin, Poland

PhD Dr. Habil. Agata Bartyzel,

University of Maria Curie-Skłodowska, Poland

PhD Dr. Habil. Daniel Ayuk Mbi Egbe,

Linz Institute for Organic Solar Cells, Austria

Dr. Eduardo V. Ludeña,

Escuela Superior Politécnica del Litoral Ecuador

Dr. Hatem M.A. Amin

Faculty of Chemistry and Biochemistry, Ruhr-University Bochum, Germany

Dr. Mauricio Heriberto Cornejo Martinez,

Escuela Superior Politécnica del Litoral Ecuador

PhD Pabitra Saha

RWTH Aachen University, Aachen, Germany

PhD Flavio Massignan

Eötvös Loránd University, Budapest, Hungary

ORGANIZATION COMMITTEE

Assoc. Prof. Dr. Dolunay Sakar Dasdan

Yıldız Technical University – Turkey

Conference Chair

Assoc. Prof. Dr. Yelda Yalcin Gurkan

Namık Kemal University – Turkey

Chemistry Department

Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of “**6th International Conference on New Trends in Chemistry**”, to be held as based on Online Presentations dates between October 17-18, 2020

*Conference was originally planned for April 2020 but due to the global spread of COVID-19 (Corona Virus) and The Council of Higher Education's declaration on “Measures to be Taken in Higher Education Institutions about COVID-19” (March 6, 2020) the conference is postponed to this **current date and will be organized based on online presentations.***

All informations are available in conference web site. For more information please do not hesitate to contact us. icntcconference@gmail.com and info@icntcconference.com.

Limited number of oral and poster studies with the below mentioned topics will be accepted for our conference:

- Polymer Chemistry and Applications
- Pharmaceutical Chemsitry
- Computational Chemistry
- Bio Chemistry
- Physical Chemistry
- Analytical Chemistry
- Inorganic Chemistry
- Organic Chemistry
- Material Chemistry
- Environmental Chemistry

The most distinctive feature of ICNTC Conferences from other conference organizations is that the academicians working interdisciplinary can also attend to presentations performed in different speciality fields and they will also have the opportunity to meet with other academicians coming from various parts of the world.

Selected papers presented oral will be published in one of the Science Citation Index Expanded Journal.

We kindly wait for your attendance to our conference to be held on 16 –18th of October 2020,

Respectfully Yours,

On Behalf of the Organization Committee of ICNTC Conference

Assoc. Prof. Dr. Dolunay SAKAR DASDAN

6th ICNTC 2020 | Conference Chair

Yıldız Technical University – Istanbul / Turkey

Chemistry Department

SCIENTIFIC PROGRAM

17 OCTOBER 2020 SATURDAY

Online access : with given username and password.

08:50 – 09:00

Welcome Speech
Chair

: Assoc. Prof. Dr. Dolunay SAKAR DASDAN / Conference
Yildiz Technical University, Turkey

09:00 – 09:40

Keynote Speaker
Algeria

: Assoc. Prof. Dr. Sameh BOUDIBA / Tebessa University,

Speech Title
Applications

: Anthracene Based Conjugated Polymers for Optoelectronic

09:40 – 09:45

B R E A K

SESSION A

SESSION CHAIR	Assoc. Prof. Dr. Dolunay SAKAR DASDAN Yildiz Technical University	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
09:45– 10:00	Effect of Incorporation of Zinc Oxide on the Properties of PHBV	Semra KIRBOGA
10:00– 10:15	Green synthesis of ZnO particles and their application as catalysts in the transesterification of methyl benzoates	Mohamed Soliman , Elisabete Alegria, Ana Ribeiro, Marta Alves, Fátima Montemor and Armando Pombeiro
10:15– 10:30	Antibacterial Activity and Physical Properties of Bovine Gelatine-Chitosan Wound Dressing Films Supplemented With Propolis	Ilknur KUCUK , Nigar YILDIRIM
10:30– 10:45	The Effects of Additives on Particle Size and Morphology of Barium Sulfate Crystals	Egemen OYMAN, Emel AKYOL
10:45– 11:00	Computational Examination of Degradation Reactions of Precious Endocrine Disruptors Molecules Through Surface Water	Simal KURUMOGLU , Yelda YALCIN GURKAN
11:00– 11:15	Molecular Sensors: Design, Synthesis and Practical Applications	Erman KARAKUS
11:15– 11:30	Theoretical and Molecular Docking Analysis of Silver-nhc Complexes as a Potential Anticancer Agent	Neslihan SAHIN , Elvan USTUN
11:30– 11:45	Structure of Drug-Polymer Composites Prepared by Nano Spray Dryer	Mirella MIRANKO , Laszlo TRIF, Judit TOTH, Tivadar FECZKO
11:45– 12:00	Polymorphism and Topochemical Reactivity in Fusedring Heteroaromatics	Fabio BORBONE , Roberto CENTORE, Emmanuele PARIS, Antonio CARELLA

17 OCTOBER 2020 SATURDAY

Online access : with given username and password

SESSION B

SESSION CHAIR	Prof.Dr.Sevil YUCEL Yildiz Technical University	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
13:00-13:15	Biodegradable Zwitterionic Nanoparticles With a Biologically Relevant Ucs at Physiological Salt Concentration	Mattia SPONCHIONI , Umberto CAPASSO PALMIERO, Davide MOSCATELLI
13:15 – 13:30	New Voltammetric Method for Determination and Electrochemical Behaviors of Oxaliplatin by cpt-bdd Electrode	Mehmet ASLAN , Abdulkadir LEVENT
13:30 – 13:45	Synthesis of Poly (Methyl Vinyl Ether-Co-Maleic Anhydride)-Cu+2-Bovine Serum Albumin Biocomplex and Investigation of Different pHs and Salt Concentration Effects on The Stability of Poly (Methyl Vinyl Ether-Co-Maleic Anhydride)-Cu+2-Bovine Serum Albumin Biocomplex in Aquous Solutions	Rahime Bilge BORKLU, Dolunay SAKAR DAsDAN , Mesut KARAHAN
13:45 – 14:00	Development of Nanostructured-Graphene-Supported Silver Nanoparticles as Catalysts for Electroreduction of Oxygen in Alkaline Electrolyte	Sylwia ZOLADEK , Magdalena BLICHARSKA-SOBOLEWSKA, Agnieszka ZLOTOROWICZ, Iwona Agnieszka RUTKOWSKA, Krzysztof MIECZNIKOWSKI, Enrico NEGRO, Vito DI NOTO, Pawel KULESZA
14:00 – 14:15	Preparation and Co2 Permeabilities of Pebax Mixed Matrix Membranes With Metal Organic Frameworks	Nagehan CELIK , Sennur DENİZ
14:15 – 14:30	Novel Electrochemical Biosensing of Tyramine Based on Fe ₂ O ₃ NPs-Multiwall Carbon Nanotubes-Hexaammineruthenium-Chitosan Modified Glassy Carbon Electrode	Berna DALKIRAN
14:30-14:45	Stabilization and Harvesting of Hesperetin Microrods From the Hesperetin Stabilised Via Plantacare 2000 Solution by Using Template-Assisted Particle Infiltration Method	Yesim KARAHAN , Marcel POURASGHAR, Marc SCHNEIDER, Cornelia M. KECK, Dolunay SAKAR DAsDAN
14:45– 15:00	One Pot Synthesis of Piperidine Derivatives and Evaluation of Their Anticancer Potential	Zulfiqar Ali KHAN

15:00-15:15	B R E A K
--------------------	------------------

17 OCTOBER 2020 SATURDAY

Online access : with given username and password

SESSION C

SESSION CHAIR	Mattia SPONCHIONI Politecnico di Milano	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
15:15– 15:30	Optimization of Drying Process for Green Bricks Using Response Surface Methodology	Bercem KIRAN YILDIRIM , Ebru MANCUHAN, Sibel TITIZ SARGUT
15:30– 15:45	Water Quality in the Armutlu Beach	Esin BOZKURT KOPUZ
15:45– 16:00	New Voltammetric Strategy for Determination and Electrochemical Behaviors of Metformin by Pencil Graphite Electrode	Yalcin ALTUNKAYNAK , Omer YAVUZ, Abdulkadir LEVENT
16:00– 16:15	Facile Access to O-Heterocycles Using N-Methyl-1-(Methylthio)-2-Nitroethenamine (NMSM)	Musawwer KHAN , Saigal and Sumbulunnesa SHAREEF
16:15– 16:30	Bodipy Functionalized Molecular Metal Oxides: Synthesis, Characterization and Properties	Seda CETINDERE
16:30– 16:45	Antiproliferative Silver-NHC Complexes: Structural and Global Reactivity Descriptor Analysis and Molecular Docking Study	Elvan USTUN , Neslihan SAHIN
16:45– 17:00	Thermal and Mechanical Properties of Continuous Glass Fiber/Pet Composites	Melis Eldem HEPER , Sennur DENİZ
17:00– 17:15	Iridium Oxide Immobilized On Cerium Oxide For Enhanced Water Oxidation	Kadriye Özlem HAMALOĞLU , Rukiye BABACAN TOSUN, Ali TUNCEL
17:15–17:30	Temperature Control In Polystyrene Polymerization Reactor By Using Neural Network Model Predictive Algorithm	Erkin ETIKE, Gülşay ÖZKAN , Hale HAPOĞLU

17 OCTOBER 2020 SATURDAY

Online access : with given username and password

POSTER SESSION A

SESSION CHAIR	Prof. Dr. Mustafa GAZI Eastern Mediterranean University Assoc. Prof. Dr. Yelda YALCIN GURKAN Namik Kemal University Assoc. Prof. Dr. Elvan ÜSTÜN Ordu University	5 min oral presentation after that questions from participants
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
17:30-18:30	Effect Of N-Butanolic Extract Of A Plant Growing Spontaneously In Central Algeria As An Additive In Electrodeposition	Karima HANINI1 , Sameh BOUDIBA, Merzoug BENAHMED, Hocine LAOUER and Louiza BOUDIBA
	Electrochemical Oxidation of Vildagliptin on Pencil Graphite Electrode: Extremely Sensitive Determination in Drugs and Human Urine With Square Wave Voltammetry	Yalcin ALTUNKAYNAK , Omer YAVUZ, Abdulkadir LEVENT
	Computational Examination of Degradation Reactions of Butralin	Simal KURUMOGLU , Yelda YALCIN GURKAN
	The Properties of Phbv/Caco3 Composites Prepared by Melt Processing	Semra KIRBOGA , Mualla ONER
	Determination of Hexanal as Marker of Lipid Oxidation in Edible Oils by Headspace Gas Chromatography	Birute BUGELYTE , Gintare PIPIRAITE, Vilius POSKUS, Vida VICKACKAITE
	Synthesis and Characterisation of a Glutathione-Transferase (Hgtp1-1) Single NUCLEOTIDE Polymorph	Sadhna MATHURA
	Investigation of Structural and Magnetic Properties of Nickel Doped Iron Oxide Nanoparticles Depending on the Amount of Dope Values	Nurcan DOGAN , Namik DIKTAŞ, Ceren ERSEN , Ayhan BINGOLBALI
	Analysis of Molecular Orbital Energies, Global Reactivity Descriptors, and Electronic Transitions of [Mn(CO) ₃ (bpy)(N-benzimidazole)]PF ₆ Complex by DFT/TDDFT-Based Computational Methods	Dolunay ŞAKAR DAŞDAN , Elvan ÜSTÜN
	Bitter Vetch Seed Oil (Vicia Ervilia L.) – A New Source of Bioactive Components	Zhana PETKOVA , Ginka ANTOVA, Olga TENEVA, Maria ANGELOVA-ROMOVA
	Different Response of A 2-Ureido-4-Ferrocenyl Pyrimidine Sensor to CF ₃ SO ₃ H and CF ₃ CO ₂ H Guests	Soma J. KESZEI , Szabolcs BALOGH , Csaba FEHER , Livia NAGY , Nikolay TUMANOV, Johan WOUTERS, Gyorgy

		LENDVAY ,Rita SKODA- FOLDES
--	--	--------------------------------

18 OCTOBER 2020 SUNDAY

09:00 – 09:30

Invited Speaker : **Prof. Dr. Mustafa GAZI** / Eastern Mediterranean University – North Cyprus

Speech Title : Chitosan Based Adsorbents for Boron Removal from Aqueous Solutions

SESSION D

SESSION CHAIR	Prof. Dr. Huriye ICIL Eastern Mediterranean University	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
09:30– 09:45	Polyphosphazene Based Fuel Cell Membranes	Elif Busra CELEBI , Ferda HACIVELIOGLU
09:45– 10:00	Zn-Chitosan Nanoparticles as Ecofriendly Priming Agent: Re-Modulate Antioxidant Potential and Biochemical Attributes in Wheat Seeds for Sustainable Productivity	Hameed ARRUJE, Khalid ALVINA, Hameed AMJAD, Ahmed TOHEED, Farooq TAHIR
10:00- 10:15	Mechanical Properties of Biodegradable PLA/PCl Blend Films Prepared With A-Tocopherol	Nudem DENIZ , Sennur DENIZ
10:15– 10:30	Synthesis and Alpha-Glucosidase Inhibition Studies of 1,2-Benzothiazine Derivatives	Matloob AHMAD
10:30– 10:45	Sodium Nitroprusside Mediated Priming Memory Invokes Water-Deficit Stress Acclimation in Wheat Plants Through Physio-Biochemical Alterations	Hameed ARRUJE , Farooq TAHIR, Hameed, Amjad Sheikh Munir AHMAD
10:45– 11:00	Antimony Adsorption Study of Chitosan Produced From Caridea and Brachyura Shells	Zehra Ozden OZYALCIN , Azmi Seyhun KIPCAK
11:00– 11:15	Processability Improvement of Natural Rubber in Mastication Step by Residual Carbon Black Addition	Merve PEHLIVAN , Bora ATALIK, Sezgin GOKCESULAR
11:15– 11:30	Susceptibility of 99mtc-Ciprofloxacin for Common Infection Causing Bacterial Strains Isolated from Clinical Samples: An in Vitro and in Vivo Study	Syed Ali Raza NAQVI , Aysha AZIZ, Hassina SABIR

11:30 – 11:45	B R E A K
---------------	------------------

18 OCTOBER 2020 SUNDAY

Online access : with given username and password

SESSION E

SESSION CHAIR	Assist.Prof.Dr.Sennur Deniz Yildiz Technical University	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:45- 12:00	A Computational Study on the Structural and Spectral Properties of 2-Hydroxy-4-(2-Hydroxyethoxy)-2-Methylpropiophenone	Asim MANSHA, Noreen AKRAM, Sadia ASIM
12:00– 12:15	Production of Biocomposite Tissue Scaffolds by Using Boron-Containing Bioactive Glass and Collagen/Gelatin Hybrid Polymer for Bone Tissue Engineering	Eda GUNEY, Ceren KECECILER, Dilan ALTAN, Sevil YUCEL
12:15– 12:30	Novel N-4-Piperazinyl-Ciprofloxacin-Aniline Hybrids: Synthesis and in Vitro Biological Evaluation as Anticancer Agents	Rabia AKHTAR, Ameer Fawad ZAHOOOR, Azhar RASUL, Matloob AHMAD, Muhammad Naveed ANJUM, Muhammad AJMAL and Zohaib RAZA
12:30- 12:45	A Novel Nanozyme for Colorimetric Detection Of L-Histidine	Duygu YILDIRIM, Cigdem KIP, Ali TUNCCEL
12:45- 13:00	Optical Molecular Imaging: Fluorescent Smart Probes for Pathogen Detection	Muhammed UCUNCU

13:00 – 13:45	LUNCH BREAK
---------------	-------------

SESSION F

SESSION CHAIR	Prof. Dr. Mustafa GAZI Eastern Mediterranean University	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
13:45– 14:00	Cyclodextrin-Calixarene Nanosponges for the Adsorption of Lead Ion From Aqueous Solution	Salvatore CATALDO, Alberto PETTIGNANO, Paolo Lo MEO, Demetrio MILEA
14:00– 14:15	Catalytic Effect of Amines on a Co2bol Absorption Performance	Ozge YUKSEL ORHAN
14:15– 14:30	Experimental and Theoretical Analysis of a Refrigeration System With Phase Change Material (PCM) Integration	Tugce NOYA, Bercem KIRAN YILDIRIM, Ebru MANCUHAN, Sibel TITIZ SARGUT
14:30– 14:45	Synthesis, Characterization and Structure of Chlorido Platinum(II) Saccharinate Complex Bearing 1,1-Bis(Diphenylphosphino) Methane	Ceyda ICSEL
14:45– 15:00	Application Of Bismuth Film	Gunay ONAL, Yalcin

	Electrode in Determination Of Loratadine by Cathodic Stripping Voltammetry in the Presence of Cationic Surfactant	ALTUNKAYNAK, Abdulkadir LEVENT
15:00- 15:15	Effect of Temperature and Reaction Time on Structural, Morphological and Magnetic Properties of zn-doped Fe_3O_4 Nanoparticles ($Zn_{0.25}Fe_{2.75}O_4$) Synthesized by the Hydrothermal Method	Nurcan DOGAN, Gulsum CALISKAN

18 OCTOBER 2020 SUNDAY

Online access : with given username and password

15:15 – 15:45

Invited Speaker : **Prof. Dr. Huriye ICIL** / Eastern Mediterranean University – North Cyprus

Speech Title : Novel Bay-Substituted Perylene Bisimides

15:45 - 16:00	B R E A K
---------------	------------------

SESSION G

SESSION CHAIR	Prof.Dr.Nursen SARI Gazi University	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
16:00- 16:15	Production of Novel Composite Films Based on Pva-Biosilica	Enver Can KILIC, Emel AKYOL, Burcu KARAKUZU IKIZLER, Ali Can OZARSLAN, Sevil YUCEL
16:15– 16:30	A Facile Method to Prepare Bismuth Doped ZnO Photocatalysts and Their Photocatalytic Property	Nazli TURKTEN
16:30– 16:45	Chemical Reaction in Powder Mixtures of Calcium Hydroxyapatite and Potassium Hydrosulfate Under Mechanical Activation in Acetone Medium	Tatiana SAFRONOVA, Marat AKHMEDOV, Tatiana SHATALOVA, Snezhana TIKHONOVA, Gilyana KAZAKOVA
16:45– 17:00	A Computational Study Of 2,3-Dihydrospiro[Carbazole-1,2'-[1,3]Dithiolan]-4(9H)-One Compound: Structure, FT-IR, NMR, NLO, and NBO Analyses	Goncagul SERDAROGLU, Nesimi ULLUDAG
17:00– 17:15	The Hydrolysis of Tert-Butylamine Borane By Using Ni-Zr-B Catalyst for Hydrogen Production	Hatice Begum MURATHAN, Goksel OZKAN
17:15 – 17:30	Rh-Based Ternary Catalyst for the Catalytic Dehydrogenation of Hydrazine Borane as an Chemical Hydrogen Storage Material	Merve Rabia GURLUK, Gülay OZKAN, Goksel OZKAN

17:30– 17:45	New Triazolo-Triazole Derivatives: Redox and Emission Properties and Cu(I) Complexes	Sandra FUSCO , Emmanuele PARISI , Sabato VOLINO , Carla MANFREDI , Roberto CENTORE
--------------	--	--

18 OCTOBER 2020 SUNDAY

Online access : with given username and password

POSTER SESSION B

SESSION CHAIR	Prof. Dr. Huriye ICIL Eastern Mediterranean University Dr. Emel Akyol Yıldız Technical University Assoc. Prof. Dr. Nurcan DOĞAN İstanbul Kültür Sanatları Akademisi Yıldız Technical University	5 min oral presentation after that questions from participants
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
17:45-18:45	A Spectrophotometric Investigation of the Interaction Between DNA and the Anticancer Drug Candidate Schiff Bases and Their Pt (II) Complexes	Elvan HASANOGLU OZKAN, Suheyra Pinar CELIK, Leyla ACIK, Ali DISLI, Nursen SARI
	Interactions of New Tetrazolato Complexes Containing VIII B Group Transition Metals With DNA	Elvan HASANOGLU OZKAN , Suheyra CELIK, Leyla ACIK, Ali DISLI, Nursen SARI
	The Contribution of Electronegative Groups on The Synthesis and the Antimicrobial Effects of Tetrazol Compounds Containing Different Substituent Groups	Elvan HASANOGLU OZKAN , Hatice OGUTCU, Ali DISLI, Nursen SARI
	Effect of Mixer Rotor Wing Types on Compound Properties	Merve PEHLIVAN , Bora ATALIK, Sezgin GOKCESULAR
	The Effects of Naphthenic Oil, BR, NR and Content of Vinyl in S-SBR on Passenger Tread Compounds	Duygu KABAKOGLU , Sezgin GOKCESULAR
	Electroanalytical Determination of Progesterone Hormone Using Boron-Doped Diamond Electrode	Muhlis UCAR , Abdulkadir LEVENT
	Synthesis of 16 α -Substituted-Pregnenolone Derivatives Via Ionic Liquid-Catalyzed Aza-Michael and Thio-Michael Addition	Lilla MAKSO , Rita SKODA-FOLDES
	Investigation of Switchable Polarity Solvents and Their Application in Claisen-Schmidt	David ISPAN , Rita SKODA-FOLDES

	Reaction of Steroids	
	Aminocarbonylation in the Presence Of Supported Palladium Catalyst	Eniko Nagy , Bernadett ADAMCSIK, Mate PAPP, Bela URBAN, Rita SKODA-FOLDES
	CO ₂ Methanation With Ce Promoted Ni Catalyst Supported on Mixed Materials of Al ₂ O ₃ and Y ₂ O ₃	Nyamsuren BATTUMUR , Enkhsaruul BYAMBAJAV
	Antioxidant Activity of New Glycoconjugates Containing Selenium	Luigia SERPICO , Mauro De NISCO, Flavio CERMOLA, Michele MANFRA, Claus JACOB, Silvana PEDATELLA
	Preparation of Calcium Polyphosphate Powder Containing Amorphous Carbon	Tatiana SAFRONOVA , Yanis PAIANIDI, Tatiana SHATALOVA, Yaroslav FILIPPOV, Gilyana KAZAKOVA, Umarali UMIROV, Otabek TOSHEV
	Synthesis And Characterization Of Phosphazene-Based Epoxy Binders	Elif Busra CELEBI , Halil DUYAR, Cengiz AYAR Rumeysa BARAN, Ferda HACIVELIOGLU
	Tetra 7-Oxy-4-(Pyridin-3-Yl)Coumarin Substituted Copper (I) and Cobalt (I) Phthalocyanines: Synthesis, Spectroscopic Properties and Theoretical Study	Yelda YALCIN GURKAN , Simal KURUMOGLU, Caner Yahya BOYAR, Yasemin KESKEK KARABULUT, Meryem CAMUR

CONTENTS

1-NOVEL BAY-SUBSTITUTED PERYLENE BISIMIDES	
Huriye ICIL	22
2-CHITOSAN-BASED ADSORBENTS FOR BORON REMOVAL	
Mustafa GAZI, Akeem Adeyemi OLADIPO.....	23
3- ANTHRACENE BASED CONJUGATED POLYMERS FOR OPTOELECTRONIC APPLICATIONS.....	
BOUDIBA Sameh , BOUDIBA Louiza , BOUGUESSA Sabrina, GETACHEW Adam, ULBRICHT Christoph, ENENGL Sandra, ENENGL Christina, SARICIFTCI Niyazi Serdar, A.K. GOUASMIA Abdelkrim and A. M. Egbe Daniel.....	24
4-OPTIMIZATION OF DRYING PROCESS FOR GREEN BRICKS USING RESPONSE SURFACE METHODOLOGY.....	
Berçem KIRAN-YILDIRIM, Ebru MANÇUHAN, Sibel TİTİZ SARGUT	25
5-PREPARATION and CO ₂ PERMEABILITIES of PEBA MIXED MATRIX MEMBRANES WITH METAL ORGANIC FRAMEWORKS.....	
Nagehan ÇELİK, Sennur DENİZ.....	26
6-MECHANICAL PROPERTIES of BIODEGRARABLE PLA/PCL BLEND FILMS PREPARED WITH α-TOCOPHEROL.....	
Nudem DENİZ, Sennur DENİZ	27
7-DEVELOPMENT OF NANOSTRUCTURED-GRAPHENE-SUPPORTED SILVER NANOPARTICLES AS CATALYSTS FOR ELECTROREDUCTION OF OXYGEN IN ALKALINE ELECTROLYTE	29
SYLWIA ZOLADEK, MAGDALENA BLICHARSKA-SOBOLEWSKA, AGNIESZKA ZLOTOROWICZ, IWONA AGNIESZKA RUTKOWSKA, KRZYSZTOF MIECZNIKOWSKI, ENRICO NEGRO, VITO DI NOTO, PAWEŁ KULESZA.....	29
8-NOVEL ELECTROCHEMICAL BIOSENSING OF TYRAMINE BASED ON Fe ₂ O ₃ NPs-MULTIWALL CARBON NANOTUBES-HEXAAMMINERUTHENIUM-CHITOSAN MODIFIED GLASSY CARBON ELECTRODE.....	
Berna DALKIRAN.....	30
9-SYNTHESIS, CHARACTERIZATION and STRUCTURE of CHLORIDO PLATINUM(II) SACCHARINATE COMPLEX BEARING 1,1-BIS(DIPHENYLPHOSPHINO)METHANE	
Ceyda İÇSEL	31
10-SYNTHESIS OF POLY (METHYL VINYL ETHER-CO-MALEIC ANHYDRIDE)-Cu ⁺² -BOVINE SERUM ALBUMIN BIOCOMPLEX AND INVESTIGATION OF DIFFERENT pHs AND SALT CONCENTRATION EFFECTS ON THE STABILITY OF POLY (METHYL VINYL ETHER-CO-MALEIC ANHYDRIDE)-CU ⁺² -BOVINE SERUM ALBUMIN BIOCOMPLEX IN AQUOUS SOLUTIONS	
Rahime Bilge BÖRKLÜ, Dolunay ŞAKAR DAŞDAN, Mesut KARAHAN.....	32
11-A NOVEL NANOZYME FOR COLORIMETRIC DETECTION OF L-HISTIDINE	
Duygu YILDIRIM, Çiğdem KİP, Ali TUNCEL	33
.....	
12-PRODUCTION OF BIOCOMPOSITE TISSUE SCAFFOLDS BY USING BORON-CONTAINING BIOACTIVE GLASS AND COLLAGEN/GELATIN HYBRID POLYMER FOR BONE TISSUE ENGINEERING	
Eda GÜNEY, Ceren KEÇECİLER, Dilan ALTAN, Sevil YÜCEL.....	34

<u>13</u> -POLYPHOSPHAZENE BASED FUEL CELL MEMBRANES.....	
Elif Büşra ÇELEBİ, Ferda HACİVELİOĞLU	35
<u>14</u> -ANTIPROLIFERATIVE SILVER-NHC COMPLEXES: STRUCTURAL AND GLOBAL REACTIVITY DESCRIPTOR ANALYSIS AND MOLECULAR DOCKING STUDY.....	
Elvan ÜSTÜN, Neslihan ŞAHİN.....	36
<u>15</u> -TEMPERATURE CONTROL IN POLYSTYRENE POLYMERIZATION REACTOR BY USING NEURAL NETWORK MODEL PREDICTIVE ALGORITHM	
Erkin ETİKE, Gülay ÖZKAN, Hale HAPOĞLU	37
<u>16</u> -MOLECULAR SENSORS: DESIGN, SYNTHESIS AND PRACTICAL APPLICATIONS.....	
Erman KARAKUŞ	38
<u>17</u> -WATER QUALITY IN THE ARMUTLU BEACH	
Esin BOZKURT KOPUZ.....	39
<u>18</u> -POLYMORPHISM AND TOPOCHEMICAL REACTIVITY IN FUSED-RING HETEROAROMATICS	
Fabio BORBONE, Roberto CENTORE, Emmanuele PARISI, Antonio CARELLA	41
<u>19</u> -A COMPUTATIONAL STUDY OF 2,3-DIHYDROSPIRO[CARBAZOLE-1,2'-[1,3]DITHIOLAN]-4(9H)-ONE COMPOUND: STRUCTURE, FT-IR, NMR, NLO, AND NBO ANALYSES	
Goncagül Serdaroğlu Nesimi Uludağ.....	42
<u>20</u> -THE HYDROLYSIS OF TERT-BUTYLAMINE BORANE BY USING Ni-Zr-B CATALYST FOR HYDROGEN PRODUCTION.....	
Hatice Begüm MURATHAN, Göksel ÖZKAN.....	43
<u>21</u> -FACILE ACCESS TO O-HETEROCYCLES USING N-METHYL-1-(METHYLTHIO)-2-NITROETHENAMINE (NMSM)	
Md. Musawwer Khan, Saigal and Sumbulunnesa Shareef.....	44
<u>22</u> -SODIUM NITROPRUSSIDE MEDIATED PRIMING MEMORY INVOKES WATER-DEFICIT STRESS ACCLIMATION IN WHEAT PLANTS THROUGH PHYSIO-BIOCHEMICAL ALTERATIONS	
Hameed Arruje, Farooq Tahir, Hameed, Amjad Sheikh Munir Ahmad,.....	45
<u>23</u> -ZN-CHITOSAN NANOPARTICLES AS ECOFRIENDLY PRIMING AGENT: RE-MODULATE ANTIOXIDANT POTENTIAL AND BIOCHEMICAL ATTRIBUTES IN WHEAT SEEDS FOR SUSTAINABLE PRODUCTIVITY	
Hameed Arruje, Khalid Alvina, Hameed Amjad, Ahmed Toheed, Farooq Tahir	46
<u>24</u> -A COMPUTATIONAL STUDY ON THE STRUCTURAL AND SPECTRAL PROPERTIES OF 2-HYDROXY-4- (2-HYDROXYETHOXY)-2-METHYLPROPIOPHENONE.....	
Asim MANSHA, Noreen AKRAM, Sadia ASIM,	47
<u>25</u> -THE EFFECTS OF ADDITIVES ON PARTICLE SIZE AND MORPHOLOGY OF BARIUM SULFATE CRYSTALS	
Egemen OYMAN, Emel AKYOL,.....	48
<u>26</u> -OPTICAL MOLECULAR IMAGING: FLUORESCENT SMART PROBES FOR PATHOGEN DETECTION	
Muhammed ÜÇÜNCÜ	49
<u>27</u> -BODIPY FUNCTIONALIZED MOLECULAR METAL OXIDES: SYNTHESIS, CHARACTERIZATION AND PROPERTIES	
Seda ÇETİNDERE	50

<u>28</u> -PRODUCTION OF NOVEL COMPOSITE FILMS BASED ON PVA-BIOSILICA.....	
Enver Can KILIÇ, Emel AKYOL, Burcu KARAKUZU İKİZLER, Ali Can ÖZARSLAN, Sevil YÜCEL.....	51
<u>29</u> -COMPUTATIONAL EXAMINATION OF DEGRADATION REACTIONS OF PRECIOUS ENDOCRINE DISRUPTORS MOLECULES THROUGH SURFACE WATER	
Simal KURUMOĞLU, Yelda YALCIN GURKAN.....	52
<u>30</u> -ONE POT SYNTHESIS OF PIPERIDINE DERIVATIVES AND EVALUATION OF THEIR ANTICANCER POTENTIAL.....	
Zulfiqar Ali KHAN	53
<u>31</u> -EFFECT OF MIXER ROTOR WING TYPES ON COMPOUND PROPERTIES	
Merve PEHLIVAN ,Bora ATALIK, Sezgin GOKCESULAR	54
<u>32</u> -PROCESSABILITY IMPROVEMENT OF NATURAL RUBBER IN MASTICATION STEP BY RESIDUAL CARBON BLACK ADDITION	
Merve PEHLIVAN, Bora ATALIK, Sezgin GOKCESULAR	56
<u>33</u> -ANTIBACTERIAL ACTIVITY AND PHYSICAL PROPERTIES OF BOVINE GELATINE-CHITOSAN WOUND DRESSING FILMS SUPPLEMENTED WITH PROPOLIS.....	
İlknur KÜÇÜK, Nigar YILDIRIM	58
<u>34</u> -IRIDIUM OXIDE IMMOBILIZED ON CERIUM OXIDE FOR ENHANCED WATER OXIDATION	
Kadriye Özlem HAMALOĞLU, Rukiye BABACAN TOSUN, Ali TUNCEL	59
<u>35</u> -APPLICATION OF BISMUTH FILM ELECTRODE IN DETERMINATION OF LORATADINE BY CATHODIC STRIPPING VOLTAMMETRY IN THE PRESENCE OF CATIONIC SURFACTANT	
Günay ÖNAL, Yalçın ALTUNKAYNAK, Abdulkadir LEVENT	60
<u>36</u> -SYNTHESIS AND ALPHA-GLUCOSIDASE INHIBITION STUDIES OF 1,2-BENZOTHAZINE DERIVATIVES..	
Matloob AHMAD	61
<u>37</u> -BIODEGRADABLE ZWITTERIONIC NANOPARTICLES WITH A BIOLOGICALLY RELEVANT UCST AT PHYSIOLOGICAL SALT CONCENTRATION.....	
Mattia SPONCHIONI ¹ , Umberto CAPASSO PALMIERO ² , Davide MOSCATELLI ¹	62
<u>38</u> -THERMAL and MECHANICAL PROPERTIES of CONTINUOUS GLASS FIBER/PET COMPOSITES.....	64
Melis Eldem HEPER, Sennur DENİZ	64
<u>39</u> -Rh-BASED TERNARY CATALYST FOR THE CATALYTIC DEHYDROGENATION OF HYDRAZINE BORANE As an CHEMICAL HYDROGEN STORAGE MATERIAL.....	
Merve Rabia GÜRLÜK, Gülay ÖZKAN, Göksel ÖZKAN	65
<u>40</u> -NEW VOLTAMMETRIC STRATEGY FOR DETERMINATION AND ELECTROCHEMICAL BEHAVIORS OF METFORMIN BY PENCIL GRAPHITE ELECTRODE.....	
Yalçın ALTUNKAYNAK, Ömer YAVUZ, Abdulkadir LEVENT	66
<u>41</u> -STRUCTURE OF DRUG-POLYMER COMPOSITES PREPARED BY NANO SPRAY DRYER	
Mirella Mirankó, László Trif, Judit Tóth, Tivadar Feczkó	67
<u>42</u> -GREEN SYNTHESIS OF ZNO PARTICLES AND THEIR APPLICATION AS CATALYSTS IN THE TRANSESTERIFICATION OF METHYL BENZOATES.....	

Mohamed Soliman, Elisabete Alegria, Ana Ribeiro, Marta Alves, Fátima Montemor and Armando Pombeiro	68
<u>43-EFFECT OF TEMPERATURES AND REACTION TIMES ON STRUCTURAL, MORPHOLOGICAL AND MAGNETIC PROPERTIES OF ZN-DOPED Fe_3O_4 NANOPARTICLES ($\text{Zn}_{0.25}\text{Fe}_{2.75}\text{O}_4$) SYNTHESIZED BY THE HYDROTHERMAL METHOD</u>	
Nurcan DOGAN, Gulsum CALISKAN,.....	69
<u>44-A FACILE METHOD TO PREPARE BISMUTH DOPED ZNO PHOTOCATALYSTS AND THEIR PHOTOCATALYTIC PROPERTY</u>	
Nazli TURKTEN	70
<u>45-THEORETICAL AND MOLECULAR DOCKING ANALYSIS OF SILVER-NHC COMPLEXES AS A POTENTIAL ANTICANCER AGENT.....</u>	
Neslihan ŞAHİN ¹ , Elvan ÜSTÜN ²	71
<u>46-NEW VOLTAMMETRIC METHOD FOR DETERMINATION AND ELECTROCHEMICAL BEHAVIORS OF OXALIPLATIN BY CPT-BDD ELECTRODE.....</u>	
Mehmet ASLAN, Abdulkadir LEVENT	72
<u>47-CATALYTIC EFFECT OF AMINES ON A CO_2 BOL ABSORPTION PERFORMANCE</u>	
Ozge YUKSEL ORHAN,.....	73
<u>48-ANTIMONY ADSORPTION STUDY OF CHITOSAN PRODUCED FROM <i>CARIDEA</i> AND <i>BRACHYURA</i> SHELLS</u>	
Zehra Ozden OZYALCIN, Azmi Seyhun KIPCAK	74
<u>49-NOVEL N-4-PIPERAZINYL-CIPROFLOXACIN-ANILINE HYBRIDS: SYNTHESIS AND <i>IN VITRO</i> BIOLOGICAL EVALUATION AS ANTICANCER AGENTS.....</u>	
Rabia AKHTAR, Ameer Fawad ZAHOR, Azhar RASUL, Matloob AHMAD, Muhammad Naveed ANJUM, Muhammad AJMAL and Zohaib RAZA.....	75
<u>50-SYNTHESIS AND CHARACTERISATION OF A GLUTATHIONE-S-TRANSFERASE (hGSTP1-1) SINGLE NUCLEOTIDE POLYMORPH</u>	
Sadhna MATHURA.....	76
<u>51-CYCLODEXTRIN-CALIXARENE NANOSPONGES FOR THE ADSORPTION OF LEAD ION FROM AQUEOUS SOLUTION.....</u>	
Salvatore Cataldo, Alberto Pettignano, Paolo Lo Meo, Demetrio Milea	78
<u>52-NEW TRIAZOLO-TRIAZOLE DERIVATIVES: REDOX AND EMISSION PROPERTIES AND Cu(II) COMPLEXES</u>	
Sandra FUSCO, Emmanuele PARISI, Sabato VOLINO, Carla MANFREDI, Roberto CENTORE	79
<u>53-INVESTIGATION OF SWITCHABLE POLARITY SOLVENTS AND THEIR APPLICATION IN CLAISEN-SCHMIDT REACTION OF STEROIDS.....</u>	
Dávid ISPÁN, Rita SKODA-FÖLDES	81
<u>54-SYNTHESIS AND CHARACTERIZATION OF PHOSPHAZENE-BASED EPOXY BINDERS</u>	
Elif Büşra Çelebi, Halil Duyar, Cengiz Ayar, Rümeysa Baran, Ferda Hacivelioglu	83
<u>55-TETRA 7-OXY-4-(PYRIDIN-3-yl)COUMARIN SUBSTITUTED COPPER (II) and COBALT (II) PHTHALOCYANINES: SYNTHESIS, SPECTROSCOPIC PROPERTIES and THEORETICAL STUDY</u>	

Yelda YALCIN GURKAN, Şimal KURUMOĞLU, Caner Yahya BOYAR, Yasemin KESKEK KARABULUT, Meryem CAMUR,.....	84
<u>56-EFFECT OF N-BUTANOLIC EXTRACT OF A PLANT GROWING SPONTANEOUSLY IN CENTRAL ALGERIA AS AN ADDITIVE IN ELECTRODEPOSITION</u>	
Karima HANINI, Sameh BOUDIBA, Merzoug BENAHMED, Hocine LAOUER and Louiza BOUDIBA	85
<u>57-DETERMINATION OF HEXANAL AS MARKER OF LIPID OXIDATION IN EDIBLE OILS BY HEADSPACE GAS CHROMATOGRAPHY</u>	
Birutė BUGELYTĖ, Gintarė PIPIRAITĖ, Vilius POŠKUS, Vida VIČKAČKAITĖ	86
<u>58-ANALYSIS OF MOLECULAR ORBITAL ENERGIES, GLOBAL REACTIVITY DESCRIPTORS, AND ELECTRONIC TRANSITIONS OF [MN(CO)₃(BPY)(N-BENZIMIDAZOLE)]PF₆] COMPLEX BY DFT/TDDFT-BASED COMPUTATIONAL METHODS</u>	
Dolunay ŞAKAR DAŞDAN, Elvan ÜSTÜN	87
<u>59-THE EFFECTS OF NAPHTHENIC OIL, BR, NR AND CONTENT OF VINYL IN S-SBR ON PASSENGER TREAD COMPOUNDS</u>	
Duygu KABAKOĞLU, Sezgin GÖKÇESULAR	88
<u>60-AMINOCARBONYLATION IN THE PRESENCE OF SUPPORTED PALLADIUM CATALYST</u>	
Enikő Nagy, Bernadett Adamcsik, Máté Papp, Béla Urbán, Rita Skoda-Földes,	90
<u>61-ANTIOXIDANT ACTIVITY OF NEW GLYCOCONJUGATES CONTAINING SELENIUM</u>	
Luigia SERPICO, Mauro De NISCO, Flavio CERMOLA, Michele MANFRA, Claus JACOB, Silvana PEDATELLA.....	91
<u>62-THE CONTRIBUTION OF ELECTRONEGATIVE GROUPS ON THE SYNTHESIS AND THE ANTIMICROBIAL EFFECTS OF TETRAZOL COMPOUNDS CONTAINING DIFFERENT SUBSTITUTENT GROUPS</u>	
Elvan HASANOĞLU ÖZKAN, Hatice ÖĞÜTÇÜ, Ali DİŞLİ, Nurşen SARI.....	92
<u>63-INTERACTIONS OF NEW TETRAZOLATO COMPLEXES CONTAINING VIII B GROUP TRANSITION METALS WITH DNA</u>	
Elvan HASANOĞLU ÖZKAN, Süheyla ÇELİK, Leyla AÇIK, Ali DİŞLİ, Nurşen SARI	94
<u>64-A SPECTROPHOTOMETRIC INVESTIGATION OF THE INTERACTION BETWEEN DNA AND THE ANTICANCER DRUG CANDIDATE SCHIFF BASES AND THEIR Pt (II) COMPLEXES</u>	
Elvan HASANOĞLU ÖZKAN, Süheyla Pınar ÇELİK, Leyla AÇIK, Ali DİŞLİ, Nurşen SARI	96
<u>65-COMPUTATIONAL EXAMINATION OF DEGRADATION REACTIONS OF BUTRALIN</u>	
Şimal KURUMOĞLU, Yelda YALCIN GURKAN.....	97
<u>66-SYNTHESIS OF 16A-SUBSTITUTED-PREGNENOLONE DERIVATIVES VIA IONIC LIQUID-CATALYZED AZA-MICHAEL AND THIO-MICHAEL ADDITION</u>	98
Lilla MAKÓ ¹ , Rita SKODA-FÖLDES ² ,.....	98
<u>67-INVESTIGATION OF STRUCTURAL AND MAGNETIC PROPERTIES OF NICKEL DOPED IRON OXIDE NANOPARTICLES DEPENDING ON THE AMOUNT OF DOPE VALUES</u>	
Nurcan DOĞAN, Namık DİKTAŞ, Ceren ERŞEN , Ayhan BİNGÖLBALİ	99
<u>68-CO₂ METHANATION WITH Ce PROMOTED Ni CATALYST SUPPORTED ON MIXED MATERIALS OF Al₂O₃ AND Y₂O₃</u>	
Nyamsuren Battumur, Enkhsaruul Byambajav	100

<u>69</u> -ELECTROANALYTICAL DETERMINATION OF PROGESTERONE HORMONE USING BORON-DOPED DIAMOND ELECTRODE	
Muhlis UÇAR, Abdulkadir LEVENT	101
<u>70</u> -THE PROPERTIES OF PHBV/CaCO ₃ COMPOSITES PREPARED BY MELT PROCESSING	
Semra KIRBOGA, Mualla ÖNER	102
<u>71</u> -DIFFERENT RESPONSE OF A 2-UREIDO-4-FERROCENYL PYRIMIDINE SENSOR TO CF ₃ SO ₃ H AND CF ₃ CO ₂ H GUESTS.....	
Soma J. Keszei, Szabolcs Balogh, Csaba Fehér, Livia Nagy, Nikolay Tumanov, Johan Wouters, György Lendvay and Rita Skoda-Földes	104
<u>72</u> -PREPARATION OF CALCIUM POLYPHOSPHATE POWDER CONTAINING AMORPHOUS CARBON	
Tatiana SAFRONOVA, Yanis PAIANIDI, Tatiana SHATALOVA, Yaroslav FILIPPOV, Gilyana KAZAKOVA, Umarali UMIROV, Otabek TOSHEV	105
<u>73</u> -ELECTROCHEMICAL OXIDATION OF VILDAGLIPTIN ON PENCIL GRAPHITE ELECTRODE: EXTREMELY SENSITIVE DETERMINATION IN DRUGS AND HUMAN URINE WITH SQUARE WAVE VOLTAMMETRY	
Yalçın ALTUNKAYNAK, Ömer YAVUZ, Abdulkadir LEVENT	106
<u>74</u> -BITTER VETCH SEED OIL (<i>VICIA ERVILIA</i> L.) – A NEW SOURCE OF BIOACTIVE COMPONENTS	
Zhana PETKOVA, Ginka ANTOVA, Olga TENEVA, Maria ANGELOVA-ROMOVA	107
<u>75</u> -CHEMICAL REACTION IN POWDER MIXTURES OF CALCIUM HYDROXYAPATITE AND POTASSIUM HYDROSULFATE UNDER MECHANICAL ACTIVATION IN ACETONE MEDIUM	
Tatiana SAFRONOVA, Marat AKHMEDOV, Tatiana SHATALOVA, Snezhana TIKHONOVA, Gilyana KAZAKOVA	108
<u>76</u> -STABILIZATION AND HARVESTING OF HESPERETIN MICRORODS FROM THE HESPERETIN STABILISED VIA PLANTACARE 2000 SOLUTION BY USING TEMPLATE-ASSISTED PARTICLE INFILTRATION METHOD	
Yesim KARAHAN, Marcel POURASGHAR, Marc SCHNEIDER, Cornelia M. KECK, Dolunay SAKAR DASDAN	109
<u>77</u> -EFFECT OF INCORPORATION OF ZINC OXIDE ON THE PROPERTIES OF PHBV	
Semra KIRBOGA	110
<u>78</u> -SUSCEPTIBILITY OF 99MTC-CIPROFLOXACIN FOR COMMON INFECTION CAUSING BACTERIAL STRAINS ISOLATED FROM CLINICAL SAMPLES: AN IN VITRO AND IN VIVO STUDY.....	
Syed Ali Raza NAQVI, Aysha AZIZ, Hassina SABIR	112
<u>79</u> -EXPERIMENTAL AND THEORETICAL ANALYSIS OF A REFRIGERATION SYSTEM WITH PHASE CHANGE MATERIAL (PCM) INTEGRATION.....	
Tuğçe NOYA, Berçem KIRAN YILDIRIM, Ebru MANÇUHAN, Sibel TİTİZ SARGUT	113

NOVEL BAY-SUBSTITUTED PERYLENE BISIMIDES

Huriye İCİL

Eastern Mediterranean University, Faculty of Arts and Science, Department of
Chemistry, Magosa-North Cyprus, Mersin 10, TURKEY

E-mail: huriye.icil@emu.edu.tr

Abstract

Novel, one bay-substituted perylene bisanhydride and two bay-substituted perylenebisimides have been successfully synthesized with a large and swallow tail type, 2-decyl-1-tetradecanoyl substituents at the bay area (1 and 7 positions). The non-bay-substituted perylene bisimides with the same N-substituents were prepared as model compounds. Absorption and fluorescence, electrochemical, spectroelectrochemical, morphological properties of the compounds were investigated, and then, DFT simulations were conducted. The bay-substituted perylene compounds have shown J-aggregated featureless, very broad absorbance through the UV-Vis-NIR region with a strong fluorescence quenching attributed to efficient intramolecular electron transfer from electron donor 2-decyl-1-tetradecanoyl substituent to PDI acceptor and scaffolds allow pi intermolecular interactions, induced molecular aggregation [1, 2]. Obviously, observed optical characteristics are due to a delicate interplay of different intermolecular and intramolecular interactions in the bay-substituted symmetrical perylene dyes as compared to the non-bay-substituted symmetrical N,N'-substituted perylene bisimides with the similar substituents. The synthesized compounds can be exploited as an off-on fluorescence probes for photonic applications.

Key Words: Bay-substituted perylene bisimides; Fluorescence quenching; Electrochemistry; Spectroelectrochemistry; DFT.

References

- [1] S. Chen, B. Hong, H. Guo, F. Yang, The mesomorphic and photophysical properties of perylene liquid crystals with different bay-rigid spacers. *Liq. Cryst.* 45(6) (2018) 793–800.
<https://doi.org/10.1080/02678292.2017.1383522>
- [2] M. Matussek, M. Filapek, P. Gancarz, S. Krompiec, J.G. Malecki, S. Kotowicz, M. Siwy, S. Maćkowski, A. Chrobok, E. Schab-Balcerzak, A. Słodek, Synthesis and photophysical properties of new perylene bisimide derivatives for application as emitting materials in OLEDs. *Dyes Pigments* 159 (2018) 590–599. <https://doi.org/10.1016/j.dyepig.2018.07.006>.

Chitosan-based Adsorbents for Boron Removal

Mustafa GAZI, Akeem Adeyemi OLADIPO

Polymeric Materials Research Laboratory, Department of Chemistry, Faculty of Arts and Sciences, Eastern Mediterranean University, Famagusta TR North Cyprus, via Mersin 10, Turkey

Abstract

Boron is an essential element that is widely distributed in rocks, soils and natural bodies of water. For livestock and plant growth, trace amounts of boron are extremely significant. However, when present in concentrations above tolerable levels, it can be harmful [1]. As stipulated by the World Health Organization (WHO), the tolerable concentration of boron in drinking water varies from 0.3 to 0.5 ppm, whereas that of highly sensitive to very tolerant plants vary from 0.5 to 10 ppm [1-3]. Excessive boron toxicity has terrible effects on humans, including blood chemistry disorders and neurological effects [3-5]. Boron occurs predominantly in mononuclear forms at concentrations lower than 216 ppm, which are remarkably difficult to remove from the aqueous environment due to their high solubility. Boron also exists as a poly-nuclear or ringed forms in aqueous solutions at higher concentrations, requiring boron-selective adsorbents [2]. For the removal of boron from aqueous solutions, various adsorbents (layered double hydroxides, clays, cellulose, metal-based ferrites and other minerals) have been successfully applied [4-6]. However, some of these materials are limited in their stability, selectivity, and regenerability. In particular, adsorbents containing vicinal diols have been documented to form a powerful boron complex in aqueous media [1-4]; and chitosan is perfect for extracting boron because of its modifiable hydroxyl groups. This paper provides a thorough analysis of both trace and concentrated boron adsorbents based on chitosan from synthetic and actual water bodies. Different methods for improving chitosan are explored and the mechanism of adsorption is checked to enhance its affinity for boron. In particular, the discussion also focuses on the extraction of boron from saline water; the output of chitosan-based adsorbents when competing metal ions and anions are interfered with based in light of recently published results.

Key Words: *Chitosan-based materials; boron-selective adsorbents; functionalized polymers; mechanisms; adsorption kinetics*

Acknowledgement: *The authors acknowledge the financial support of Scientific and Technical Research Council of Turkey (TUBITAK 1001 Project no: 114Z461).*

References

- [1] Oladipo AA, Gazi M (2016) *Reactive and Functional Polymers* 109:23–32.
- [2] Oladipo AA, Gazi M (2017) *Chemical Engineering Research and Design* 121: 329–338.
- [3] Gazi M, Shahmohammadi S (2012) *Reactive and Functional Polymers* 72:680–686.
- [4] Gazi M, Galli G, Bicaç N (2008) *Separation and Purification Technology* 62: 485–489.
- [5] Yüksel S, Yürüm Y (2009) *Separation and Purification Technology* 45: 105–115.
- [6] Irawan C, Liu JC, Wu CC (2011) *Desalination* 276: 322–327.

ANTHRACENE BASED CONJUGATED POLYMERS FOR OPTOELECTRONIC APPLICATIONS

BOUDIBA Sameh^{1*}, BOUDIBA Louiza², BOUGUESSA Sabrina¹, GETACHEW Adam³, ULBRICHT Christoph³, ENENGL Sandra³, ENENGL Christina³, SARICIFTCI Niyazi Serdar³, A.K. GOUASMIA Abdelkrim¹ and A. M. Egbe Daniel⁴

sameh.boudiba@univ-tebessa.dz, boudibasameh@gmail.com

Abstract

The research in progress on silicon derivatives employed as active layer in solar cells has concentrated on semiconductor organic materials [1], doped polymers among others [2], due to the energy gain and sustainable development. This work aims the synthesis of a serial of organic conjugated polymers containing in their structure anthracene moiety. The results of this investigation revealed that the introduction of this moiety, which can be adjusted by its positioning between two triple bonds into the polymer backbone has a remarkable influence on its planarity, affecting the energy gap and the charges transport in the polymer. The electrochemical study exhibited a quasi-reversible redox as well as a total reversibility for the synthesized polymers, probably due to the low stability of the oxidized anthracene due to the non-stability of the "holes" in its skeleton. Nevertheless, an increasing conductivity up to 0.69 S.cm⁻¹ for P4 was obtained through iodine vapor doping. Additionally to the thermogravimetric analysis suggesting a relatively good thermal stability of all studied polymers, the photo-physical properties and behavior of the anthracene unit in different polymer structures by shifting its position (P4 and P5), confirmed that these products appear to be more suitable for photovoltaics. The use of **P1** with PC₆₁BM in photovoltaic cells, displayed that the heterojunction has good yields, about 2.3 to 2.5% without optimization. The performance in efficiency is analogous to the results attained for the photovoltaic mass heterojunction of P3HT: PC₆₁BM.

Key Words: *Organic semiconductor materials, conjugated polymers, anthracene, optoelectronics, photovoltaic.*

References

- [1] Travis L. Benanti, D. Venkataraman (2006) Photosynthesis Research 87: 73–81.
- [2] Cindy G. Tang, Mervin C. Y. Ang, Kim-Kian Choo, Venu Keerthi, Jun-Kai Tan, Mazlan Nur Syafiqah, Thomas Kugler, Jeremy H. Burroughes, Rui-Qi Png, Lay-Lay Chua, Peter K. H. Ho (2016) Nature 539(7630) : 536-540.

OPTIMIZATION OF DRYING PROCESS FOR GREEN BRICKS USING RESPONSE SURFACE METHODOLOGY

Berçem KIRAN-YILDIRIM¹, Ebru MANÇUHAN², Sibel TİTİZ SARGUT³

^{1,2,3}Marmara University, Chemical Engineering Dept., Istanbul, Turkey

¹bercem.kiran@marmara.edu.tr

²emancuhan@marmara.edu.tr

³sibel.sargut@marmara.edu.tr

Abstract

Drying process is of significant importance in terms of the quality of the products such as bricks, roof tiles etc. This process conditions should be under control due to possible occurring shrinkage which can result in cracks, deformations and so on. The properties of the brick bodies such as initial moisture content, clay percentage etc. are of also great contribution on the shrinkage beside especially the drying air properties such as temperature, velocity etc. Moreover, these properties are also considered to optimize the drying time of green bricks which can lead to minimize the energy consumption of the process. Therefore, in this study, we have focused on the effects of the clay content of brick samples, temperature and velocity of the drying air on the drying time. The experimental study was performed under five different values of each parameter. In a laboratory scale tunnel dryer, the green brick samples with 40 % - 60 % clay contents were dried by using different drying air temperatures (50 °C - 70 °C) with various air velocities (1 m/s - 3 m/s).

The evaluation of combined effect of the clay content of green brick sample, temperature and velocity of the drying air on the drying time is more complicated. For this purpose, response surface methodology (RSM) based on Central-Composite Design (CCD) was used to determine the optimal conditions for drying process of green bricks. Moreover the model equation representing drying time of the green brick was developed as function of three parameters such as brick clay content, temperature and velocity.

Key Words: Tunnel Dryer; Green Brick; Central-Composite Design, Drying time

PREPARATION and CO₂ PERMEABILITIES of PEBA MIXED MATRIX MEMBRANES WITH METAL ORGANIC FRAMEWORKS

Nagehan ÇELİK¹, Sennur DENİZ¹

¹Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering,
Chemical Engineering Department, 34220, Esenler, İstanbul-Turkey
e-mail: f2019015@std.yildiz.edu.tr; deniz@yildiz.edu.tr

Abstract

Gas mixtures are separated in industrial systems by the use of cryogenic distillation, adsorption and polymeric membranes. Membrane technologies take a great deal of attention in gas separation, because membrane-based systems have advantages such as low energy consumption, low cost, easy installation and small footprint [1]. The most important parameters emphasized when examining the efficiency of membrane systems are selectivity and permeability. These parameters of membrane material affects the economy of a gas separation membrane process. Permeability is the rate at which any compound penetrates through a membrane, it depends on thermodynamic and kinetic factors. Selectivity is the ability of a membrane to perform a particular distinction. Membrane systems can be used in many fields. In the researches conducted on these systems, carbon dioxide gas separation is the most crucial and interesting area due to the concerns on global warming. Mixed-matrix membranes (MMMs) are based on polymeric membranes filled with inorganic particles as a means to improve their gas separation performance. Metal organic frameworks (MOFs) are highly porous crystalline networks containing metal clusters interconnected by organic linkers [2]. In this study, poly(ether-*b*-amide) (PEBA) was selected as a membrane matrix to prepare the polymer nanocomposite membranes containing with MOF particles. Cu-MOF nanocrystals was synthesized by the solvo-thermal method using with two different modulators (acetic acid or trimethylamine) [2,3]. Copper-based metal organic framework (Cu-MOF) nanocrystals were added to the PEBA membrane matrix to increase the separation performance depending on the selectivity and permeability parameters. PEBA/Cu-MOF membranes were fabricated by the loading of Cu-MOF with different weight ratios (10, 20, 30 wt.%) in PEBA matrix. The effects of CuMOF loading and structures were investigated on the morphologies and CO₂ gas permeabilities of PEBA MMMs. To compare with pure PEBA membrane, CO₂ permeabilities of PEBA/Cu-MOF membranes were measured at 35°C and 3 bar feed pressure.

Key Words: *Mixed-matrix membranes, PEBA, Cu-MOF, Gas separation, Permeability*

References

- [1] Keizer K, Uhlhorn RJR, Burggraaf TJ. (1995) Membrane Science and Technology 2:553-588.
- [2] Tovar TM, Zhao J, Nunn WT, Barton HF, Peterson GW, Parsons GN, LeVan MD (2016) Journal of The American Chemical Society 138(36):11449-11452.
- [3] Wang F, Guo H, Chai Y, Li Y, Liu C (2013) Microporous and Mesoporous Materials 173:181-188.

MECHANICAL PROPERTIES of BIODEGRADABLE PLA/PCL BLEND FILMS PREPARED WITH α -TOCOPHEROL

Nudem DENİZ¹, Sennur DENİZ¹

¹Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering,
Chemical Engineering Department, 34220, Esenler, İstanbul-Turkey
e-mail: f2018025@std.yildiz.edu.tr; deniz@yildiz.edu.tr

Abstract

With the increasing use of petroleum-derived polymers, the variety of products in the packaging industry has also increased with the aim of providing for desired mechanical properties. The wide use of conventional petroleum-based polymers and their environmental impact due to their inconvenient disposal are already alarming, but one alternative could be the promising route of development and use of biodegradable polymers as raw materials for packaging. Poly(lactic acid) (PLA) and poly(ϵ -caprolactone) (PCL) are two well-known biodegradable polyesters with interesting and complementary properties [1,2]. PLA is a semi crystalline thermoplastic that can be obtained from renewable resources such as corn starch [1]. PLA can be used in a wide range of applications in different fields because of its great tensile strength and high modulus [3]. However, PLA is very brittle and this can limit some of its applications [3]. In order to use of PLA as flexible packaging material, it is necessary to add different additives or to blend flexible polymers such as PCL, which presents high flexibility, low melting point and good compatibility with other polymers. For this purpose, additions should be made that can bring flexibility to the same time, but do not decrease the strength.

In this study, biodegradable blends of PLA and PCL were prepared by solution-blending method based on the complementary mechanical properties between both rigid PLA and ductile PCL. PLA/PCL blend films was prepared using different mass fraction of each component. We then evaluated the addition of α -tocopherol as antioxidant agent in the blends. The mechanical properties of PLA/PCL biodegradable films were investigated by adding α -tocopherol in the range of 1.5-3.5 wt%. Referring to previous studies, it has been shown that the introducing of α -tocopherol increases the strength of PLA blends, and it can be used for food packaging. Also, the use of α -tocopherol, which has antioxidant properties, in the packaging films can help to extend the life of the food during its release [2]. Based on this, α -tocopherol was added to improve the mechanical and barrier properties of the PLA/PCL blend films. With the increase of PCL ratio in PLA/PCL blends, the modulus of elasticity decreased and the elongation at break increased. In addition, it was observed that the opacity of the film increased with increasing PCL ratio. With the addition of α -tocopherol to PLA20/PCL80 blend, the elongation at break decreased. As a result, PLA/PCL blend films can be obtained by adding PCL and α -tocopherol to biodegradable PLA matrix for desired mechanical properties of packaging film.

Key Words: PLA, PCL, Biodegradable packaging films, α -Tocopherol, Mechanical properties

References

- [1] Auras R, Lim LT, Selke SEM, Tsuji H (2010) Poly(lactic acid): Synthesis, Structures, Properties, Processing, and Applications, A John Wiley&Sons Inc. Publication.
- [2] Manzanarez-López F, Soto-Valdez H, Auras R (2011) Journal of Food Engineering 104(4): 508-517.
- [3] Garlotta D (2001) Journal of Polymer and The Environment 9(2):63-84.

Development of Nanostructured-Graphene-Supported Silver Nanoparticles as Catalysts for Electroreduction of Oxygen in Alkaline Electrolyte

SYLWIA ZOLADEK¹, MAGDALENA BLICHARSKA-SOBOLEWSKA¹, AGNIESZKA ZLOTOROWICZ¹, IWONA AGNIESZKA RUTKOWSKA¹, KRZYSZTOF MIECZNIKOWSKI¹, ENRICO NEGRO², VITO DI NOTO², PAWEŁ KULESZA¹

¹ Faculty of Chemistry, University of Warsaw, Pasteura 1, PL-02-093 Warsaw, Poland

² Section of Chemistry for the Technology (ChemTech), Department of Industrial Engineering, University of Padova, Via Marzolo 9, I-35131 Padova (PD), Italy

There has been growing interest in the field of oxygen electroreduction, particularly with respect to potential applications in the science and technology of low-temperature fuel cells. Obviously, many efforts have been made to develop suitable alternative electrocatalysts efficient enough to replace electrocatalysts based on scarce strategic elements such as platinum-group metals. Despite intensive research in the area, there are still a number of fundamental problems to be resolved and the practical oxygen reduction catalysts still utilize systems based on platinum.

The present study refers to a novel and unique approach of fabrication and deposition of silver nanoparticles on different carbon supports: carboxylated-graphene, SiO₂-doped reduced-graphene-oxide (Gr/SiO₂) and chemically reduced graphene oxide. Among important issues is application of inorganic (rather than organic) capping ligand, heteropolytungstate to modify and stabilize silver nanoparticles as well as to link them with the hydroxyl groups on graphene surface. During operation in alkaline medium polyoxometallates disappear but catalytically highly active silver remains and it exhibits excellent stability. The resulting material has occurred to show highly potent electrocatalytic properties toward electroreductions of oxygen in alkaline solution. It was apparent from XRD data that silver nanoparticles are crystalline in nature and have face-centered-cubic structure enriched with high-index Ag(111) facets known to facilitate ORR. The major advantage of the proposed chemical synthetic method is the integration of the superb properties of both silver nanoparticles and graphene supports in a single-step synthesis with a 100% usage of the silver precursor (AgNO₃) according to the coupled plasma mass spectrometer (ICP-MS). What is even more important is that carbon supports have occurred to act effectively as carriers for silver nanostructures. Mutual activating interactions are feasible. The conclusions are reached on the basis of diagnostic electrochemical (e.g. rotating ring disk voltammetry), spectroscopic (FTIR) and microscopic (SEM, TEM) experiments.

A series of comparative experiments with different carbon carriers and model catalytic materials (e.g. Vulcan-supported platinum) have also been performed. With respect to oxygen reduction, our diagnostic experiments at different concentrations of H₂O₂, support a view that the effect of the fast following chemical (H₂O₂-reductive-decomposition) reaction could be the dominating factor in explaining the observed positive potential shift during the oxygen reduction. The fact, that the optimum graphene-based catalytic system produced the oxygen reduction peak current comparable to that observed at the model platinum containing catalyst, would imply the efficient four-electron-type reduction mechanism.

Acknowledgments:

This work has been supported by the National Science Center (NCN, Poland) under Opus Project 2018/29/B/ST5/02627. We also acknowledge the European Commission through the Graphene Flagship - Core 1 project [Grant number GA-696656]. K. Miecznikowski appreciates partial support from National Science Center (Poland) under Project No. 2015/19/B/ST4/03758.

Key Words: Graphene; silver nanoparticles; oxygen reduction; alkaline
NOVEL ELECTROCHEMICAL BIOSENSING OF TYRAMINE BASED
ON Fe₂O₃ NPs-MULTIWALL CARBON NANOTUBES-
HEXAAMMINERUTHENIUM-CHITOSAN MODIFIED GLASSY
CARBON ELECTRODE

Berna DALKIRAN

Ankara University, Faculty of Science, Department of Chemistry, 06560, Tandoğan, Ankara, TURKEY
e-mail: bernadalkiran@gmail.com

Abstract

Tyramine, a biogenic amine, is the decarboxylation of tyrosine. The level of tyramine in many foods can be used as a biomarker for the indication of food quality because tyramine content increases in easily perishable products [1]. In addition, a high concentration of tyramine in food can cause various diseases such as high blood pressure, migraine, hypertension, etc. Therefore, the development of a suitable method for the detection of tyrosine is of importance [2]. Compared with other analytical techniques, electrochemical biosensors are rapid, cost-effective, highly sensitive and selective [1]. In recent years, the applications of nanomaterials to biosensors have received growing interest, due to their excellent properties such as high surface activity, fast electron transfer and good biocompatibility [3]. Redox mediators, together with nanomaterials-based electrochemical biosensors, are also widely used in biosensor construction because they are able to catalyze the oxidation of substrates at a low potential, thus preventing potentials interference [4].

This study is focused on the development of new matrices based on iron oxide nanoparticles (Fe₂O₃NPs), multiwall carbon nanotubes (MWCNT), and hexaammineruthenium (III) chloride (RUT), in the modification of glassy carbon electrodes (GCE). In the fabrication process of the biosensor chitosan (CH) was used to disperse Fe₂O₃NPs, MWCNT and RUT. A known amount of homogeneous solution was dropped casted onto the GCE surface. This modified electrode, with the best architecture, was characterized by cyclic voltammetry and electrochemical impedance spectroscopy. To construct the tyramine biosensor, the prepared tyrosinase solution was immobilized onto the modified electrode. The determination of tyramine was performed by the oxidation of enzymatically generated H₂O₂. The influence of experimental parameters such as enzyme amount, pH, working potential were examined. Optimum applied potential and pH were found to be -0.25 V and 7.0, respectively. The analytical performance of the biosensor was investigated and also they were compared with literature. In conclusion, the presented biosensor can be used for monitoring various food samples.

Key Words: Tyramine, nanomaterials, mediator, biosensor, amperometry

References

- [1] Dalkiran B, Erden PE, Kaçar C, Kılıç E (2019) *Electroanalysis* 31(7):1324-1333.
- [2] Anand SK, Mathew MR, Radecki J, Radecka H, Kumar KG (2020) *Journal of Electroanalytical Chemistry* 878:114531.
- [3] Shrivastava S, Jadon N, Jain R (2016) *TrAC Trends in Analytical Chemistry* 82:55-67.
- [4] Chaubey A, Malhotra B (2002) *Biosensors and Bioelectronics* 17(6-7):441-456.

SYNTHESIS, CHARACTERIZATION and STRUCTURE of CHLORIDO PLATINUM(II) SACCHARINATE COMPLEX BEARING 1,1-BIS(DIPHENYLPHOSPHINO)METHANE

Ceyda İCSEL¹

¹Department of Chemistry, Faculty of Arts and Sciences, Bursa Uludag University, Görükle, Bursa
e-mail: cydicsel@uludag.edu.tr

Abstract

Platinum(II) complexes of phosphines received great attention due to their applications in various fields of chemistry and material science [1]. In addition, the mixed-ligand complexes of platinum(II) with the artificial sweetening agent, saccharin (sacH) also displayed significant anticancer activity compared to cisplatin [2]. The synthesis, characterization, structures and anticancer potentials of platinum(II) complexes containing both 1,1-bis(diphenylphosphino)methane (dppm) and sac were reported earlier [3]. The complexes were obtained in the neutral form $[\text{Pt}(\text{sac})_2(\text{dppm})]$ and cationic form $[\text{Pt}(\text{dppm})_2](\text{sac})_2$. These complexes can be obtained by changing the ratio of the bis(phosphine) ligand. In this study, a new platinum(II) complex bearing dppm, sac and chlorido ligands was reported. This complex was synthesized from the reaction of $[\text{PtCl}(\text{sac})(\text{COD})]$ (COD = 1,5-cyclooctadiene) with dppm. The new complex $[\text{PtCl}(\text{sac})(\text{dppm})]$ was characterized by elemental analysis and common spectroscopic techniques such as FTIR, ^1H , ^{13}C and ^{31}P NMR, and ESI-MS. In addition, the structure of the complex was determined by single crystal X-ray crystallography. In the complex, the platinum(II) ion was coordinated by a bidentate chelating dppm ligand, and anionic sac and chlorido ligands, forming a distorted square planar coordination geometry (Figure 1).

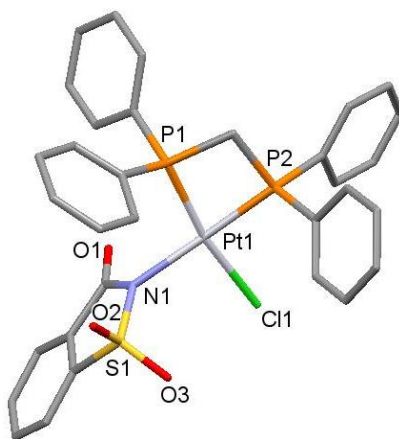


Figure 1. Molecular structure of $[\text{PtCl}(\text{sac})(\text{dppm})]$

Key Words: *Platinum(II); 1,1-bis(diphenylphosphino)methane; saccharin; crystal structure*

References

- [1] BW Malerbi MA (1965) *Platinum Metals Review* 9(2):47–50.
- [2] Yilmaz VT, Icel C, Turgut OR, Aygun M, Erkisa M, Turkdemir MH, Ulukaya E (2018) *European Journal of Medicinal Chemistry* 155:609–622.
- [3] Icel C, Yilmaz VT, Aygun M, Cevatemre B, Alper P, Ulukaya E (2018) *Dalton Transactions* 47:11397–11410.

SYNTHESIS OF POLY (METHYL VINYL ETHER-CO-MALEIC ANHYDRIDE)-Cu⁺²-BOVINE SERUM ALBUMIN BIOCOMPLEX AND INVESTIGATION OF DIFFERENT pHs AND SALT CONCENTRATION EFFECTS ON THE STABILITY OF POLY (METHYL VINYL ETHER-CO-MALEIC ANHYDRIDE)-Cu⁺²-BOVINE SERUM ALBUMIN BIOCOMPLEX IN AQUEOUS SOLUTIONS

Rahime Bilge BÖRKLÜ¹, Dolunay ŞAKAR DAŞDAN^{*2}, Mesut KARAHAN¹

¹Uskudar University, Faculty of Health Science, Department of Nutrition and Dietetics, İstanbul, Turkey.

²Yıldız Technical University, Faculty of Art and Science, Chemistry Department, 34210, İstanbul, Turkey.

*email:dolunaykar@yahoo.com

Abstract

Synthetic peptides with short or long chain of amino acids used in synthetic vaccine systems do not have sufficient size in terms of immunogenic activity. In order to develop the immune response, their molecular weights and diameters need to be increased. Therefore, biopolymer systems are used to stimulate immunity and stimulate the production of antibodies against peptides. Water soluble synthetic polyelectrolyte - metal - protein complexes are functional biopolymer systems. Polyelectrolytes show an adjuvant effect that stimulates immunity. Polyelectrolyte-metal-protein triple biocomplexes, one of the functional biopolymer systems, are structures representing a specific class of conjugates and complexes that have been investigated in many studies as an application area. These structures; synthetic vaccine development, protein purification, enzyme immobilization, drug delivery systems. It is the subject of many studies in the field of medicine, pharmacology and biotechnology [1-4].

In this study, it was determining the stability of PMVEMA-BSA conjugate and PMVEMA-Cu⁺²-BSA biocomplex at different pH and salt concentrations. The data obtained will contribute to the studies on biocomplex, especially synthetic polymeric vaccine systems, It is aimed to obtain preliminary information for the development of more effective and more stable biocomplexes. For this purpose; The PMVEMA-BSA conjugate was synthesized with poly (methyl vinyl ether co-maleic anhydride) (PMVEMA) and bovine serum albumin (BSA), a water-soluble synthetic polyelectrolyte, and PMVEMA-Cu⁺²-BSA biocomplex in the presence of copper ions (Cu⁺²). The stability of polydispersity, particle size, mobility and zeta potential of the aqueous solutions of the prepared conjugates and biocomplexes at varying pH and salt concentrations were measured with Brookhaven 90 Zeta PALS Zetasizer device. It was observed that pH and salt concentrations affect the stability of the conjugate and biocomplex.

Key Words: PMVEMA-BSA conjugate, PMVEMA-Cu⁺²-BSA biocomplex, stability, zetasizer

FUNDING: This work was supported by Research Fund of the Yildiz Technical University. Project Number: 2012-01-02-GEP04.

References

- [1] Morawetz, H., & Hughes Jr, W. L., (1952). The Interaction Of Proteins With Synthetic Polyelectrolytes. I. Complexing Of Bovine Serum Albumin. *The Journal Of Physical Chemistry*, 56(1), 64-69.
- [2] Mustafaev, M. I., & Norimov, A., (1990). Polymer-Metal Complexes Of Protein Antigens New Highly Effective Immunogens. *Biomedical Science*, 1(3), 274-278.
- [3] Reis, C. P., Neufeld, R. J., Ribeiro, A. J., & Veiga, F., (2006). Nanoencapsulation I. Methods For Preparation Of Drug-Loaded Polymeric Nanoparticles. *Nanomedicine: Nanotechnology, Biology And Medicine*, 2 (1), 8-21.
- [4] Şakar Daşdan, D., Karahan, M., Noyan Tekeli, F., & Gölbaşı Şimşek, G., (2019). Modeling Particle Size Of Polyacrylic Acid-Copper (I)-Bovine Serum Albumin Ternary Complex In Salt Solution. *Journal Of The Indian Chemical Society*.

A NOVEL NANOZYME FOR COLORIMETRIC DETECTION OF L-HISTIDINE

Duygu YILDIRIM¹, Çiğdem KİP², Ali TUNCEL³

¹Chemical Engineering Department, Hacettepe University, 06800, Ankara, Turkey, duygu-yildirim@hacettepe.edu.tr

²Chemical Engineering Department, Hacettepe University, 06800, Ankara, Turkey, cigdemg@hacettepe.edu.tr

³Chemical Engineering Department, Hacettepe University, 06800, Ankara, Turkey, atuncel@hacettepe.edu.tr

Abstract

L-histidine plays an important role in the central-nervous system, tissue healing, and growth in humans and other mammals [1]. Abnormal levels of L-histidine are seen as biomarkers of many diseases such as acute renal failure, rheumatism, AIDS, and Alzheimer. Therefore, the determination of L-histidine is crucial for biological research [2]. Hydrogels were used in different fields including biosensors, drug delivery and tissue engineering [3]. In our study, Cu(II) immobilized poly(vinyl phosphonic acid-co-2-hydroxyethyl methacrylate) (poly(VPA-co-HEMA)) hydrogels were synthesized with a one pot reaction. The peroxidase-like activity behavior of the hydrogels were investigated. The colored product 2,3-diaminophenazine (DAP) is produced with the reaction of o-phenylenediamine (OPDA), as a synthetic substrate, and hydrogen peroxide (H₂O₂). DAP, which is the product of colorimetric reaction catalyzed by hydrogel nanozyme, can be detected at 416 nm using UV-Visible spectrophotometer. When hydrogel nanozymes are modified with copper (II) ions, the selective and reversible interaction between copper ions and L-histidine is achieved by binding of L-histidine to Cu sites of Cu-hydrogel nanozyme. Then the active sites of the nanozyme providing catalytic activity decreases by the adsorption of L-histidine onto the nanozyme. The linear calibration plot based on colorimetric response versus L-histidine concentration was prepared using this behavior of Cu-hydrogel nanozymes. Colorimetric determination of L-histidine concentration in buffer media was performed using Cu-hydrogel nanozyme.

Key Words: *Hydrogels, L-Histidine, Colorimetric detection, Peroxidase-like activity, Nanozyme*

References

- [1] Liu YR, Hu R, Liu T, Zhang XB, Tan W, Shen GL, Yu RQ (2013) Talanta 107:402-407
- [2] Sun J, Yang F, Zhao D, Chen C, Yang X (2015) ACS Applied Material Interfaces 7:6860-6866
- [3] Yuan W, Li Z, Xie X, Zhang ZY, Bian L (2020) Bioactive Materials 5:819-831

PRODUCTION OF BIOCOMPOSITE TISSUE SCAFFOLDS BY USING BORON-CONTAINING BIOACTIVE GLASS AND COLLAGEN/GELATIN HYBRID POLYMER FOR BONE TISSUE ENGINEERING

Eda GÜNEY¹, Ceren KEÇECİLER¹, Dilan ALTAN¹, Sevil YÜCEL¹

¹Yildiz Technical University, Faculty of Chemical and Metallurgical Engineering, Department of Bioengineering, Esenler-ISTANBUL, e-mail: eda.gguney@gmail.com

Abstract

Millions of patients experience bone tissue loss every year due to some reasons such as surgery, some diseases, or trauma. Bone has the ability to heal itself, but an external intervention is required to heal large bone defects. Bone grafts are used frequently to repair bone defects caused by trauma or tumour resection [1]. The selection of biomaterials and manufacturing techniques used in the production of scaffolds is very important for tissue regeneration capacity. The aim of this study was to produce tissue scaffolds by using collagen, gelatine, and boron-containing bioactive glass by solvent casting/particulate leaching method. To increase bone formation capacity modified bioactive glasses with boron was used.

In this study, solvent casting/particle leaching method was chosen as the scaffold production technique, thus pore size and porosity were kept under control. Bioactive glass was produced by sol-gel technique. Collagen and gelatine hybrid polymers in different proportions were combined with boron-doped bioactive glass. Characterization of Boron-doped bioactive glass was carried out with AAS (Atomic Absorption Spectroscopy), FTIR (Fourier Infrared Transformation Spectroscopy), BET (Brunner-Emmett-Teller) analysis, XRD (X-Ray Diffraction), TGA (Thermogravimetric Analysis) / DSC (Differential Scanning Calorimetry), and SEM (Scanning electron microscopy). While the structure of the biocomposite tissue scaffolds was characterized by SEM, XRD, and FTIR analysis; swelling capacity and biodegradability tests were also performed. In addition, Hydroxyapatite accumulation on the surface of scaffolds to determine bioactivity was examined by using simulated body fluid (SBF). The effects of biocomposite tissue scaffolds on viability of human osteoblast-like cell line (SaOS-2) were evaluated by MTT cell viability assay.

FTIR, XRD, and SEM analysis results revealed produced scaffold surfaces have good apatite-forming ability. All the results of tests showed that the composite tissue scaffolds containing collagen/ gelatine/ boron-doped bioactive glass can be a promising material to support the healing process of bone defects.

Key Words: *Collagen, gelatine, boron-containing bioactive glass, composite tissue scaffolds, bone tissue regeneration*

References

[1] Şimşek, A., Çakmak, G., & Cila, E. (2004). Kemik Greftleri ve Kemik Greftlerinin Yerini Tutabilecek Maddeler. TOTBİD (Türk Ortopedi ve Travmatoloji Birliği Derneği) Dergisi, 3, 3-4.

Polyphosphazene Based Fuel Cell Membranes

Elif Büşra Celebi, Ferda Hacıvelioğlu

Gebze Technical University Department of Chemistry, 41400, Gebze, Kocaeli, Turkey
bsracelebi@gmail.com

Abstract

Introduction of acid functionality to phosphazenes make them competitors of perfluorosulfonic acid membranes (PFSA), which are widely used in polymer electrolyte membrane fuel cells (PEMFCs). Because, sulfonic and phosphonic acid substituted polyphosphazenes can ensure high resistivity against to chemical oxidation, high thermal stability and close proton conductivity to the PFSA while providing lower fuel crossover. [1] Nevertheless, there is a synthetic challenge to prepare and control the acid functionality on phosphazenes. Because, a simple nucleophilic displacement reaction of an acid containing alkoxy, aryloxy or amine reagent with phosphazene can give mixture of the products and/or crosslinked derivatives. [2] Therefore, protection of the acid functionality and de-protection after the nucleophilic displacement reaction is the safest method to prepare acid functional phosphazenes. Recently we described the control of the phosphonic acid substitution degree on polyaryloxyphosphazenes for preparation of proton conducting polymer electrolyte membranes by covalent protection of the phosphonic acid functionality. [3] Sulfonic acid functional polymers are a logical choice for PEM materials, because strong acidity is required in order to provide high ionic conductivity and thermal stability associated with the sulfonic acid group. There are numerous examples of sulfonated organic polymers such as PSS, sPEEK, PES, sPI and various others developed as an alternative to PFSA membranes for PEM fuel cells. [4] However, polyphosphazenes differ from their organic counterparts in their thermal stability and flexibility associated with the inorganic main chain and in terms of their preparation. In the present study we are going to report some new results from our recent research.

Key Words: Polyphosphazene; PEMFC;

Acknowledgment: We greatly acknowledge TUBITAK for their support on our research (project code 118Z711).

References

- [1] Neburchilov V, Martin J, Wang H, Zhang J (2007) Journal of Power Sources 169:221.
- [2] Ganapathiappan S, Chen K, Shriver DF (1988) Macromolecules 21:2299.
- [3] Hacıvelioğlu F, Okutan E, Çelik SÜ, Yeşilot S, Bozkurt A, Kılıç A (2012) Polymer 53: 3659.
- [4] Çelebi EB, Hacıvelioğlu F, (2017) Polym. Chem. 8:3022.

Antiproliferative Silver-NHC Complexes: Structural and Global Reactivity Descriptor Analysis and Molecular Docking Study

Elvan ÜSTÜN¹, Neslihan ŞAHİN²

¹ Ordu University, Faculty of Science and Arts, Department of Chemistry, 52200 Ordu, Turkey

² Department of Basic Education, Faculty of Education, Sivas Cumhuriyet University, 58140, Sivas, Turkey

Abstract

N-Heterocyclic Carbenes (NHCs) is a well-known ligand family of organometallic chemistry thanks to its catalytic activity [1]. Recently, studies on the biological activity of NHCs and the change of activity depends on both ring size and substituent type are remarkable. The antimicrobial, antitumor, antioxidant and antiviral activities of the benzimidazole derivative NHC molecules were also recorded [2, 3]. On the other hand, the antimicrobial effects of silver salts are historically known, and this is the motivation for studying the bioactivity of NHC-Ag molecules [4].

Since cancer is one of the most fatal diseases in the world, it is an important area that many researchers work on. Breast cancer is one of the most deathful disease among women worldwide. Chemotherapy drugs are important in cancer treatment and are frequently used in conjunction with radiotherapy and surgical applications. In studies about anti-cancer activity, the effects of the molecule on the healthy cells are as important as the effects on the cancerous cell [5]. Therefore, the most suitable molecule must be designed before synthesis and analysis. For this purpose, designing molecules by computational methods saves time, material and labour and theoretical analysis of structure-activity connections are valuable.

In this study, synthesized and characterized Ag-NHC molecules [6] with benzimidazole derivative ligands were theoretically analysed. Both ligand and complex molecules were optimized, their electronic and structural properties were examined, and DNA interactions were investigated by docking methods on DNA, thioredoxin reductase and VEGFR-2 enzymes, which are considered as important in cancer treatment.

Key Words: *N-heterocyclic Carbenes, Silver Complexes, Benzimidazole, DFT/TDDFT, Molecular Docking*

Acknowledgments: This work was supported by the Technological and Scientific Research Council of Turkey TÜBİTAK-3001(118R045).

References

- [1] Hopkinson MN, Richter C, Schedler M, Glorius F (2014) Nature 510:485-496.
- [2] Bouche M, Bonnefont A, Achard T, Bellemin-Laponnaz S (2018) Dalton Trans. 47:11491-11502.
- [3] Asekunowo PO, Haque RA, Razali MR, Avicor SW, Wajidi MFF (2018) Eur. J. Med. Chem. 150:601-615.
- [4] Nomiya K, Morozumi S, Yanagawa Y, Hasegawa M, Kurose K, Taguchi K, Sakamoto R, Mihara K, Kasuga NC (2018) Inorg. Chem. 57:1322-11332.
- [5] Mostafa AS, Gomaa RM, Elmorsy MA (2019) Chem. Biol. Drug Des. 93:454-463.
- [6] Yıldız EÇ, Şahin N, Bölükbaşı SŞ (2020) Journal of Molecular Structure 1199:126987.

TEMPERATURE CONTROL IN POLYSTYRENE POLYMERIZATION REACTOR BY USING NEURAL NETWORK MODEL PREDICTIVE ALGORITHM

Erkin ETIKE, Gülay ÖZKAN, Hale HAPOĞLU

¹Ankara University, Faculty of Engineering, Department of Chemical Engineering,
06100 Maltepe, Ankara, Turkey, e-mail : gozkan@eng.ankara.edu.tr

Abstract

In this work the dynamic behavior and temperature control of free radical solution polymerisation of styrene in a jacketed 1.6 L batch reactor [1] is studied both theoretically and experimentally. In the theoretical part, the analytic model of the process is determined and implemented to MATLAB® Simulink® environment. Heat is introduced to the model in PRBS form and reactor temperature change is recorded. These data are used for system identification in order to build an artificial neural network (NN) model [2,3] which will be used by the control algorithm having heat introduced as the manipulated variable and reactor temperature as the controlled variable. In the experimental part, neural network model predictive control algorithm is written by Visual Basic programming language. Experimental control of the reactor temperature on optimal temperature profile was achieved successfully by neural network model predictive control algorithm.

Key Words: *Neural Network Model Predictive Control, Online Application, Polymerization of Styrene, System identification*

References

- [1] Özkan, G., Tekin, Ö., Hapoğlu, H. (2009). Korean Journal Chemical Engineering, 26, 1201-1207
- [2] Özkan G, Uçan L, Özkan G (2010) Neural Computing and Applications, 1-9
- [3] Mete, T., Ozkan, G. Hapoglu H., Alpbaz M.,(2011) Computer Applications in Engineering Education, 19, 1-10

Molecular Sensors: Design, Synthesis and Practical Applications

Erman KARAKUŞ

Organic Chemistry Laboratory, Chemistry Group, The Scientific and Technological Research Council of Turkey, National Metrology Institute, (TUBITAK UME),
41470, Gebze, Kocaeli, Turkey erman.karakus@tubitak.gov.tr

Abstract

In recent years, the construction of molecular sensors for the detection of environmentally and biologically important species has received a great deal of attention [1]. Among these species, metal ions are the most common. Heavy metal contaminants may be released as waste in the industry, drinking water, or soil threatens human health and the future of the ecosystem. It is known that some metal ions such as Hg^{2+} , Cd^{2+} , Pb^{2+} , Au^{3+} , and As^{3+} are highly toxic and even trace amounts can cause serious fatal diseases [2]. Reactive oxygen/nitrogen/sulfur species such as HOCl , $^1\text{O}_2$, NOO , H_2O_2 , H_2S are also dangerous to human health like heavy metal ions [3]. Therefore, reliable and straightforward methods are highly essential to detect these species. Molecular sensors are very popular compared to traditional instrumental techniques as molecular probes have many preferable advantages such as low cost, simplicity, high sensitivity and reproducibility. Several molecular sensors utilizing various fluorophore units including rhodamine, BODIPY, fluorescein, anthracene and coumarin dyes have been developed over the last few years [4-6].

In view of such information, we have designed and synthesized various molecular sensors to detect different types of analytes and made a significant contribution to the literature. In this context, it will be examined the photophysical and photochemical features of these probes in detail and discuss practical applications.

Key Words: Molecular Sensors, Fluorescent Probes, Fluorometric Determination, Metal Ion Detection, Living-cell Application

References

- [1] Wu D, Sedgwick AC, Gunnlaugsson T, Akkaya EU, Yoon J, James TD (2017) Chemistry Society Reviews 46:7105-7123.
- [2] Quang DT, Kim JS (2010) Chemistry Review 110:6280-6301.
- [3] Wu L, Sedgwick AC, Sun X, Bull SD, He XP, James TD (2019) Accounts of Chemical Research 52:2582-2597.
- [4] Karakuş E, Üçüncü M, Emrulloğlu M (2014) Chemical Communication 50:1119-1121
- [5] Çetintaş C, Karakuş E, Üçünüc M, Emrulloğlu M (2016) Sensors and Actuators B: Chemical 234:109-114.
- [6] Karakuş E, Gunduz S, Liv L, Ozturk T (2020) Journal of Photochemistry & Photobiology A: Chemistry 400:112702.

WATER QUALITY IN THE ARMUTLU BEACH

Esin BOZKURT KOPUZ¹

¹Marmara University Engineering Faculty esin.bozkurt@marmara.edu.tr

Abstract

There is an ongoing relationship in terms of fishing, tourism and transportation both socially and economically on the coasts. It is important to investigate the dynamics of the coasts in terms of people who use them as recreation areas and aquatic creatures that use them as living spaces. For this purpose, the water quality was examined by measuring the sea water temperature, pH, dissolved oxygen, salinity, and concentrations of As, Cd, Cu, Pb, Ni, and Zn daily between 5-14 August 2020 in Armutlu, Yalova. The levels of parameters were close to the previous studies. The order of heavy metal concentrations was: As > Pb > Zn > Cu > Ni > Cd. Armutlu coastline should be saved from pollution, destruction, and crass development.

Key Words: *sea water; water quality; heavy metals*

References

- [1] Taskin E, Tsiamis K, Orfanidis S. Ecological quality of the Sea of Marmara (Turkey) assessed by the Marine Floristic Ecological Index (MARFEI). J Black Sea/Mediterranean Environment 2018;24: 97-114.
- [2] Milliyet news. Accessed 09.09.2020. Available from URL. <https://www.milliyet.com.tr/the-others/marmarada-tanker-faciast-5258847>
- [3] Yalcin Erik N. Petrol tanker kazaları ve neden olduğu çevre kirliliği. Mavi Gezegen Yerbilim Dergisi 2015;20:1-11.
- [4] Bilecenoglu M, Cinar ME, Ozturk B. Endangered species of the Marmara Sea. In: Ozsoy E, Cagatay MN, Balkis N, Balkis N, Ozturk B, editors. The Sea of Marmara, Marine Biodiversity, Fisheries, Conservation and Governance, Istanbul: Turkish Marine Research Foundation Publication; 2016, p.919-934.
- [5] Acarli D, Kale S. Species composition of artificial reef models specifically designed for Homarus gammarus (Crustacea: Decapoda: Nephropidae) in the Sea of Marmara. Research in Marine Sciences 2020;5:625 – 635.
- [6] Song H, Wignall PB, Song H, Dai X, Chu D. Seawater Temperature and Dissolved Oxygen over the Past 500 Million Years. Journal of Earth Science 2019;30:236–243.
- [7] Spencera LH, Horwithb M, Lowec AT, Venkataramana YR, Timmins-Schiffmand E, Nunnd BL, Robertsa SB. Pacific geoduck (Panopea generosa) resilience to natural pH variation. Comparative Biochemistry and Physiology - Part D 2019;30:91-101.
- [8] Jin-Jun L, Zeng-Hui D, Xiang-Rong X, Qun X. Effects of dissolved oxygen, salinity, nitrogen and phosphorus on the release of heavy metals from coastal sediments. Science of the Total Environment 2019;666:894–901.
- [9] Lowe AT, Bos J, Ruesink J. Ecosystem metabolism drives pH variability and modulates longterm ocean acidification in the Northeast Pacific coastal ocean. Scientific Reports 2019;9:1-11.
- [10] Sikder MNA, Al MA, Xu G, Hu G, Xu H. Spatial variations in trophic-functional patterns of periphytic ciliates and indications to water quality in coastal waters of the Yellow Sea. Environmental Science and Pollution Research 2019;26:2592–2602.

- [11] Adefemi OS, Asaolu SS, Olaofe O. Assessment of the physico-chemical status of water samples from major dams in Ekiti State, Nigeria. *Pakistan Journal of Nutrition* 2007;6:657 - 659.
- [12] Atputhanathan M, Chitravadivelu K. Fishes of the Thondaimannar lagoon. *Proc. Sri Lanka Association of Advancement of Science* 1968;25:68.
- [13] Culha ST, Karaduman FR. The influence of marine fish farming on water and sediment quality: Ildir Bay (Aegean Sea). *Environ Monit Assess* 2020;192:1-10.
- [14] Taskin E, Tan I, Minareci E, Mineraci O, Cakır M, Polat Beken C. Ecological quality status of the Turkish coastal waters by using marine macrophytes (macroalgae and angiosperms). *Ecological Indicators* 2020;112:1-9.
- [15] Hair JF, Black WC, Babin BJ, Anderson RE. *Multivariate Data Analysis*. ISBN-13: 978-8131776483, ISBN-10: 8131776484 7th ed. : Pearson; 2009.
- [16] Bozkurt Kopuz E, Pursa A, Yilmaz B, Ozdemir E, Ozturk D. Current Trends in Science and Landscape Management. In: Efe R, Zencirkiran M, Wendt JA, Tumsavas Z, Unal H, Borisova B, editors. *Current Trends in Science and Landscape Management*, Sofia: St. Kliment Ohridski University Press; 2017, p.417.
- [17] State of Turkey. *Turkey Recreational Standards* 2006;Annexes 1,1.
- [18] State of Turkey. *General Quality Criteria of Sea Water in Turkey Regulation on Water Pollution Control Annexes*, 2004;Table 4.
- [19] U.S. EPA. *Quality criteria for water Appendix A*, 1986;233.
- [20] Pekey H, Karakas D, Bakoglu M. Source apportionment of trace metals in surface waters of a polluted stream using multivariate statistical analyses. *Marine Pollution Bulletin* 2004;49:809-818.
- [21] Ergul HA, Ay U, Karademir A, Cayir B, Topcuoglu S, Telli B, Terzi M. Heavy metal concentrations in biota, sediment and sea water samples from Dil Iskelesi region. *Rapp. Comm. int. Mer Médit* 2010;39:246.

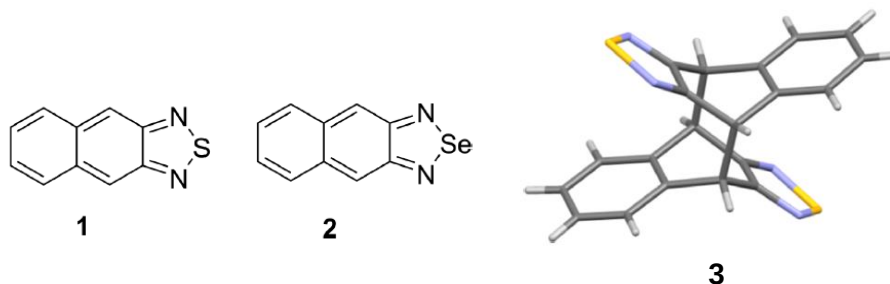
POLYMORPHISM AND TOPOCHEMICAL REACTIVITY IN FUSED-RING HETEROAROMATICS

Fabio BORBONE¹, Roberto CENTORE¹, Emmanuele PARISI¹, Antonio CARELLA¹

¹Department of Chemical Sciences, University of Napoli Federico II, Complesso Monte S. Angelo Via Cintia 80126 – Napoli, Italy - e-mail: fabio.borbone@unina.it

Abstract

The structural study of fused-ring aromatics has been evergreen and gained renewed attention in recent years in relation to their semiconducting properties.[1,2] Beside the classic aromatic hydrocarbon systems showing noteworthy electron/hole transport properties, heteroaromatic derivatives offer the possibility to modulate such properties by tuning the HOMO/LUMO bandgap. However, the introduction of heteroatoms such as nitrogen or sulfur may also lead to modification of the packing modes of the pure hydrocarbon fused-ring aromatics, mainly based on the number and type of rim H atoms.[3,4] This effect can be due to new and stronger interactions which may arise and overcome the usual weak C-H $\cdots\pi$ and $\pi\cdots\pi$ ones, by driving the packing through hydrogen and/or chalcogen bond. In this work naphtho[2,3-c][1,2,5]thiadiazole (1) and naphtho[2,3-c][1,2,5]selenadiazole (2) were synthesized and their solid-state structural properties were investigated. Three different polymorphs of 1 were isolated while only one crystal phase of 2 could be obtained. This result was due to different possible combinations of $\pi\cdots\pi$, C-H $\cdots\pi$, C-H $\cdots$ N, S $\cdots$ N interactions in 1, while in 2 the packing was driven by the strongest Se $\cdots$ N interaction of the chalcogen bond. Fused-ring hydrocarbons have been reported to undergo cycloaddition reactions. In this case, by leaving 1 in chloroform, under visible light at room temperature, single crystals formed which resulted to be a C_{2h} butterfly dimer (3). This reaction also occurred in the solid state under irradiation with UV lamp. The diverse packings of 1 affected its topochemical reactivity, varying from nonreactive packings to packings giving rise to the topochemical reaction.



In this regard, high transverse displacement component and reduced transverse oscillational freedom of the molecules in the crystal can be the reasons behind the photostability of the nonreactive polymorph.

Key Words: *Heterocycle, fused-ring, polymorphism, topochemical reactivity, chalcogen bond*

References

- [1] Chen M, Yan L, Zhao Y, Murtaza I, Meng H, Huang W (2018) J. Mater. Chem. C 6:7416–7444.
- [2] Okamoto H, Kawasaki N, Kaji Y, Kubozono Y, Fujiwara A, Yamaji M (2008) J. Am. Chem. Soc. 130:10470–10471.
- [3] Desiraju GR, Gavezzotti A (1989) J. Chem. Soc., Chem. Commun. 621–623.
- [4] Desiraju GR, Gavezzotti A (1989) Acta Crystallogr., Sect. B: Struct. Sci. B45:473–482.

A Computational Study of 2,3-dihydrospiro[carbazole-1,2'-[1,3]dithiolan]-4(9H)-one compound: Structure, FT-IR, NMR, NLO, and NBO Analyses

Goncagül Serdaroğlu¹ Nesimi Uludağ²

¹Sivas Cumhuriyet University, Department of Science Education, 58140, Sivas, Turkey;
e-mail: goncagul.serdaroglu@gmail.com

²Namık Kemal University, Department of Chemistry, 59030, Tekirdag, Turkey; e-mail: nuludag@nku.edu.tr

Abstract

The substituted carbazole compound has a vital role in synthetic chemistry because the D- π -A bridge provides the charge-transport capability of them, resulting in the potential applications in the field of pharmaceutical or medicinal chemistry [1]. Besides, these group compounds have used in the synthesis of the uleine type alkaloids [2,3], which are obtained from natural sources also for a long time because of their pharmacological importance [4,5]. The 2,3-dihydrospiro[carbazole-1,2'-[1,3]dithiolan]-4(9H)-one compound as a polycyclic aromatic alkaloid, was investigated by using the quantum chemical tools. All calculations were performed by DFT hybrid functionals (B3LYP and M06HF) [6-9] and HF [10,11] method, in three solvent environments (vacuum, chloroform, DMSO), with using the 6-31+G(d,p) and 6-311++G(d,p) basis sets. The calculated FT-IR and NMR [12] spectral data of the compound are compared with those of the observed values. The frontier molecular orbital amplitudes show that the nucleophilic attack site is mostly located over the dithiolane ring, and electrophilic attack site is mainly located on all rings and oxygen atom of the studied compound. NLO [13] analysis indicates that the title compound might be used as an available material in the optoelectronic tools because of the higher $\beta=10.70 \times 10^{-30}$ esu by B3LYP level.

Keywords: FT-IR, NMR, NLO, FMO, donor- acceptor interactions,

Acknowledgments

The author thanks to Scientific Research Projects Department of Cumhuriyet University (Project No: CUBAP: EĞT-090). The all calculations have been conducted at TUBITAK ULAKBIM, High Performance and Grid Computing Center.

References

- [1] Z. A. Kaplancıklı, Marmara Pharmaceutical Journal, **15**, 105-109 (2011).
- [2] N. Uludag, R. Yilmaz, O. Asutay, N. Colak, Chem. Heterocycl. Compd. **52**, 196-199 (2016).
- [3] H-K. Cho, N. T. Tam, G-G. Cho Bull. Korean. Chem. Soc. **31**, 3382-3384 (2010).
- [4] R. Eckermann and T. Gaich, Synthesis, **45**, 2813-2823 (2013).
- [5] D. Maes and R. Maes, Rev. Bras. Farmacogn. **25**, 42-46 (2015).
- [6] A. D. Becke, J. Chem. Phys., **98**, 5648-52 (1993).
- [7] C. Lee, W. Yang, R. G. Parr, Phys. Rev. **B37**, 785-789 (1988).
- [8] Y. Zhao and D. G. Truhlar, J. Phys. Chem. A, **110**, 13126-30 (2006).
- [9] Y. Zhao and D. G. Truhlar, J. Phys. Chem., **110**, 5121-29 (2006).
- [10] C. C. J. Roothaan, Rev. Mod. Phys., **23**, 69 (1951).
- [11] J. A. Pople and R. K. Nesbet, J. Chem. Phys., **22**, 571-72 (1954).
- [12] C. M. Rohlfing, L. C. Allen, R. Ditchfield, Chem. Phys. **87**, 9-15 (1984).
- [13] A. J. Garza, O. I. Osman, A. M. Asiri, G. E. Scuseria, J. Phys. Chem. B. **119**, 1202-1212 (2015).

THE HYDROLYSIS OF TERT-BUTYLAMINE BORANE BY USING Ni-Zr-B CATALYST FOR HYDROGEN PRODUCTION

Hatice Begüm MURATHAN¹, Göksel ÖZKAN¹

¹ Gazi University, Department of Chemical Engineering, 0570, Maltepe, Ankara, Turkey

begummurathan@gazi.edu.tr, gozkan@gazi.edu.tr

Abstract

Hydrogen has been favoured as an energy carrier due to its high-energy capacity, clean burning qualities, and renewable nature. However, the most important issue that hinders the applicability of hydrogen is the storage of hydrogen. Several studies have recently been carried out in the field of hydrogen storage materials [1,2,3,4,5,6]. Chemical storage is the storage of hydrogen in hydrides, amides/imides, hydrocarbons, and boron-based materials [7,8]. From these substances, hydrogen can be released by hydrolysis, thermolysis or alcoholysis. The most remarkable aspect of the hydrolysis, half of the produced hydrogen is obtained from water. Catalytic hydrolysis provides high hydrogen generation yields in low temperatures. This work focuses on the catalytic hydrolysis of tert-butylamine borane (TBAB, $C_4H_9NH_2BH_3$) with Ni-Zr-B catalyst. The catalyst mixture was prepared by co-precipitation method with $NaBH_4$ containing 40% Ni and 60% Zr by mass. The effects of temperature, reaction time and catalyst amount on the hydrogen production yield were investigated. Reaction rate was also calculated as a zero order which was suitable for exponential kinetics [5]. Activation energy, ΔH^{++} and ΔS^{++} were calculated as $52.34 \text{ kJ.mol}^{-1}$, $49.71 \text{ kJ.mol}^{-1}$ and $-178.11 \text{ J.mol}^{-1}.\text{K}^{-1}$ respectively. Turnover frequency value was $789 \text{ mol H}_2.\text{mol Ni}^{-1}.\text{min}^{-1}$ at 55°C . Catalyst was characterized with XRD.

Key Words: *tert-Butylamine Borane, Hydrogen Storage, Hydrolysis, Dehydrogenation*

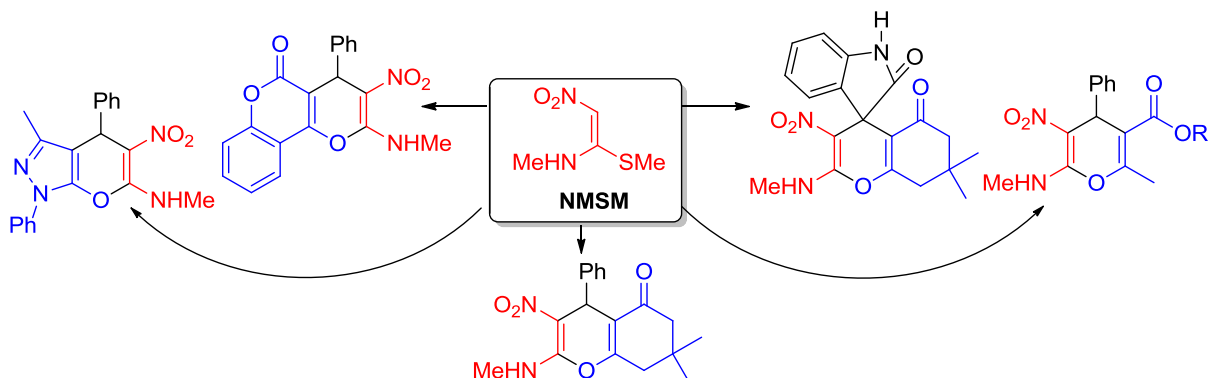
References

- [1] Murathan, H. B., Özkan, G., Akkuş, M. S., Özgür, D. Ö., & Özkan, G., (2018), International Journal of Hydrogen Energy 43: 10728-10733.
- [2] Drost, K. J.(2017) U.S. Patent No. 9,604,850. 28 Mar. 2017.
- [3] Özgür, D. Ö., & Özkan, G., (2017) International Journal of Chemical Kinetics 2017;49(12): 875-883.
- [4] Özkan, G. Akkuş, M.S, Özkan, G, (2019) International Journal of Hydrogen Energy, 44 9811-9816
- [5] Akkuş, M.S, Murathan, H.B, Özgür, D., Özkan, G, Özkan, G. (2018) International Journal of Hydrogen Energy, 43, 10734-10740
- [6] Özgür, D.Ö, Şimşek, T, Özkan, G, Akkuş, M.S, Özkan, G. (2018) International Journal of Hydrogen Energy Volume 43,10765-10772
- [7] Najjar, Y. S.,(2013) . International Journal of Hydrogen Energy, 2013; 38 : 10716-10728.
- [8] Yadav,M., & Xu, Q.,(2012) Energy and Environmental Science, 5: 9698-9725.

Facile Access to O-Heterocycles Using N-Methyl-1-(Methylthio)-2-Nitroethenamine (NMSM)

Md. Musawwer Khan, Saigal and Sumbulunnesa Shareef

Department of Chemistry, Aligarh Muslim University, Aligarh-202002, India
E-mail: musawwer@gmail.com



Abstract

Heterocycles, especially oxygen containing heterocyclic compounds are important molecules and widely distributed in natural products. They exhibit a broad spectrum of biological activities like antitumor, antibiotic, antidepressant, anti-malarial, anti-HIV, anti-microbial, antiviral, anticancer, antitubercular, anti-diabetic and anti-inflammatory. In this presentation, we would like to share our recent works that is synthesis of O-containing heterocycles using N-Methyl-1-(Methylthio)-2-Nitroethenamine (NMSM) is an ambiphilic building block and it belongs to a class of nitroketene *N,S*-acetal.[1]

We have successfully developed practical and green methods for the synthesis of highly functionalized pyrazole-and coumarin-fused 4H-pyrans [2,3], 4H-chromene-5-one [4] under solvent and catalyst free conditions and novel fused spiro 4H-pyrans [5] by the reaction of NMSM with other reacting partners.

The developed protocols have important features such as short reaction time, good to excellent yields, elimination of the use of toxic catalysts or solvents, easy isolation of compounds without traditional column purification and applicability to a broad range of substrates.

Key Words: Green Chemistry; NMSM; 4H-pyrans; 4H-chromene-5-one

References

- [1] Saigal, Khan S, Rahman H, Shafiullah, Khan MM (2019) RSC Adv, 9, 14477–14502.
- [2] Khan MM, Shareef S, Saigal, Sahoo SC (2019) RSC Adv, 9, 26393–26401.
- [3] Khan MM, Saigal, Shareef S, Khan S, Sahoo SC (2019) J. Heterocyclic Chem. 56, 1020-1029.
- [4] Khan MM, Saigal, Shareef S, Khan S, Sahoo SC (2018) Synth. Commun. 48, 2683–2694.
- [5] Saigal, Irfan M, Khan, P, Abid, M, Khan MM (2019) ACS Omega, 4, 16794–16807

Sodium nitroprusside mediated priming memory invokes water-deficit stress acclimation in wheat plants through physio-biochemical alterations

Hameed Arruje,^{1*} Farooq Tahir, Hameed, Amjad³ Sheikh Munir Ahmad,⁴

¹Department of Biochemistry, Government College University, Faisalabad, Pakistan;

²Department of Applied Chemistry, Government College University, Faisalabad, Pakistan

³Nuclear Institute for Agriculture and Biology (NIAB), Jhang Road Faisalabad, Pakistan;

⁴Institute of molecular biology and Biotechnology (IMBB), University of Lahore, Lahore, Pakistan

*Correspondence: arrujetahirfsd@gmail.com, arrujeh@yahoo.com

Abstract

Water-deficit stress has been considered as the most devastating factor that adversely affects plant growth causing yield losses and low crop productivity.¹ In this study, we employed sodium nitroprusside (SNP)² as a seed priming agent for the acclimation of water-deficit stress in wheat plants by invoking priming memory. The SNP-primed (75, 100, and 125 μ M) and non-primed controls were allowed to grow in pots under water deficit as well as normal conditions. The flag leaves of 98-days matured plants were used for biochemical and physiological studies following the well-established methods.³⁻⁵ The antioxidant and hydrolytic enzymes⁶ were upregulated while reducing sugars, total sugars, and glycine betaine⁷ increased significantly in flag leaves of wheat plants originated from SNP-treated seeds compared to control under water deficit stress. However, a significant reduction in MDA and proline contents represented a lesser ROS production which resulted in enhanced cell membrane stability. Consequently, a significant enhancement in yield, plant biomass, and 100 grains weight of wheat plants was observed under water deficit stress. The improvement in yield parameters indicates the induction of priming memory in SNP-primed seeds which elicit water deficit tolerance till the maturity of plants thus ensures sustainable productivity of wheat.

Key Words: Stress-memory, seed priming, wheat, sustainable productivity, water deficit stress tolerance

References

1. Teh, S. Y.; Koh, H. L., Climate change and soil salinization: impact on agriculture, water and food security. *International Journal of Agriculture, Forestry and Plantation* **2016**, 2, 1-9.
2. Wu, S.; Hu, C.; Tan, Q.; Xu, S.; Sun, X., Nitric oxide mediates molybdenum-induced antioxidant defense in wheat under drought stress. *Frontiers in plant science* **2017**, 8, 1085.
3. Giannopolitis, C. N.; Ries, S. K., Superoxide dismutases: I. Occurrence in higher plants. *Plant Physiology* **1977**, 59 (2), 309-314.
4. Heath, R. L.; Packer, L., Photoperoxidation in isolated chloroplasts: I. Kinetics and stoichiometry of fatty acid peroxidation. *Archives of Biochemistry and Biophysics* **1968**, 125 (1), 189-198.
5. Dubois, M.; Gilles, K.; Hamilton, J.; Rebers, P.; Smith, F., A colorimetric method for the determination of sugars. *Nature* **1951**, 168 (4265), 167-167.
6. Varavinit, S.; Chaokasem, N.; Shobsngob, S., Immobilization of a thermostable α -amylase. *Science Asia* **2002**, 28 (3), 247-251.
7. Grieve, C.; Grattan, S., Rapid assay for determination of water soluble quaternary ammonium compounds. *Plant and Soil* **1983**, 70 (2), 303-307.

Zn-chitosan nanoparticles as ecofriendly priming agent: re-modulate antioxidant potential and biochemical attributes in wheat seeds for sustainable productivity

Hameed Arruje,¹ Khalid Alvina,¹ Hameed Amjad,² Ahmed Toheed,³ Farooq Tahir^{3,*}

¹Department of Biochemistry, Government College University, Faisalabad, Pakistan;

²Nuclear Institute for Agriculture and Biology (NIAB), Jhang Road Faisalabad, Pakistan;

³Department of Applied Chemistry, Government College University, Faisalabad, Pakistan;

*Correspondence: Tahir Farooq; email: tahirfarooqfsd@gmail.com

Abstract

Wheat is a major staple food and its seed germination, seedling growth and plant development also experience the abiotic stress-induced negative impacts which ultimately result in low yield [1-2]. Seed priming is a facile seed preconditioning approach which prepares the seeds to counter environmental and eco-toxicological stresses. Priming requires little amount of priming agents (usually synthetic agrochemical) and minimizes the eco-toxicological effects on soil fertility. In this study, Zn-chitosan nanoparticles (Zn-CNPs) have been employed as eco-friendly nano-priming agents to modulate biochemical changes for the enhancement of seed quality [3-4]. The wheat seeds were primed with 0.12% and 0.16% Zn-CNPs for eight hours. The controlled and sustained releasing of Zn from bioactive CNPs increased total soluble proteins, sugars and enhanced the activity of hydrolytic enzymes compared to control. Further, priming treatments up-regulated the antioxidant enzymes, increased TPC as non-enzymatic antioxidant and reduced MDA in wheat seeds. Hence, Zn-CNP treatments induced the synthesis of important biomolecules, boosted antioxidant defense potential and controlled ROS production. All these priming-induced biochemical changes are anticipated to produce positive effects on growth and germinating parameters in wheat seedling under normal and stress conditions. The micronutrient encapsulating biopolymer-based nano-system has been suggested as a smart priming agent for a number of applications without compromising soil fertility and environmental safety.

Keywords: Wheat priming, Zn-chitosan nanoparticles, nano-priming, antioxidants, chitosan

References:

1. Amirjani, M.; Mahdijeh, M., Antioxidative and biochemical responses of wheat to drought stress. *Journal of Agricultural and Biological Science* **2013**, 8 (4), 291-301.
2. Guo, Q.; Wang, Y.; Zhang, H.; Qu, G.; Wang, T.; Sun, Q.; Liang, D., Alleviation of adverse effects of drought stress on wheat seed germination using atmospheric dielectric barrier discharge plasma treatment. *Scientific Reports* **2017**, 7 (1), 16680.
3. Choudhary, R. C.; Kumaraswamy, R.; Kumari, S.; Sharma, S.; Pal, A.; Raliya, R.; Biswas, P.; Saharan, V., Zinc encapsulated chitosan nanoparticle to promote maize crop yield. *International Journal of Biological Macromolecules* **2019**, 127, 126-135.
4. Rahmani, F.; Sayfzadeh, S.; Jabbari, H.; Valadabadi, S. A.; Masouleh, E. H., Alleviation of Drought Stress Effects on Safflower Yield by Foliar Application of Zinc. *International Journal of Plant Production* **2019**, 13 (4), 297-308.

A computational study on the structural and spectral properties of 2-Hydroxy-4-(2-hydroxyethoxy)-2-methylpropiophenone

Asim MANSHA¹, Noreen AKRAM¹, Sadia ASIM²,

¹Department of Chemistry, Government College University Faisalabad, Pakistan

²Department of Chemistry, Government College Women University Faisalabad, Pakistan

Abstract

In the current research work explored the conformational, structural, vibrational, electronic, and thermodynamic parameters of 2-hydroxy-4-(2-hydroxy)-2-methylpropiophenone (Irgacure 2959). The potential energy surface (PES) scan of the Irgacure-2959 molecule was carried out, followed by the geometric optimization of the title compound. The fourier transform (FT)-Infrared and FT-Raman spectra of the title molecule was recorded and computed. The observed and calculated vibrational numbers were assigned and tabulated. The frontier molecular orbital analysis was carried out to elucidate the electronic properties which further used to explore the chemical reactivity and kinetic stability. The stability of the molecule resulting from hyperconjugative interactions and charge delocalization was analysed by the natural bond orbital analysis. The effect of solvent on the UV-Vis spectrum and dipole moment of the title molecule was analysed. The molecular electrostatic potential map was engendered to identify the electrophilic and nucleophilic sites in the title molecule. The thermodynamic functions of the title molecule were obtained by the statistical methods in the range of 50 to 500 K.

Key Words: DFT, FT-IR, FT-Raman, MESP

THE EFFECTS OF ADDITIVES ON PARTICLE SIZE AND MORPHOLOGY OF BARIUM SULFATE CRYSTALS

Egemen OYMAN¹, Emel AKYOL¹,

¹Yildiz Technical University, Department of Chemical Engineering, Davutpasa-Istanbul, Turkey

Abstract

Barium sulfate (BaSO_4) is a very important inorganic compound that is mainly used in the petrol industry but in other industries like paint and pharmaceutical as well [1-2]. As an undesired product in the petrol industry, barium sulfate is a preferred compound in various other fields. Since additives of both organic and inorganic nature play an important role in crystallization, there are plenty of studies related to the use of additives for the production or inhibition of BaSO_4 crystals [3-4].

In the present study, the effects of polystyrene and alginate on particle size and morphology of barium sulfate crystals were investigated. As a second step of this research, the effects of polyacrylic acid (PAA), polyvinyl sulphonic acid (PVS) and polyethylene glycol were investigated to figure out their effect on reducing the rate of barium sulfate crystallization. The crystallizations were made at a constant temperature and pH. SEM analysis of the crystals was made to determine the effect of additives on the particle size and the morphology. The degree of inhibition is measured as the reduction in initial crystallization rate, determined by conductivity of the crystallizing solution. The results have shown that the additives that we used were effective in order to minimize the particle size of the crystals and reducing the rate of barium sulfate crystallization.

Key Words: *Crystallization; barium sulfate; additives; particle size; morphology.*

References

- [1] Gupta A, Singh P, Shivakumara C, (2010) Solid State Communications 150:9-10.
- [2] Merdhan ABB, Yassin AM, (2009) Journal of Petroleum Science and Engineering 70(1-2):79-88.
- [3] Akyol E, Aras Ö, Oner, M (2014) Desalination and Water Treatment 52: 5965–5973.
- [4] Akyol E, Cedimagar MA (2016) Crystal Research and Technology 6: 393–399.

OPTICAL MOLECULAR IMAGING: FLUORESCENT SMART PROBES FOR PATHOGEN DETECTION

Muhammed ÜCÜNCÜ

¹ Department of Analytical Chemistry, Faculty of Pharmacy, Izmir Katip Celebi University, Izmir, Turkey
muhammed.ucuncu@ikcu.edu.tr

² School of Chemistry, University of Edinburgh, Joseph Black Building, David Brewster Road, Edinburgh, EH9 3FJ, United Kingdom

Abstract

Infectious diseases caused by microorganisms including bacteria and fungi result in serious public health problems and economic burden. The emerging increase in antimicrobial resistance (AMR) due to the excessive or misuse of antibiotics have increased the morbidity and mortality rates globally. [1] Early-stage diagnosis and the correct identification of the type of pathogens will play a crucial role to in personalised medicine and a reduction in AMR by allowing the correct prescription and treatment. Culture-based methods are the gold standard in pathogen diagnosis however they require a long culture period. [2] Another important tool is the polymerase chain reaction (PCR) provides quick and accurate detection. However it requires sophisticated instrumentation and reagents, which are often inaccessible, especially in developing countries. [3] Thus the development of new and practical methods for the early-stage diagnosis of pathogens-based diseases is in high demand.

Optical molecular imaging has become popular as a diagnostic tool due to its high sensitivity and selectivity towards target species (e.g. bacteria, fungi). Besides these, ease of applicability and low-cost instrumentations makes it a significant alternative to current diagnostic methods. [4-6] In this regard, we have developed a variety of fluorescent “*smart probes*” that enable the detection and identification of pathogens *in vitro* and *in ex vivo* models. In our “*smart probe*” design the high target specificity was achieved by conjugating fluorescence reporter molecules covalently to target specific-moieties.

Key Words: *Optical Molecular Imaging, Fluorescent “Smart Probes”, Diagnosis, Infectious Diseases, Pathogens*

References

- [1] Aminov R (2010) *Frontiers in Microbiology* 1:134:1 – 7.
- [2] Leck A (2015) *Community Eye Health* 28(89): 8–9.
- [3] Perfect JR (2013) *Current Medical Research and Opinion* 29: 3 – 11.
- [4] Mills B, Bradley M, Dhaliwal K (2016) *Clinical Translational Imaging* 4: 163 – 174.
- [5] Baibek A, Ucuncu M, Blackburn EA, Bradley M, Lilienkamp A (2020) *Peptide Science* e24167.
- [6] Mills B, Megia-Fernandez A, Norberg D, Duncan S, Marshall A, Akram AR, Quinn T, Young I, Bruce AM, Scholefield E, Williams GOS, Krstajić N, Choudhary TR, Parker HE, Tanner MG, Harrington K, Wood HAC, Birks TA, Knight JC, Haslett C, Dhaliwal K, Bradley M, Ucuncu M, Stone JM (2020) *European Journal of Nuclear Medicine and Molecular Imaging* <https://doi.org/10.1007/s00259-020-05021-4>.

BODIPY FUNCTIONALIZED MOLECULAR METAL OXIDES: SYNTHESIS, CHARACTERIZATION AND PROPERTIES

Seda CETİNDERE

¹Gebze Technical University Department of Chemistry 41400 Gebze, Kocaeli
sdemirer@gtu.edu.tr

Abstract

Molecular metal oxides, so called polyoxometalates (POMs), are inorganic metal-oxo cluster anions of the general formula $[M_xO_y]^{n-}$ representing a class of compounds that is unique in its topological and electronic versatility [1]. These polynuclear metal-oxo anions contain highly symmetrical core assemblies of $[MO_x]$ units which are mostly based on early transition metals M such as molybdenum, tungsten and vanadium in their highest oxidation states (generally d^0 , d^1). These high-valent transition metals are often referred to as *addenda* atoms [2]. Functionalization of POMs using organic ligands provides a smart strategy to achieve POM-based inorganic-organic hybrid materials. They combine advantages of organic molecules such as good processability and fine-adjustable structures together with chemical stability and high redox activity of inorganic POM clusters [3]. Boron dipyrromethene (BODIPY) compounds are fluorescent organic dyes which have interesting spectral properties such as high quantum yields (0.6-1.0), large extinction coefficients (60000-80000 M⁻¹cm⁻¹) and narrow emission bands. Absorption and emission properties of these compounds can be adjustable by substitution of different groups into the BODIPY core [4].

The aim of this study is preparation of BODIPY functionalized molecular metal oxides and investigation of their properties to define their application areas [Figure 1].

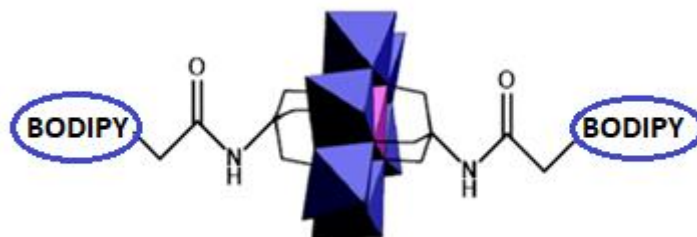


Figure 1. Structure of BODIPY functionalized Anderson type POM.

Key Words: BODIPY, POM, hybrid material, transition metal, addenda atom.

References

- [1] Pope MT, Müller A (1991), Angewandte Chemie International Edition., 103: 56–70.
- [2] Pope MT (2005), Encyclopedia of Inorganic Chemistry, ed. R. B. King, John Wiley & Sons, Inc., Chichester, 2nd edn.
- [3] Pope MT, Jeannin Y, Fournier M (1983), Heteropoly and isopoly oxometalates, Springer-Verlag Berlin, Heidelberg.
- [4] Loudet A, Burgess K (2007), Chemical Reviews, 107:4891-4932.

PRODUCTION OF NOVEL COMPOSITE FILMS BASED ON PVA-BIOSILICA

Enver Can KILIÇ¹, Emel AKYOL¹, Burcu KARAKUZU İKİZLER², Ali Can ÖZARSLAN²,
Sevil YÜCEL²

¹Yildiz Technical University, Department of Chemical Engineering, Davutpasa-Istanbul, Turkey

²Yildiz Technical University, Department of Bioengineering, Davutpasa-Istanbul, Turkey

Abstract

PVA films have been commonly studied in glucose sensors, immuno-isolation membranes, contact lenses and drug delivery systems applications [1-2]. There are various ceramic filler have been studied in order to stabilize or enhance some properties of polymer films such as chemical, thermal and mechanical stabilities[3].

In this study, PVA/silica gel composite films were prepared. Tetraethoxysilane (TEOS), tetramethoxysilane (TMOS) or sodium silicate solutions are generally used in production of composite silica films as silica sources. Sodium silicate solution was produced from rice hull ash which is a cheap agricultural waste by alkali extraction method [4]. Sodium silicate solutions were gelated at pH 7 with HCl addition by sol-gel method. Silica gels were added to PVA films at first time with this study which is different than the literature studies. Composite films were produced by using obtained gels and PVA with three different viscosity grades. PVA, has different viscosity and same hydrolysis degrees; 5:88, 26:88 and 40:88. PVA/silica gel films were obtained by drying at room temperature for 24 hours and in vacuum. Structural characteristics of prepared PVA/silica gel films were determined by FT-IR analysis and their surface morphology was determined by SEM. Films obtained with high viscosity PVA showed homogeneous structure and slightly higher absorption capacity.

Key Words: *P VA Films; Sodium Silicate Solution; Sol-Gel Method; Silica; Absorption.*

References

- [1] Narayanaswam R, Torchilin VP (2019) Molecules 24(3):603.
- [2] Kashyap N, Kumar N, Ravi Kumar MNV (2005) Critical Reviews in Therapeutic Drug Carrier Systems 22(2):107-49.
- [3] Chrissafis K, Bikiaris DN,(2011) Thermochimica Acta 523(1-2):1-24.
- [4] Özgül-Yücel S, Tolay M, Erdağ S, Türkay S (2004) Journal of The American Oil Chemists Society, 81, 619-620.

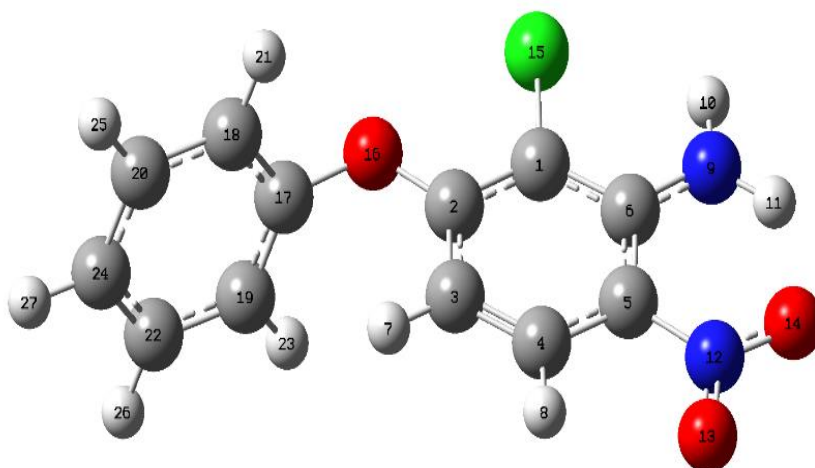
COMPUTATIONAL EXAMINATION OF DEGRADATION REACTIONS OF PRECIOUS ENDOCRINE DISRUPTORS MOLECULES THROUGH SURFACE WATER

Simal KURUMOGLU¹, Yelda YALCIN GURKAN¹

¹Tekirdag Namik Kemal University, Department of Chemistry, Tekirdag, Turkey, e-mail: simalsencan@hotmail.com

Abstract

Degradation reactions of molecules to be investigated will be examined by molecular modeling methods and theoretical approaches will be proposed for reaction pathways. For this purpose, possible reactions were calculated using Gaussian09 package program. DFT method was used in the theoretical study. In this study, possible reaction paths in the reaction between drug active substances and OH radical were determined. Fragmentation reaction requires energy. OH radicals are used to degrade drug active substances. The lowest energy molecule has the most stable structure. According to this, when we list the drug active substances from the most stable to most unstable, they are Bifenox, Bis(2-ethylhexyl)phthalate, Khlorfenvinphos, Trifluralin, Aklonifen, Heptachlor epoxide, Perfluorooctanesulfonic acid, Klorprifos, Quinoxifen, Terbutrin. These results will guide experimental workers and determine the mechanism of fragmentation.



The geometric shapes of molecule obtained because of optimization

Key Words: Gaussian09; DFT.

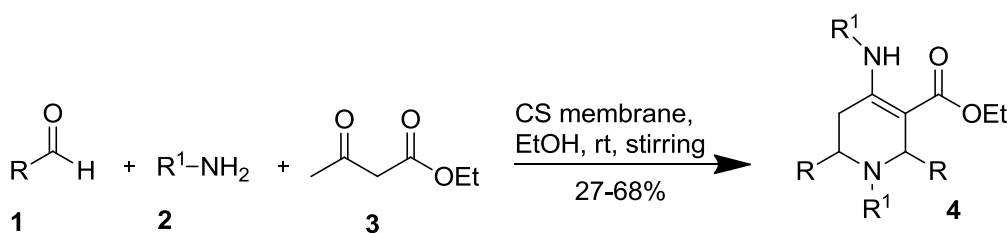
One pot synthesis of piperidine derivatives and evaluation of their anticancer potential

Zulfiqar Ali KHAN¹

¹Department of Chemistry, Government College University, Faisalabad and e-mail: zulfiqarchem@gamil.comd

Abstract

A series of ten piperidines **4** were synthesized via single step multicomponent reaction in 27-68% and 29-59% yields by using Chitosan (CS) membrane and chitosan (CS) film respectively as catalysts [1]. The piperidines **4** were prepared by following the Scheme 1. Structures of the synthesized piperidines were analyzed by ¹H NMR, ¹³C NMR, mass spectroscopy and elemental analysis. Anti-proliferative and pro-apoptotic potential of all the synthesized compounds was evaluated by MTT and Hoechst 33258 staining assay. The synthesized compounds showed good potential against HeLa cancer cell line [2].



Scheme 1

Key Words: Piperidines, Chitosan membrane catalysts, multicomponent reaction, MTT assay, anticancer agent.

References

- [1] Bari A, Iqbal A, Khan ZA, Shahzad SA, Yar M (2020), Synthetic Communications, 50, 2572-2589.
- [2] Iqbal A, Khan ZA, Shahzad SA, Khan SA, Naqvi SAR, Bari A, Amjad H, Umar MI (2019), Journal of Molecular Structure, 1197, 271-281.

EFFECT OF MIXER ROTOR WING TYPES ON COMPOUND PROPERTIES

Merve PEHLIVAN^{1,2}, Bora ATALIK², Sezgin GOKCESULAR²

¹Yildiz Technical University, Chemical Engineering Department, Davutpasa Campus, Esenler/Istanbul, 34220 Turkey, Tel. +90 212 383 4747 m.pehlivan@brisa.com.tr (M. Pehlivan)

²Brisa Bridgestone Sabanci Tire Company, İzmit/Kocaeli, 41310, Turkey, Tel. +90 262 316 4040; emails: b.atalik@brisa.com.tr (B. Atalık), s.gokcesular@brisa.com.tr (S. Gokcesular)

Abstract

The tyre compounds consist of various ingredients as raw material such as rubber, carbon black, silica, antioxidants, antiozonants, curing agents, etc. Generally, the ingredients of the compounds are mixed at least two steps. In rubber processing, mixing is an essential step to obtain a uniform compound. The mixing step provides the development of physical and chemical properties of compounds by reducing the non-uniformity of the ingredients [1,2].

In the rubber industry, internal mixers are widely used for mixing steps. Basically, internal mixers consist of mixing rotors, a mixing chamber, a feeding hooper, a ram, and a drop door. The most important parts of internal mixers are mixing rotors. There are two main designs of mixing rotors; non-intermeshing (tangential) and intermeshing [1,3].

The internal mixer with tangential rotors were widely used in the rubber processing area for the tire industry. For internal mixers, there are various tangential rotor types, depends on their design parameters such as number of wings, position of wing and length of wing. F. H. Banbury designed the traditional internal mixers in the beginning of 20th century and their tangential rotor equipped with two wings. In recent years, the usage of internal mixers with intermeshing rotors increases due to new trends in raw materials of tires [4,5]. Basically, the differences between tangential and intermeshing rotors are wing types and gap between the wing tips. The mixing rotor types differences affect the mixing time, mixing energy, viscosity index, and silica dispersion of compound [5,6].

In the present study, the effects of tangential rotor types with two different wings design investigated on compound properties. For this aim, a compound with two steps as masterbatch and final batch was chosen. By the combination method of tangential rotor types with two different wings design, compounds were produced with four different ways. Then, the rheological and dynamic properties, curing characteristics, and tensile properties of produced compounds were compared with data obtained from characterization studies using Mooney viscometer, Rubber Process Analyzer (RPA) Analysis, Moving Die Rheometer (MDR), and Tensometer.

Key Words: *Internal mixer; intermeshing rotor; tangential rotor; rheological properties; tensile properties*

References

- [1] S.R. Das (2016) Investigation of design and operating parameters in partially-filled rubber mixing simulations, The Graduate Faculty of The University of Akron, Master of Science, Akron, OH.
- [2] M.J. Hannon (1997) Mixing of tire compounds, *The Mixing of Rubber*, 187-200.
- [3] H. Publishers (2006) Rubber Compounding, *Van Nostrand's Sci. Encycl.* 255–267.
- [4] C. Koolhiraan (2000) J.L. White, Comparison of intermeshing rotor and traditional rotors of internal mixers in dispersing silica and other fillers, *J. Appl. Polym. Sci.* 78:1551–1554.
- [5] D. Berkemeier (2012) *Mixing of Rubber Compounds, Internal Mixer – Configuration and Design*, First Edit, Carl Hanser Verlag GmbH & Co. KG, 1-46.
- [6] T. Moribe (2012) Advanced Intermeshing Mixers for Energy Saving and Reduction of Environmental Impact, *Mitsubishi Heavy Ind. Tech. Rev.* 49:38–43.

PROCESSABILITY IMPROVEMENT OF NATURAL RUBBER IN MASTICATION STEP BY RESIDUAL CARBON BLACK ADDITION

Merve PEHLIVAN^{1,2}, Bora ATALIK², Sezgin GOKCESULAR²

¹Yildiz Technical University, Chemical Engineering Department, Davutpasa Campus, Esenler/Istanbul, 34220 Turkey, Tel. +90 212 383 4747 m.pehlivan@brisa.com.tr (M. Pehlivan)

²Brisa Bridgestone Sabanci Tire Company, İzmit/Kocaeli, 41310, Tel. +90 262 316 4040; emails: b.atalik@brisa.com.tr (B. Atalik), s.gokcesular@brisa.com.tr (S. Gokcesular)

Abstract

Rubbers are known as complex systems containing various constituents. The main chemical components of rubbers are elastomers or “elastic polymers” that are characterized by nonlinear stress-strain curves, high ability to recover its original shape and strain hardening. Rubbers are the main components of automobile, vehicle, aircraft, and bicycle tires [1,2].

Rubbers are classified by the obtained method such as exudations of plants (natural rubber, NR) or derived from petroleum, etc (synthetic rubber). In addition to this, processing of rubber consists of four basic steps. These are mastication, mixing (master batching, remilling and final mixing), shaping (extruding and calendaring) and curing, respectively. The first step of NR processing is mastication or polymer ‘breakdown’. This step is important and necessary for obtain a homogenous compound and developing the mechanical and viscoelastic properties of rubber [1,3,4].

In the rubber industry, using the reinforcing filler provides improvements in processing. The most frequently used reinforcing filler is carbon black (CB), which was discovered in the early 20th century [5]. There are various types of CB using as a reinforcing filler in rubber and they were classified by their grade, particle size, surface area, aggregate structure etc. [5]. The addition of CB into the rubbers improves the mechanical properties of compound such as tensile strength, modulus, tear strength, abrasion resistance and etc [1,6].

After mastication step, the rubber sheet stick each other and it cause processing problem and production loss. The aim of this study is to improve natural rubber processability by addition of residual CB. For this purpose, specified amount of residual CB was added to natural rubber in the mastication step. This relevant residual CB obtained from dust collector in the process and it is consisting of various types of carbon mixtures. Firstly, the properties of residual CB were analyzed by Brunauer–Emmett–Teller (BET) surface area analysis. Then, the effects of residual CB addition step changing (mastication or master batching) on natural rubber and produced compound properties were compared. The rheological and thermal behaviors of natural rubber were analyzed by Rubber Process Analyzer (RPA) and Thermogravimetric Analyzer (TGA). Finally, the physical and chemical properties of compounds, which use natural rubber with added residual CB, were investigated.

Key Words: Carbon black; mastication step; natural rubber compound; rheological behaviour; viscoelasticity

References

- [1] F. de M. Carolina, J.G.Z. Aldo, Fernando Galembeck (2019) Nanostructures and compatibility in rubber nanocomposites containing carbon nanofillers, in: Carbon-Based Nanofillers Their Rubber Nanocomposites Fundam. Appl., Elsevier Inc., 1–26.
- [2] L. Valentini, M.A.L. Manchado (2019) Classification of rubbers and components for harsh environmental systems, Elsevier Inc.
- [3] N.H. Peter A. Ciullo (1999) Rubber Processing, The Rubber Formulary, 49-55.
- [4] D.K. Arti, A.S. Hidayat, I.M. Ulfah, H. Susanto, L.A. Wisojodharmo, A. Dandi (2020) Mastication Process of Natural Rubber/Butadiene Rubber Blending: Validation Method on Influence of Peptizer, Macromol. Symp. 391:1–5.
- [5] I.M. Ulfah, R. Fidyaningsih, S. Rahayu, D.A. Fitriani, D.A. Saputra, D.A. Winarto, L.A. Wisojodharmo (2015) Influence of Carbon Black and Silica Filler on the Rheological and Mechanical Properties of Natural Rubber Compound, Procedia Chem. 16:258–264.
- [6] S. Sattayanurak, J.W.M. Noordermeer, K. Sahakaro, W. Kaewsakul, W.K. Dierkes, A. Blume (2019) Silica-Reinforced Natural Rubber: Synergistic Effects by Addition of Small Amounts of Secondary Fillers to Silica-Reinforced Natural Rubber Tire Tread Compounds, Adv. Mater. Sci. Eng.

Antibacterial Activity and Physical Properties of Bovine Gelatine-Chitosan wound dressing Films Supplemented with Propolis

İlknur KÜÇÜK¹, Nigar YILDIRIM²

¹Yıldız Technical University, Department of Chemical Engineering, Istanbul Turkey,
kucuk@yildiz.edu.tr

²Yıldız Technical University, Department of Chemical Engineering, Istanbul Turkey

Abstract

Material selection is an important step to design an ideal wound dressing. Prevention of bacterial infection is one of the primary goals of an ideal wound dressing and wound dressings with antimicrobial properties are emerging as valuable options to prevent wound infection. To address this issue, here we describe the preparation of Bovine Gelatine (BGE)-Chitosan (CS) wound dressing films supplemented with propolis (PE) which is a well-known anti-bacterial agent. Propolis supported wound dressing films were prepared by using solvent casting technique. As wound dressing film structures were confirmed by FTIR and optical microscope. Also, physical properties of the films such as thickness, mass, water vapor permission rate (WVPR), water absorption capacity, water content and dressing pH were determined. Furthermore, the antibacterial activities of the BGE-CS-PE films were determined by the agar disc diffusion method against gram positive (*S. Aureus*, *B. Subtilis*) and gram negative (*S. Typhi*, *E. Coli*) microorganisms. Inhibition zone indicated that propolis supported wound dressing film possessed much higher antimicrobial activity than that of BGE-CS films. Taken together, our finding suggested that the BGE-CS-PE film showed strong potential as a wound dressing.

Key Words: Antibacterial Activity, Bovine Gelatine, Chitosan, Propolis

References

- [1] Verlee, A., Mincke, S., Stevens, C.V., (2017). Recent developments in antibacterial and antifungal chitosan and its derivatives, *Carbohydrate Polymers*, 164:268-283.
- [2] Oryan, A., Alemzadeh, E., Moshiri, A., (2018). Potential role of propolis in wound healing: Biological properties and therapeutic activities, *Biomedicine & Pharmacotherapy*, 98:469-483.
- [3] Li, H., Cheng, F., Gao, S., Wu, Z., Dong, L., Lin, S., Luo, Z., Li, X., (2017). Preparation, characterization, antibacterial properties, and hemostatic evaluation of ibuprofen-loaded chitosan/gelatin composite films, *J. Appl. Polym. Sci.*, 134, 45441.

IRIDIUM OXIDE IMMOBILIZED ON CERIUM OXIDE FOR ENHANCED WATER OXIDATION

Kadriye Özlem HAMALOĞLU¹, Rukiye BABACAN TOSUN², Ali TUNCEL³

¹ Hacettepe University, Chemical Engineering Department, Ankara, 06800, Turkey
ozlemnaz@hacettepe.edu.tr

² Hacettepe University, Division of Nanotechnology and Nanomedicine, Ankara, Turkey
rbabacantosun@hotmail.com

³ Hacettepe University, Chemical Engineering Department, Ankara, 06800, Turkey
atuncel@hacettepe.edu.tr

Abstract

The synthesis of reusable heterogeneous catalysts with high catalytic activity is a significant challenge in water oxidation. In order to obtain reusable heterogeneous oxidation catalysts with high catalytic activity, we developed iridium oxide nanoparticle immobilized cerium oxide microspheres. Cerium oxide microspheres were synthesized by a template-assisted method [1]. Iridium oxide nanoparticles were immobilized on cerium oxide microspheres via electrostatic attraction. The catalyst was characterized by using XRD, SEM, EDX, TEM, XPS, ICP-MS and BET. The catalytic activity was monitored by chemical water oxidation using sodium periodate. Oxygen amount evolved during water oxidation was measured with gas chromatography-mass spectrometry (GC-MS). Turnover number (TON) and turnover frequency (TOF) values were calculated as 310 and 368 h⁻¹ respectively. By performing XPS analysis, the stability of catalyst was also demonstrated. By using cerium oxide microspheres as a support for iridium oxide nanoparticles, the catalyst was reused for five runs with minor losses in the oxygen evolution. Consequently, the synthesized oxidation catalyst demonstrated high catalytic performance and reusability.

Key Words: Water oxidation, heterogeneous catalyst, iridium oxide nanoparticles, cerium oxide, sodium periodate

References

[1] Yıldırım D, Gökçal B, Büber E, Kip Ç, Demir MC, Tuncel A (2021) Chemical Engineering Journal 403:126357.

Application of bismuth film electrode in determination of Loratadine by cathodic stripping voltammetry in the presence of cationic surfactant

Günay ÖNAL¹, Yalçın ALTUNKAYNAK², Abdulkadir LEVENT³

¹ Batman University Health Services Vocational School, 72100, Batman, Turkey
gunayturmus@hotmail.com

² Batman University, Vocational School of Technical Sciences, 72100 Batman, Turkey
yalcin.altunkaynak@batman.edu.tr

³ Batman University, Faculty of Sciences and arts, Department of Chemistry, 72100, Batman, Turkey
leventkadir@hotmail.com

Abstract

Loratadine, histamine - H1 antihistamine receptors it is being used for many years in the treatment of an allergic condition illustrating the effects on [1]. When the literature is reviewed, there are limited number of studies on Loratadine based on electrochemistry [2-5]. Stripping voltammetry is a very sensitive and selective method for determining drugs and organic / inorganic substances in biological fluids. The electrochemical behavior of Loratadine with BiFE in different supporting electrolyte and pH values, and its performance characteristics in electroanalytical determinations were investigated by cyclic voltammetry and linear sweep cathodic stripping voltammetry (LS-CSV) methods. LS-CSV measurements on the BiFE surface of 6.5×10^{-4} M Loratadine in 0.04 M BR buffer (pH 7.0) and 4 mM cationic surfactant (CTAB) were taken between 0.0 V and -2.0 V. Loratadine gave a voltammetric response about at -1.486 V. The limit of detection was found $LOD = 1.2 \times 10^{-7}$ M* at the BIFE surface at liner concentration range [1.305×10^{-6} M – 14.3×10^{-6} M, $r = 0.998^*$ ($n = 11$)]. This voltammetric method, developed under optimum conditions, has been successfully applied to pharmaceutical formulations of Loratadin as fast, easy to apply, sensitive and environmentally friendly.

Keywords: Loratadine, BiFE, Voltammetry, pharmaceutical formulation

***It was corrected by presented author.**

References

- [1] Michael E.El-Kommos, Samia M.El-Gizawy, Noha N.Atia, Noha M.Hosny, 2015. Analytical Chemistry Research, 3, 1-12
- [2] Ghoneim, M.M., Mabrouk , M.M., Hassanein, A.M., Tawfik, A., 2001. Journal of Pharmaceutical and Biomedical Analysis, 25 (933–939).
- [3] Eisele, A.P.P., E.R. Sartori, 2015. Anal. Methods 7, (8697–8703)
- [4] Roushani, M., Nezhadali, A., Jalilian, Z., Azadbakht, A., 2017. Materials Science and Engineering C 7(1106–1114)
- [5] Hassanpour,A., Baj ,R.F.B., Abolhasani,J., 2019. Journal of Analytical Chemistry, 74, 12, 1223–1231.

Synthesis and Alpha-Glucosidase Inhibition Studies of 1,2-Benzothiazine Derivatives

Matloob AHMAD

E-mail Address: Matloob.Ahmad@gcuf.edu.pk, Matloob_123@yahoo.com

Abstract

Diabetes mellitus is a chronic disease in which the infected cells do not have the ability to produce sufficient amount of insulin that results in the abnormality of carbohydrates metabolism and an increase in blood glucose level. Long time exposure to diabetes mellitus results in failure or dysfunction of different organs like kidneys, nerves, heart, eyes, etc. A common practice to cure diabetes is the use of α -glucosidase inhibitors which help in lowering the blood glucose level. In order to explore novel and more potent α -glucosidase inhibitors, we synthesized and screened a variety of 1,2-benzothiazine derivatives for their in silico α -glucosidase inhibitory potential and as a result most of the compounds showed good binding energies and interactions with the active site residues. These best compounds were then subjected to the in vitro alpha glucosidase inhibition and a good agreement was found between the results. Compound 1, 8, 9, 15, 21, 23, 25, 30, 32 and 36 showed excellent results having IC₅₀ values of 5.9, 7.8, 3.9, 6.9, 14.0, 4.2, 5.9, 29.2, 14.0 and 12.7 μ M respectively, even less than the standard acarbose (IC₅₀ = 38.31 μ M). These derivatives were also proved more potent anti-diabetic agents compared to some previously reported heterocyclic compounds. Hence, the presented derivatives may be used as lead candidates to cure diabetes.

Key Words: 1,2-Benzothiazine Derivatives, Biological Evaluation, Antidiabetic Studies, Enzyme Inhibition, Alpha-glucosidase Inhibition

Biodegradable Zwitterionic Nanoparticles with a Biologically Relevant UCST at Physiological Salt Concentration

Mattia SPONCHIONI¹, Umberto CAPASSO PALMIERO², Davide MOSCATELLI¹

¹Politecnico di Milano, via Mancinelli 7, 20131 Milano, Italy

²ETH Zürich, Vladimir-Prelog-Weg 1-10, 8093 Zürich, Switzerland

Email: mattia.sponchioni@polimi.it

Abstract

Thermo-responsive polymer nanoparticles (NPs) are attracting growing attention in the biomedical field owing to their dynamic responses upon application of thermal stimuli.[1] Despite zwitterionic NPs with an upper critical solution temperature (UCST) in physiological solutions would be highly desirable in this field, the presence of salts prevents the obtainment of phase separations in a biologically relevant temperature range (i.e. 30-45 °C).[2] This is the case of polysulfobetaine (pSB) based NPs. However, the recent discovery of polysulfobetaine (pZB) has partially covered this lack of thermo-responsive materials. In fact, pZB shows an UCST above 100 °C even in saline solutions.[3] We now discovered that by copolymerizing SB and ZB in a statistical copolymer it is possible to obtain controllable UCST in physiological media. We exploited this possibility to produce for the first time modular amphiphilic block copolymers able to self-assemble into biodegradable NPs with an UCST suitable for drug delivery applications. The synthesis was carried out *via* emulsion reversible addition-fragmentation chain transfer polymerization, enabling to finely control the copolymer microstructure. In particular, we demonstrated the possibility of controlling the NP transition temperature, size and degradation time by modulating: (i) the relative ZB/SB ratio, (ii) the number of hydrophobic units and (iii) the length of the oligoester macromonomer adopted for the hydrophobic portion, respectively (**Figure 1a**). Finally, we exploited the thermo-responsive behaviour of this formulation for controlling the release of pyrene as a drug mimic molecule. In particular, the formation of microaggregates below the cloud point (**Figure 1b**) significantly slows down the release rate making this formulation suitable for a prolonged local release (**Figure 1c**). We therefore envision the storage of this formulation below its cloud point to prevent a premature degradation and drug release, its administration as a NP suspension at 40 °C and finally the usage as a local drug delivery system at physiological temperature (**Figure 1d**).

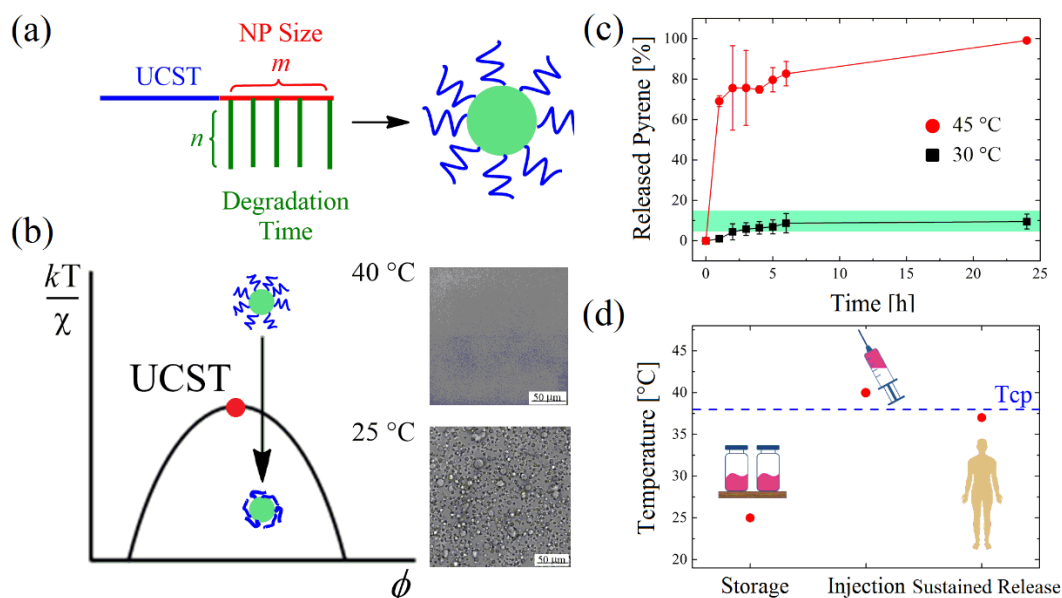


Figure 1. (a) Modular block copolymers enable the control over the main NP properties. (b) Schematic representation of the NP behaviour above and below their binodal curve. (c) Modulation of the release of pyrene by adjusting the temperature. (d) Strategy for the usage of the produced NPs as local drug delivery systems.

Key Words: Zwitterionic Nanoparticles; Thermo-responsive; UCST; Liquid-Liquid Phase Separation; Drug Delivery

References

- [1] M. Sponchioni, U. Capasso Palmiero, and D. Moscatelli, "Thermo-responsive polymers: Applications of smart materials in drug delivery and tissue engineering," *Materials Science and Engineering: C*, vol. 102, pp. 589-605, 2019/09/01/ 2019.
- [2] J. Seuring and S. Agarwal, "Polymers with Upper Critical Solution Temperature in Aqueous Solution," *Macromolecular Rapid Communications*, vol. 33, no. 22, pp. 1898-1920, 2012.
- [3] N. M. Nizardo, D. Schanzenbach, E. Schönmann, and A. Laschewsky, "Exploring Poly(ethylene glycol)-Polyzwitterion Diblock Copolymers as Biocompatible Smart Macrosurfactants Featuring UCST-Phase Behavior in Normal Saline Solution," *Polymers*, vol. 10, no. 3, p. 325, 2018.

THERMAL and MECHANICAL PROPERTIES of CONTINUOUS GLASS FIBER/PET COMPOSITES

Melis Eldem HEPER^{1,2}, Sennur DENİZ¹

¹Yıldız Technical University, Faculty of Chemical and Metallurgical Engineering,
Chemical Engineering Department, 34220, Esenler, İstanbul-Turkey, e-mail: deniz@yildiz.edu.tr
²Korteks Mensucat Sanayi ve Ticaret A.Ş., Bursa-Turkey, e-mail: meliseldem.heper@zorlu.com.tr

Abstract

The interest and demand towards the use of thermoplastic composites have been gradually increasing each day due to their high damage tolerance, energy absorption capability and strain rates compared to thermoset composites [1-2]. Although thermoplastic composites have many advantages, their high resin viscosity is a major concern to fill pores at tightly woven or unidirectional textile preforms during manufacturing of composites. Using hybrid yarns is one of the methods to overcome this problem to manufacture uniform and well impregnated thermoplastic composites [3]. In this work, it was aimed to investigate the thermal and mechanical properties of thermoplastic composites to be prepared using continuous glass fiber/poly(ethylene terephthalate) (C-GF/PET) hybrid yarns in different proportions by volume. C-GF/PET hybrid yarns containing glass fiber in different volumes (35, 45, 55 and 65%) were produced, woven and then transformed into thermoplastic composite test plates using hot press. Microstructural properties of the composites were investigated using optical microscopy analyses. Tensile, three point bending and impact tests were used to investigate the mechanical properties and TGA and DSC were used to analyze the thermal properties of the composites.

Key Words: *Glass fiber, PET, Hybrid yarn, Thermoplastic composite, Mechanical properties*

Acknowledgment

We would like to express our gratitude to Korteks Mensucat Sanayi ve Ticaret A.Ş., which provides the production and characterization of hybrid yarns within the scope of the study. This work; Supported by Yıldız Technical University Scientific Research Projects Coordination Unit. Project Number: FYL-2019-3565.

References

- [1] Boria S, Scattina A, Belingardi G (2017) Composite Structures, 167:63-75.
- [2] Sonnenfeld C, Mendil-Jakani H, Agogue R, Nunez P, Beauchene P (2017) Composite Structure, 171:298-305.
- [3] Selver E, Potluri P (2017) European Mechanical Science, 1(3):93-103.

Rh-BASED TERNARY CATALYST FOR THE CATALYTIC DEHYDROGENATION OF HYDRAZINE BORANE As an CHEMICAL HYDROGEN STORAGE MATERIAL

¹Merve Rabia GÜRLÜK, ²Gülay ÖZKAN, ¹Göksel ÖZKAN

¹Gazi University, Faculty of Engineering, Department of Chemical Engineering, Ankara,
06570, Turkey, gozkan@gazi.edu.tr

²Ankara University, Faculty of Engineering, Department of Chemical Engineering, Ankara
06100, Turkey

Abstract

Hydrogen has been favoured as an energy carrier due to its high-energy capacity, clean burning qualities, and renewable nature [1]. However, the most important issue that hinders the applicability of hydrogen is the storage of hydrogen. Several studies have recently been carried out in the field of hydrogen storage materials [2]. Organic or inorganic chemical hydrogen storage materials is given such as H₂O, hydrazine or hydrazine borane, ammonia borane, amine borane complexes, organic hydrocarbons, complex hydrides, and chemical hydrides [3]. In addition, One of the methods which is hydrogen production from boron compounds is catalytic or noncatalytic hydrolysis. The most important application problem with boron compounds, believed to be future hydrogen storage materials, is the rapid and uncontrolled production of hydrogen required for fuel cells. Accordingly, storing hydrogen efficiently and safely for future applications is a significant problem that must be solved in the prospect of a hydrogen-based economy. However, designing new materials or catalysts to meet the requirements of the technology will increase the capacity of hydrogen storage [4]. This study focuses on the synthesis of the Rh-Ni-B catalyst for the dehydrogenation of the hydrazine borane. The results reported here includes the characterization of the Rh-based catalyst by using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and BET surface properties. Furthermore, the catalytic hydrolysis experiments were conducted to investigate the hydrogen release performance of hydrazine borane. This study also shows how boron-based materials can help hydrogen production to support the development of hydrogen storage applications for low-carbon energy systems.

Key Words: Hydrazine Borane, Hydrolysis, Hydrogen, Dehydrogenation, Catalyst

References

- [1] Acar C, Dincer I. (2020) Int. J. Hydrogen Energy, 45: 3396-3406.
- [2] Murathan, H. B., Özkan, G., Akkuş, M. S., Özgür, D. Ö., & Özkan, G., (2018), International Journal of Hydrogen Energy 43: 10728-10733.
- [3] Hamilton CW, Baker RT, Staubitz A, Manners J. (2008) Chem. Soc. Rev. 38: 279–293.
- [4] Moury R, Demirci UB. (2015). Energies 8; 3118-3141.

New voltammetric strategy for determination and electrochemical behaviors of Metformin by Pencil Graphite Electrode

Yalçın ALTUNKAYNAK¹, Ömer YAVUZ², Abdulkadir LEVENT³

¹Department of Chemistry, Science Institute, Dicle University, 21280 Diyarbakir, Turkey
altunkaynak4772@gmail.com.tr

¹Batman University, Vocational School of Technical Sciences, 72100 Batman, Turkey
yalcin.altunkaynak@batman.edu.tr

²Department of Chemistry, Faculty of Science, Dicle University, 21280 Diyarbakir, Turkey
omeryavuz@gmail.com.tr

³Batman University, Faculty of Sciences and arts, Department of Chemistry, 72100, Batman, Turkey
leventkadir@hotmail.com

Abstract

Metformin(MET), an oral antidiabetic drug commonly used in the treatment of diabetes, is a drug that increases insulin sensitivity in the biguanide group [1]. MET shows its pharmacological effect by lowering the glucose level in the blood. In the literature research, there are studies using electrochemical techniques for the analysis of MET in biological fluid and drug forms[1-6]. In this study, the electrochemical properties of MET, one of the drugs used in the treatment of diabetes, were performed using a pencil graphite electrode in NaOH (0.1 M) solution. This compound was recorded with an irreversible and diffusion controlled adsorption oxidation peak at approximately +1.28 V by cyclic voltammetry. With square wave stripping voltammetry, it was observed that the peak current signals of MET in the concentration range of 2.76-24.8 μM in 0.1M NaOH solution increased linearly. At a concentration of 2.76 μM ($n = 9$), the limit of detection and relative standard deviation were calculated as 9.03 nM (1.495 ngmL⁻¹) and 3.25 %, respectively. This method has been successfully applied for MET analysis in pharmaceutical preparations and urine samples without any separation.

Key words: *Metformin, Voltammetry, Pencil Graphite Electrode, Drug, Urine*

References

- [1] Wysham C.H, Kirkman M.S (2011) Diabetes Care. 34:11–61.
- [2] Tian X.J, Song J.F, Luan X J, Wang Y.Y, Shi Q.Z (2006) Analytical and Bioanalytical Chemistry 386: 2081–2086.
- [3] Tian X.J, Song J.F (2007) Journal of Pharmaceutical and Biomedical Analysis 44: 1192-1196.
- [4] Sattarahmadya N, Heli H, Faramarzi F(2010) Talanta 82: 1126-1135.
- [5] Gholivand M.B, Behzad L.M (2013) Analytical Biochemistr 438: 53-60.
- [6] Baghayeri M, Amiri A, Razghandi H (2019) Journal of Electroanalytical Chemistry 832:142–151.

Structure of drug-polymer composites prepared by nano spray dryer

Mirella Mirankó¹, László Trif², Judit Tóth^{1,2}, Tivadar Feczko^{1,2}

¹ University of Pannonia, Research Institute of Biomolecular and Chemical Engineering, 8200 Veszprém, Egyetem u. 10., Hungary, E-mail: miranko@mukki.richem.hu, toth@mukki.richem.hu, feczko@mukki.richem.hu

² Research Centre for Natural Sciences, Institute of Materials and Environmental Chemistry, 1117 Budapest, Magyar tudósok körútja 2., Hungary, e-mail: trif.laszlo@ttk.mta.hu

Abstract

Microencapsulation of drug molecules by different biocompatible polymers is a method for improving the biological effects of drugs. The uniformly dispersed active pharmaceutical ingredient (API) is in a different state of energy in the polymer matrix, which in turn facilitates controlled diffusion of drug species in patient body. Spray drying is one of the most widely used microencapsulation techniques, since it provides rapid evaporation of the solvent and maintains low temperature during drying of heat sensitive molecules, moreover, polymers and other excipients can be directly incorporated in the process. The Nano Spray Dryer B-90 is a new innovative equipment in spray drying introduced to the market by Büchi Labortechnik AG [1]. The new technology enables the production of submicron- and nanosized particles from 300 nm and small amount of samples even with 90 % yield. The structure of components in the composite microparticles can differ from that of the raw polymer and the API [2].

Our aim was to investigate the structure of microparticles produced by nano spray drying technology. The model drug was an imidazole type of antibiotics, while hydroxypropyl methylcellulose and polyvinylpyrrolidone polymers were used as excipients. The variable operational parameters in the experiments were inlet temperature, air flow, spray rate and the composition of the solutions to be dried. The morphology (size and shape), the crystallinity and thermal behaviour were investigated to get information on the microparticle structure.

In the dried products, the active ingredient was in crystalline state incorporated into the amorphous polymer matrix. Melting point decrease phenomenon was observed by differential scanning calorimetry and peak broadening by powder X-ray diffraction measurements, which could be the result of formation of small drug crystallites [3]. The transmission electron microscopy images proved the presence of 20 - 50 nm drug crystals in the polymer matrix, which is in good correlation with the calculated coherent scattering domain sizes from the X-ray diffraction data. The melting point decreased in the dried products compared to the bulk drug, which could be interpreted with the nano-sized crystals of the active ingredient incorporated into the micron-sized particles.

Key Words: *nano spray dryer, polymer, microparticles, nanocomposite, melting point decrease*

References

- [1] X. Li, N. Anton, C. Arpagaus, F. Belleteix, T. F Vandamme, J. Controlled Release 147(2) (2010) 304–310. <https://doi.org/10.1016/j.jconrel.2010.07.113>
- [2] M.N. Singh, K.S.Y. Hemant, M. Ram, and H.G. Shivakumar, Res Pharm Sci. 5(2) (2010) 65–77.
- [3] P. Roumanille, V. Baco-Carles, C. Bonningue, M. Gougeon, B. Duployer, P. Monfraix, H. Le Trong, P. Tailhades, Inorganic Chemistry, 56(16) (2017) 9486–9496. <http://doi.org/10.1021/acs.inorgchem.7b00608>

Green synthesis of ZnO particles and their application as catalysts in the transesterification of methyl benzoates

Mohamed Soliman^{1,2}, Elisabete Alegria^{1,2}, Ana Ribeiro^{1,*}, Marta Alves¹, Fátima Montemor¹ and Armando Pombeiro¹

¹Centro de Química Estrutural, Instituto Superior Técnico, Universidade de Lisboa, Portugal

²Área Departamental de Engenharia Química, ISEL, Instituto Politécnico de Lisboa, Portugal

Abstract

Pure ZnO nanoparticles (ZnONPs) were successfully synthesized using *bravo-de-esmolfe* apple extract, in aqueous medium at room temperature. ZnO microparticles, synthesized with a pure apple phytochemical, quercetin (ZnOq), or without phytochemicals (ZnO) were synthesized for comparative purpose [1,2]. The synthesized ZnO particles were characterized by XRD, SEM, and TEM. XRD patterns indicated formation of the hexagonal wurtzite phase with high purity and SEM and TEM analyses revealed the morphology of the particles. Apple extract produced spherical ZnONPs composed of round lamina-like structures, similar to the micro sized lamina-like shape of the ZnOq and dissimilar to the flower-like shape of ZnO. The catalytic activity of the ZnONPs was evaluated towards the transesterification reaction of different carboxylic esters and their activity compared to that of microparticles [2,3]. All of the ZnO green synthesized particles are highly selective for the transesterification of an α -keto carboxylic ester (methyl benzoylformate) and, in particular, ZnOq leads to the highest product yield of *ca.* 98% within 24 h of reaction time. The re-use of apple waste for highly efficient catalysts productions, based on green synthesis routes, can be inserted in the concept of circular economy. Furthermore, is shown that micro size ZnO particles with excellent catalytic activity are achieved and the hazardous associated to the manipulation of NPs, especially relevant in industrial applications, can be overcome in transesterification reactions. Furthermore, micro size ZnO particles with excellent catalytic activity can obviate the use and hazardous associated to NPs manipulation, especially relevant in industrial applications of transesterification reactions.

Key Words: Zinc oxide nanoparticles; green-biosynthesis; catalysis; transesterification reaction; α - keto carboxylic ester

References

- [1] Alves, MM.; Andrade, SM.; Grenho, L.; Fernandes, MH.; Santos, C.; Montemor, MF. Influence of apple phytochemicals in ZnO nanoparticles formation, photoluminescence and biocompatibility for biomedical applications. *Mater. Sci. Eng. C*. **2019**, *101*, 76.
- [2] Soliman, MMA; Alegria, ECBA; Ribeiro, APC; Alves, MM; Saraiva, MS; M.F. Montemor, MS; Pombeiro, AJL, Green synthesis of zinc oxide particles with apple-derived compounds and their application as catalysts in the transesterification of methyl benzoates, *Dalton Trans.*, **2020**,49, 6488.
- [3] Soliman, MMA.; Karmakar, A.; Alegria, ECBA; Ribeiro, APC.; Rúbio, GMDM.; Saraiva, MS.; Silva, MFCG.; Pombeiro, AJL, ZnO nanoparticles: An efficient catalyst for transesterification reaction of α -keto carboxylic esters. *Catal. Today*. **2020**, *348*, 72.

Acknowledgements: This work was supported by the Fundação para a Ciência e Tecnologia (FCT), project UIDB/00100/2020 of Centro de Química Estrutural and the PTDC/QUI-QIN/29778/2017 project and by Instituto Politécnico de Lisboa (IPL/2019/STREAM_ISEL Project). APCR and MMA thank to Instituto Superior Técnico for Scientific Employment contracts IST-ID/119/2018 and IST-ID/154/2018, respectively under Decree-Law no. 57/2017.

Effect of Temperatures and Reaction Times on Structural, Morphological and Magnetic Properties of Zn-Doped Fe₃O₄ Nanoparticles (Zn_{0.25}Fe_{2.75}O₄) Synthesized by the Hydrothermal Method

Nurcan DOGAN^{1*}, Gulsum CALISKAN²,

¹Department of Physics, Faculty of Science, Gebze Technical University, 41400 Kocaeli, Turkey

²Department of Physics, Faculty of Science, Gebze Technical University, 41400 Kocaeli, Turkey

¹Email: ndogan@gtu.edu.tr

²Email: gulsumfb95@gmail.com

Abstract

Nano-crystalline Zinc doped Fe₃O₄ powders have been synthesized by hydrothermal method under different temperature and reaction time parameters [1]. The structure of magnetic powders were characterized by X-ray Diffraction Diffractometer (XRD), Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectra (FTIR) techniques, while magnetic properties were determined by using a Physical Properties Measurement System (PPMS) and Electron Spin Resonance Spectrometer (ESR). [2] The structural properties and magnetic behaviour of the obtained nanoparticles were investigated. The average particle size was determined from the Scherer's equation found to be in the range of 12-24 nm as revealed by XRD technique. The FT-IR results show a peak around 540 cm⁻¹ for in all samples even different temperatures and reaction times. The SEM result shows that all nanoparticles have a spherical geometry and the temperature rise up to 180°C led to the increasing of crystallinity of nanoparticles. Furthermore, the saturated magnetization and coercivity of Zn_{0.25}Fe_{2.75}O₄ nanoparticles were in the range of 83 emu/g and 14 Qe as confirmed by PPMS. The results show that with increasing of temperature, the crystallinity of nanoparticles and the saturation magnetization is increased. In addition, all synthesized samples exhibited a superparamagnetic character at room temperature. In this study, considering the application areas of magnetic nanoparticles, it is tried to obtain that at optimum value of nanoparticles in terms of their crystal structures and magnetic properties under different hydrothermal conditions.

Key Words: *Magnetic nanoparticles; Hydrothermal synthesis; Zn doped Fe₃O₄; Crystal structure; Magnetic properties*

References

- [1] Attarad A., Zafar H., Zia M., Haq I., Phull A. R., Ali J. S., Hussain A., (2016), "Synthesis, characterization, applications, and challenges of iron oxide nanoparticles", *Nanotechnology, Science and Applications*, 9, 49-67.
- [2] Liu J., Bin Y., Matsuo M., (2012), "Magnetic Behavior of Zn-Doped Fe₃O₄ Nanoparticles Estimated in Terms of Crystal Domain Size" *The Journal of Physical Chemistry C*, 116 (1), 134-143.

A FACILE METHOD TO PREPARE BISMUTH DOPED ZNO PHOTOCATALYSTS AND THEIR PHOTOCATALYTIC PROPERTY

Nazli TURKTEN

Department of Chemistry, Faculty of Arts and Sciences, Kirsehir Ahi Evran University, Kirsehir 40100, Turkey.
nazli.turkten@ahievran.edu.tr

Abstract

Textile and dyeing industries are the major sources of water contamination causing serious health issues [1, 2]. In recent years, the treatment of wastewater containing the dye effluents has been attracted a great interest. In this respect, heterogeneous catalysis is as an alternative method used for the removal of dyes from wastewater. [3, 4].

In this study, ZnO and bismuth doped ZnO (Bi-ZnO) photocatalysts were synthesized by a facile solvothermal method. For this purpose, three different bismuth weight percentages (0.5% 1.0% and 1.5%) of photocatalysts were prepared through an aqueous chemical growth method at low temperature and followed by precipitation. The structural and morphological properties of the photocatalysts were investigated by FTIR, SEM-EDX, XRD, and Raman spectroscopy. The photocatalytic activity of the synthesized photocatalysts was performed by the degradation of Reactive Red 194 under UV light irradiation. SEM images of the synthesized photocatalysts were nanorod like shape. The presence of phases of ZnO and Bi₂O₃ in XRD spectroscopy confirmed a successful doping. The results revealed that 1.0-Bi-ZnO photocatalyst exhibited a better photocatalytic activity compared to bare ZnO.

Keywords: Bi-ZnO, photocatalysis, reactive dye, Reactive Red 194, solvothermal method.

References

- [1] Ishak SA, Murshed MF, Akil H Md, Ismail N, Rasib SZ Md, Al-Gheethi AAS (2020) Water 12:2032.
- [2] Javaid R., Qazi U.Y. (2019)International Journal of Environmental Research and Public Health 16.
- [3] Turkten N., Cinar Z. (2017) Catalysis Today 287:169-175.
- [4] Forgacs E., Cserháti T., Oros G. (2004) Environment International 30: 953-971.

Theoretical and Molecular Docking Analysis of Silver-NHC Complexes as a Potential Anticancer Agent

Neslihan ŞAHİN¹, Elvan ÜSTÜN²

¹Department of Basic Education, Faculty of Education, Sivas Cumhuriyet University, 58140, Sivas, Turkey

²Ordu University, Faculty of Science and Arts, Department of Chemistry, 52200 Ordu, Turkey

Abstract

Cancer is one of the major leading causes of death worldwide. The International Agency for Research on Cancer of World Health Organization reported that 18.1 million new cancer cases were detected, and 9.6 million people died because of cancer in 2018 [1]. Therefore, cancer remains one of the most researched areas. The fight against the cancer is continued especially by in drug therapy, radiotherapy, and surgical applications. Cis-platin is recorded as the first metal-based anti-cancer drug [2]. The observed side effects of cis-platin, despite the good results, motivated for the synthesis of new metal-based anticancer drugs. N-heterocyclic carbenes (NHCs) are organometallic ligands that has recently been used in medicinal chemistry [3]. Silver salts are known for their antimicrobial and wound healing properties [4]. Thus, anticancer researches of NHC-Ag type complexes are not surprising idea. Computational chemistry is important in terms of providing predictions both in the follow-up studies after in-vitro activity measurement of bioactive molecules and designing and synthesis of new molecules [5].

In this study, synthesized and characterized silver complexes with benzimidazole-based N-heterocyclic carbene ligands [6] were analysed structurally by DFT / TDDFT-based and studied the interactions with DNA (PDB code: 1BNA), thioredoxin reductase (PDB code: 4CBQ) and VEGFR-2 enzyme (PDB code: 1YWN) by molecular docking methods.

Key Words: *N-heterocyclic carbenes, silver complexes, benzimidazole, DFT/TDDFT, molecular docking*

References

- [1] <https://gco.iarc.fr/>
- [2] Rosenberg B, Vancamp L, Krigas T (1965) Nature 205:698-699.
- [3] Garner ME, Niu W, Chen X, Ghiviriga I, Abboud KA, Tan W, Veigne AS (2015) Dalton Trans. 44:1914-1923.
- [4] Melaiye A, Simons RS, Milsted A, Pingitore F, Wesdemiotis C, Tessier CA, Youngs WJ (2004) J. Med. Chem. 47:973-977.
- [5] Üstün E, Demir SA, Coşkun F, Kaloğlu, Şahin O, Büyükgüngör O, Özdemir İ (2016) J Mol Struct 1123:433–440.
- [6] Bölükbaşı SŞ, Şahin N (2019) Journal of Organometallic Chemistry 891:78-84.

New voltammetric method for determination and electrochemical behaviors of oxaliplatin by CPT-BDD electrode

Mehmet ASLAN¹, Abdulkadir LEVENT²

¹Department of Chemistry, Science Institute, Dicle University, 21280 Diyarbakir, Turkey

mhtaslan2010@gmail.com.tr

²Batman University, Faculty of Sciences and arts, Department of Chemistry, 72100, Batman, Turkey
leventkadir@hotmail.com

Abstract

Various drugs made of metal compounds have been used in many diseases including cancer[1]. Studies on Oxaliplatin in the literature are these [2-6]. Oxaliplatin (OxPt), which is a platinum analogue with anti-cancer effect, was accentuated. OxPt is separated from cisplatin, one of analogues of platinum, by replacing 1,2-diaminocyclohexane with amine groups. In this study, a simple, fast and sensitive voltammetric method was developed for OxPt which shows anticancer effects with cytotoxic properties. The boron-doped diamond (BDD) electrode was activated electrochemically in cathodic direction in 0.5 M H₂SO₄ medium. Electrochemical properties of OxPt were investigated on BDD electrode surface using square-wave and cyclic voltammetry techniques. OxPt in Britton-Robinson(BR) buffer (pH 5.0) gave a well-determined voltammetric response at +1.01 V (vs. Ag/AgCl) using the square-wave voltammetry technique. The developed voltammetric technique was found to be linear with the concentration range of 1.0-3.5 µM in the BR (pH 5.0) medium and the limit of detection was 0.276 µM (0.109 µg mL⁻¹). Recommended method was successfully applied to drug forms of OxPt.

Keywords: Oxalipaltin, Boron-Doped Diamond, Voltammetry

References

- [1] Orvig C., Abrams M.J., 1999 Chem. Rev. Medicinal inorganic chemistry introduction, Chem. Rev., 99: 2201-2203
- [2] Kim P.K., Kim H.J., Kim Y.W., Bandu R., Ahn H.S., Lee J.W., 2015 Distribution study of cisplatin in rat kidney and liver cancer tissues by using liquid chromatography electrospray ionization tandem mass spectrometry *Journal of mass spectrometry*, 0.1002/jms.3594.
- [3] Sonali G.T., Rupesh V.C., Madhukar R.T., 2017. A rapid and simple HPTLC assay for therapeutic drug monitoring of capecitabine in colorectal cancer patients *Biomedical Chromatography*, 10.1002/bmc.4100
- [4] Lemoine L., Thissen E., Noben J.P., Adriaenssens P., Carleer R., Van der speeten K., 2018. A validated inductively coupled plasma mass spectrometry (ICP-MS) method for the quantification of total platinum content in plasma, plasma ultra filtrate, urine and peritoneal fluid *Journal of Pharmaceutical and Biomedical Analysis*, 152: 39-46
- [5] Zhao D., Qin Z., Ren G., Liu Q., Lu X., Zhang Q., Fan A., Lu Y., Li N., 2018 Hydrophilic interaction liquid chromatography tandem mass spectrometry method for the determination of intact oxaliplatin in cells: validated and applied in colon cancer HCT-116 cell line, *Journal of Pharmaceutical and Biomedical Analysis* 155: 7-14
- [6] Somayeh H., Zahra R., Eskandar M., Mohsen R. Farid A.D., 2019. A novel method for the simultaneous determination of 5-fluorouracil and oxaliplatin in new biodegradable PHBV/PLGA nanoparticles *Journal of the Iranian Chemical Society*, 16: 609-615

CATALYTIC EFFECT OF AMINES ON A CO₂BOL ABSORPTION PERFORMANCE

Ozge YUKSEL ORHAN,

Hacettepe University, Department of Chemical Engineering, Ankara, Turkey, oyuksel@hacettepe.edu.tr

Abstract

CO₂ emission into atmosphere is a global concern due to its direct connection with global warming [1]. CO₂ capture with aqueous alkanolamine solutions is preferred for post-combustion CO₂ capture from flue gas and industrial applications. Among solvent based CO₂ capture technologies, 30 wt. % aqueous monoethanolamine (MEA) solution is currently the accepted benchmark [2]. However, aqueous MEA (or other amine) solutions are energy intensive since the regeneration of the rich/loaded solvent necessitates reboiling. On the other hand, carbon dioxide binding organic liquids (CO₂BOLs) are novel solvents which include a super base such as amidine or guanidine and a linear alcohol such as hexanol. These solvents have high CO₂ loading capacities and they can be regenerated by simple temperature and pressure swings without a necessity to boil, thus eliminating latent heat of evaporation [3]. Their relatively low CO₂ capture rate can be increased by adding promoters [4]. The main target of this study is to develop a cost effective and high capacity CO₂ capture solvent that also has high reactivity towards to CO₂. In this work, different concentrations of 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) in 1-hexanol were prepared as a selected CO₂BOL. The effect of MEA and morpholine on reaction rates between CO₂ and CO₂BOL were investigated by using the stopped-flow equipment at 298 K. Reaction kinetics experiments were carried out for the promoted CO₂BOL systems containing different weight concentrations of MEA (or morpholine) while keeping the DBU weight percentage constant. The termolecular reaction mechanism was found to be successful in correlating the experimentally obtained pseudo first order reaction rate (k_o , s⁻¹) values. Power law kinetics was performed by plotting the natural logarithm of reaction rate constants vs. promoter (MEA or morpholine) concentration. The fractional reaction orders were determined to be between 1 and 2. The obtained results showed that the reaction rate between CO₂ and CO₂BOLs could be significantly enhanced by blending with MEA and morpholine. These promoted solvent systems are promising candidates for CO₂ removal from flue gas.

Key Words: CO₂-BOL; CO₂ reaction kinetics; CO₂ removal; morpholine; stopped-flow

References

- [1] Mukhtar, A (2020) Science of Total Environment 734:139397.
- [2] Oh HT, Ju Y, Chung K, Lee CH (2020) Energy 206:118164.
- [3] Knipe JM, Chavez KP, Hornbostel KM et al. (2019) Environmental Science and Technology 53:2926-2936.
- [4] Yuksel Orhan O, Alper E (2015) Chemical Engineering & Technology 38:1485-1489.

ANTIMONY ADSORPTION STUDY OF CHITOSAN PRODUCED FROM *CARIDEA* AND *BRACHYURA* SHELLS

Zehra Ozden OZYALCIN¹, Azmi Seyhun KIPCAK²

¹Department of Chemical Engineering, Faculty of Chemical and Metallurgical Engineering, Yildiz Technical University, Istanbul, Turkey. e-mail: zehraozyalcin@gmail.com

²Department of Chemical Engineering, Faculty of Chemical and Metallurgical Engineering, Yildiz Technical University, Istanbul, Turkey. e-mail: skipcak@yildiz.edu.tr

Abstract

Millions of tons of shellfish rich in chitin are consuming each year. Leftover parts of these shellfish are buried or disposed back into the sea. *Pandalus borealis* (pink shrimp) and *Cancer pagurus* (brown crab) are among the most common used shellfishes and have significant economic value. In this study, chitosan production yields at every stage of production and heavy metal adsorption capacity of the produced chitosan were investigated. As production parameters, 18-40, 40-60 and 60+ mesh particle size and 60, 80 and 100 °C deacetylation temperatures were chosen. Besides that, adsorption was carried out for 1, 2 and 3 hours in 20 ppm Antimony stock solution with a gram of chitosan that deacetylated at 80°C. Deacetylation yields are found between 60,28% - 93,40% for the crab shell owned chitin and between 61,43% - 90,60% for shrimp shell owned chitin. Moreover, the highest adsorption was observed with 18 mesh shrimp and 40 mesh crab with final heavy metal concentrations as 14.14 ± 0.32 and 13.65 ± 0.31 ppm, respectively.

Key Words: adsorption; antimony; chitosan; production yield; shellfish

Acknowledgement

This work was supported by Research Fund of the Yildiz Technical University. Project Number: FYL-2020-3933”

Novel *N*-4-piperazinyl-ciprofloxacin-aniline hybrids: Synthesis and *in vitro* biological evaluation as anticancer agents

Rabia AKHTAR¹, Ameer Fawad ZAHOOR^{1,*}, Azhar RASUL², Matloob AHMAD¹,
Muhammad Naveed ANJUM³, Muhammad AJMAL⁴ and Zohaib RAZA⁵

¹Department of Chemistry, Government College University, Faisalabad, Pakistan, *fawad.zahoor@gmail.com

²Department of Zoology, Government College University, Faisalabad, Pakistan

³Department of Applied Chemistry, Government College University, Faisalabad, Pakistan

⁴Department of Chemistry and Chemical Engineering, Xiamen University, Xiamen, China

⁵Department of Pharmacology, Government College University, Faisalabad, Pakistan

Abstract

Fluoroquinolones (FQ) represent an important family of antibacterial agents that displays a great activity against Gram-negative as well as Gram-positive bacterial strains [1]. However, some members of FQ family also display anti-proliferative activity. For example, ciprofloxacin (CP) which is a second generation of fluoroquinolone displays anti-proliferative and apoptic activities against several cancer cell lines. Recently, a variety of antitumor fluoroquinolones have been derived by structural modification of the antibacterial fluoroquinolones especially in the heterocyclic ring such as piperazine at the 7-position of the quinolones scaffold [2,3]. To contribute to the development of novel antitumor fluoroquinolones, a series of *N*-4-piperazinyl-ciprofloxacin-hybrids linked with a variety of anilides were synthesized and their *in vitro* antitumor activity against liver cell line (Huh-7) was screened by determination of cell viability in MTT assay. Preliminary screening showed that one of the new compounds, namely methyl 1-cyclopropyl-6-fluoro-4-oxo-7-(4-(2-oxo-2-(phenylamino)ethyl)piperazin-1-yl)-1,4-dihydroquinoline-3-carboxylate showed significant cytotoxic activity by displaying 68.36% cell viability at 100 µg/mL concentration which was then *in-silico* modelled to define the potential mechanistic insights for its anti-proliferative activity. The PASS prediction showed the topoisomerase II (TopII) as potential anticancer target of the targeted compound. The induced fit docking revealed that this compound inhibits the TopII with superior binding affinity and forms stronger contacts with active site's key residues responsible for DNA-TopII intercalation and catalytic inhibition consistent with its cytotoxic potential [4]. These results represent promising lead compounds for future in the development of potent antitumor agents.

Key Words: Fluoroquinolones; cytotoxic activity; human liver cell line; anti-cancer; induced fit docking.

References

- [1] Kerns RJ, Rybak MJ, Kaatz GW, Vaka F, Cha R, Grucz RG, Diwadkar VU, Ward TD (2003) Bioorganic & Medicinal Chemistry Letters 13:1745-1749.
- [2] Abdel-aziz M, Park S-E, Abuo-Rahma GE-DAA, Sayed MA, Kwon Y (2013) European Journal of Medicinal Chemistry 69:427-438.
- [3] Suresh N, Nagesh HN, SekharKVG, Sekhar, Kumar A, Shirazi, AN, Parang K (2013) Bioorganic & Medicinal Chemistry Letters 23:6292-6295.
- [4] Akhtar R, Zahoor AF, Rasul A, Ahmad M, Anjum MN, Ajmal M, Raza Z (2019) Pakistan Journal of Pharmaceutical Sciences 32:2215-2222.

SYNTHESIS AND CHARACTERISATION OF A GLUTATHIONE-S-TRANSFERASE (hGSTP1-1) SINGLE NUCLEOTIDE POLYMORPH

Sadhna MATHURA¹

¹University of the Witwatersrand, Johannesburg, SOUTH AFRICA, sadhna.mathura@wits.ac.za

Abstract

Glutathione-S-transferases (GSTs, E.C. 2.5.1.18) comprise a superfamily of multifunctional enzymes involved in catalytic cellular **detoxification** reactions [1, 2]. Mutations in GST proteins, particularly single nucleotide **polymorphisms** (SNP), have been linked to several human diseases and ailments such as Alzheimer's- and Parkinson's disease, asthma, cancer and so on [3-5]. Understanding the intimate **structure-function** relationship of these SNP mutations (relative to wildtype) is therefore of growing interest. What are the structural implications of GST polymorphism and the subsequent influences on its detoxification function? Consequently, in this work we aim to synthesise and characterise a single nucleotide polymorph (P124A) in the hydrophobic domain of canonical cytosolic human GST class pi (**hGSTP1-1**).

The P124 residue sits at the interface of the two protein subunits (Figure 1) and is contained in the all-helical domain of the protein subunit. Our strategy is therefore to examine the structure-function significance of the P124 residue using an interesting SNP mutation [6], P124A. We compare the structure-function features relative to those of the wild-type (WT) to elucidate how the identity of the residue at this position influences the catalytic, structural and stability properties at the binding sites. Circular dichroism and fluorescence spectra reveal minor secondary and tertiary alterations of P124A structure relative to WT.

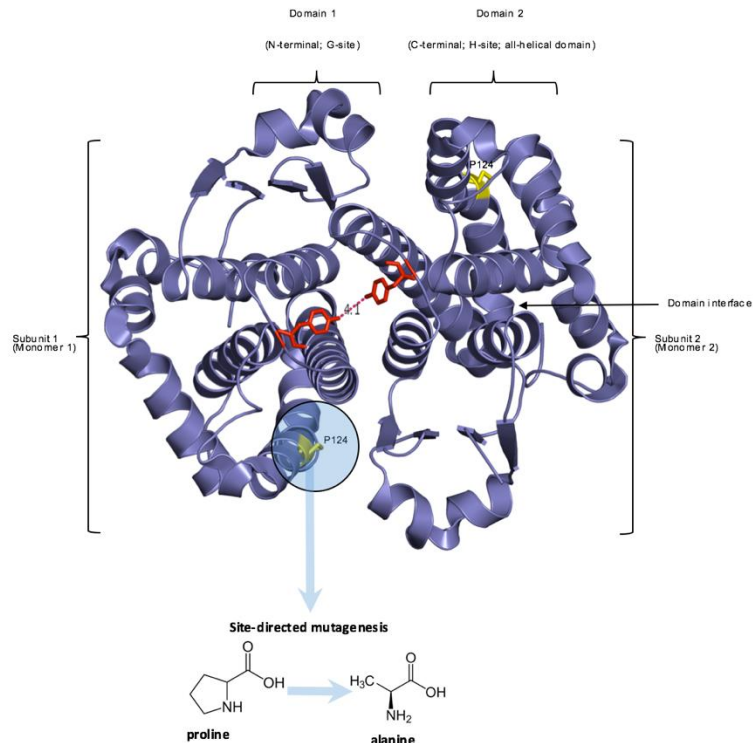


Figure 1: Quaternary structure of the homodimeric hGSTP1-1 (PDB: 2a2r). The monomer subunits, domains and interfaces are indicated. The highlighted region in yellow indicates the P124 region for site-directed mutagenesis to synthesise the P124A SNP mutant.

Key Words: *hGSTP1-1; SNP; polymorphism; structure-function relationship; detoxification proteins.*

References

- [1] Vasieva, O.; Current Molecular Medicine, 2011, 11, pp129-130.
- [2] Sheehan, D.; Meade, G.; Foley, V. M.; Dowd, C. A.; Biochem. J., 2001, 360(1); pp1-16.
- [3] Tew, K. D.; Manevich, Y.; Grek, C.; Xiong, Y.; Uys, J.; Townsend, D. M.; Free Rad. Biol. And Med., 2011, 51(2) pp299-313.
- [4] McIlwain, CC; Townsend, DM and Tew, KD; Oncogene, 2006, 25, pp1639-1648.
- [5] Hayes, J. D.; Strange, R. C.; Pharmacology, 2000, 61, pp154-166.
- [6] SNP database (<https://www.ncbi.nlm.nih.gov/snp/>)

CYCLODEXTRIN-CALIXARENE NANOSPONGES FOR THE ADSORPTION OF LEAD ION FROM AQUEOUS SOLUTION

Salvatore Cataldo,¹ Alberto Pettignano,¹ Paolo Lo Meo,² Demetrio Milea³

¹ Dipartimento di Fisica e Chimica – Emilio Segrè, Università di Palermo, viale delle scienze, 90128, Palermo -
salvatore.cataldo@unipa.it

² Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali Università di Palermo, viale delle
scienze, 90128, Palermo

³ Dipartimento di Chimica Inorganica, Chimica Analitica e Chimica Fisica, Università di Messina, Via
Ferdinando Stagno d'Alcontres, 31, 98166 Messina (Vill. S. Agata)

Abstract

Recently our research group synthesized new cyclodextrin-calixarene nanosponges (CyCaNSs): fifteen pre- and post-modified CyCaNSs with 1,2,3-triazole linker units (ACNSs) have been characterized by FT-IR, $^{13}\text{C}\{^1\text{H}\}$ CP-MAS, solid state NMR and TGA [1-2]. These materials can be useful in many fields of applications: drug carrier/delivery, devices to sensors, environment remediation, active packaging [3-4]. Their acid-base properties and their adsorption ability towards Pb^{2+} ion have been studied taking into account the changing of the molar ratio between the co-monomers, the substituent groups present on each co-monomer scaffold, and the ionizable groups introduced by chemical post-modifications.

The pH-tunability was evident even by non-modified materials, and this behavior was attributed to the presence of the triazole linkers, which may act as weak bases. This hypothesis, however, implies that triazole linkers should increase their basic strength due to their insertion in the polymeric network. Protonation constants values of CyCaNSs, calculated by ISE- H^+ potentiometric titrations data and processed with Diprotic-Like model [5], confirm this hypothesis.

The Pb^{2+} adsorption onto the selected CyCaNSs have been studied measuring the metal ion concentration in the aqueous solutions collected during batch experiments by differential pulse anodic stripping voltammetry (DPASV).

The experiments were carried out with and without the addition of background salts, at different pH, ionic strengths and temperatures. NaNO_3 and NaCl ionic media were used, changing the ionic strength in the range $0.01 - 0.1 \text{ mol L}^{-1}$. The initial pH was fixed at 3 and 5, whilst, the effect of temperature was studied in the range $283.15 - 323.15 \text{ K}$.

Key Words: Cyclodextrin; Adsorption; Nanosponges; Metal ions; Calixarene.

References

- [1] Lo Meo P, Lazzara G, Liotta L, Riela S, Noto R (2014) Polymer Chemistry 5:4499-4510.
- [2] Cinà V, Russo M, Lazzara G, Chillura Martino D, Lo Meo P (2017) Carbohydrate Polymers 157:1393-1403.
- [3] Cavalli R, Trotta F, Tumiatti W (2006) Journal of Inclusion Phenomena and Macrocyclic Chemistry 56(1-2): 209.
- [4] Subramanian S, Anandam S, Kannan K, Rajappan M (2012) Journal of Pharmacy and Pharmaceutical Sciences 15:103.
- [5] Crea F, De Stefano C, Gianguzza A, Pettignano A, Piazzese D, Sammartano S (2009) Journal of Chemical and Engineering Data 54(2):589.

New triazolo-triazole derivatives: redox and emission properties and Cu(II) complexes

Sandra FUSCO¹, Emmanuele PARISI¹, Sabato VOLINO¹, Carla MANFREDI¹, Roberto CENTORE¹

¹ Department of Chemical Sciences, University of Naples "Federico II",
Via Cintia – Complesso Universitario Monte S. Angelo- 80126 Naples
Email: sandra.fusco@unina.it

Abstract

N-rich heterocycles have attracted the interest of the researchers in the past as in the present. Mostly nowadays their use as building block in materials chemistry, *e.g.* for applications in organic solar cells and organic semiconductors, [1] and as nucleobase analogues, *e.g.* for DNA and RNA study and for therapy against cancer cells proliferation, [2] has given new inputs to their study in solid state and in solution. The most exploited characteristics are photo-absorption and emission (photochromism and photofluorism).

Particularly, following our long standing interest in five membered rings, we have focused on triazolo-triazole derivatives and their modes of packing in the solid state and their tautomerism have been investigated and described. [3,4] Herein we present three triazolo-triazole derivatives [3] (see Figure 1a) that only differ from the electronic character (electron donor or acceptor) of the substituent at 7-position of the heterobicycle. Their acid-base (see Figure 1b and Table 1), redox and emission properties are studied with the aim to highlight the structure–property relationships. [5]

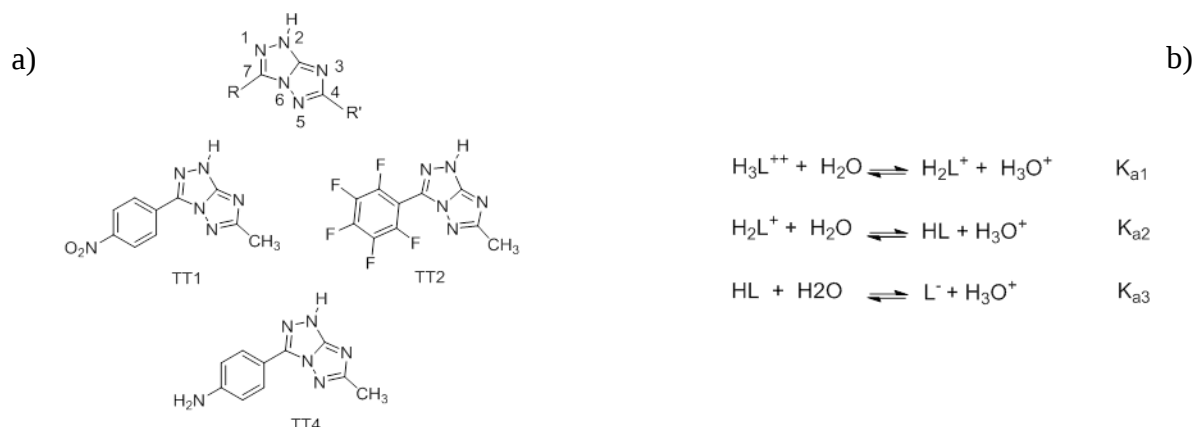


Figure 1- a) Chemical structures of triazolo-triazole derivatives [3] with atom numbering and only the 2H tautomer shown; b) Protolytic equilibria of triazolo-triazoles

Sample	pK _{a1}	pK _{a2}	pK _{a3}
TT1	-	1.18(5)	6.20(3)
TT2	-	0.77(5)	5.70(1)
TT4	1.30(3)	3.10(1)	7.10(5)

Table 1- Summary of obtained equilibrium constants, valid in 0.5 M NaCl/ethanol 4% (v/v) with estimated standard deviation in parentheses (T=25 °C)

By using spectrophotometry (in absorption and emission) and voltammetry, the study reveals that, in the class of [1,2,4]triazolo[3,2-c][1,2,4]triazoles, the electron donor/acceptor nature of the group at 7 position influences the hydrolysis reactions in the ground (Table 1) and excited state as well as the redox and emission properties. [5] Particularly, as regards the TT4

triazolo-triazole (electron donor character of the substituent), the recorded fluorescence in the whole pH range, with minimum in the pH range 4-6, allows to consider it as a potential fluorescent probe for nucleic acids study. For TT2, on the contrary, only the singly protonated species H_2L^+ is fluorescent, arising as a possible pH-induced fluorescence switch (see Figure 2). Therefore, for both TT2 and TT4, the neutral species are weak emitters. Unfortunately, for TT1 no emission is detected. [5]

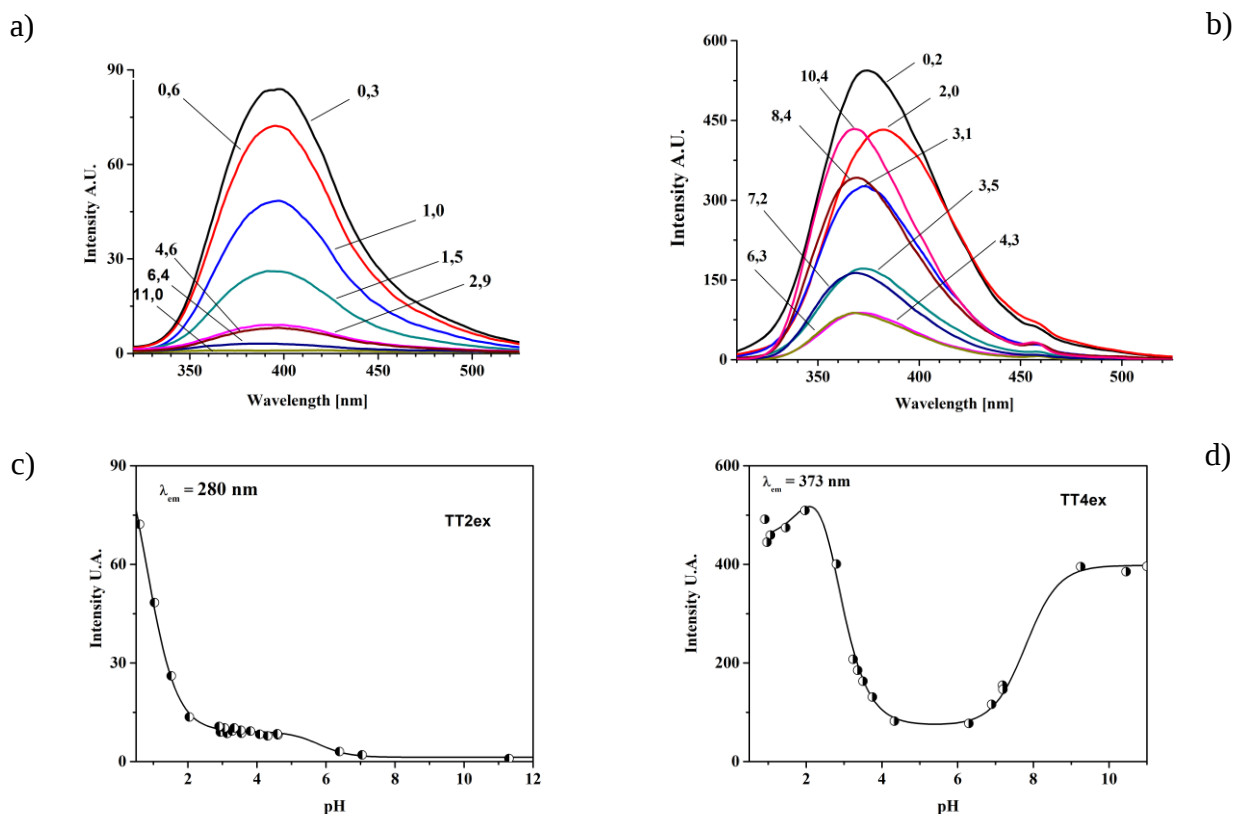


Figure 2- a) Emission spectrum of TT2 at different pH; b) Emission spectrum of TT4 at different pH; c) Emission intensity of TT2 vs pH at constant value of λ_{em} ; d) Emission intensity of TT4 vs pH at constant value of λ_{em}

Furthermore, the voltammetric current/potential ($i(A)/E(V)$) curves reveal a pH dependence of the reduction reaction of the heterobicycle moiety, at $-1.2\text{ V} < E_p < -0.9\text{ V}$, involving the same number of electrons and protons. Finally, the formation of mononuclear complexes of Cu^{2+} with TT4 triazolo-triazole, in the pH range 2-6, is highlighted. In particular, the experimental E_p / pH data collected in this study suggest a bridge copper (II) coordination for the $Cu(HL)^{2+}$ species. [5]

Key Words: Triazolo-triazole systems, Acid–base equilibria, UV–vis absorption-emission, Cu(II)-triazolo–triazole complexes, Equilibrium analysis

References

- [1] Zhao X, Chaudhry ST, Mei J (2017) *Advances in Heterocyclic Chemistry* 121: 133-171
- [2] Nakahara M, Kuboyama T, Izawa A, Hari Y, Imanishi T, Obika S (2009) *Bioorganic & Medicinal Chemistry Letters* 19: 3316–3319
- [3] Centore R, Manfredi C, Fusco S, Maglione C, Carella A, Capobianco A, Peluso A, Colonna D, Di Carlo A (2015) *Journal of Molecular Structure* 1093: 119–124
- [4] Centore R, Manfredi C, Capobianco A, Volino S, Ferrara MV, Carella A, Fusco S, Peluso A (2017) *Journal of Organic Chemistry* 82: 5155-5161
- [5] Fusco S, Parisi E, Volino S, Manfredi C, Centore R (2020) *Journal of Solution Chemistry* 49: 504–521

Investigation of switchable polarity solvents and their application in Claisen-Schmidt reaction of steroids

Dávid ISPÁN¹, Rita SKODA-FÖLDES²

^{1,2}Department of Organic Chemistry. Institute of Chemistry, University of Pannonia, P.O. Box 158, Veszprém, H-8200, Hungary

¹e-mail: ispan.david@mk.uni-pannon.hu

²e-mail: skodane@almos.uni-pannon.hu

Abstract

The switchable polarity solvent is a substance that can be converted from a non-polar to a polar ionic liquid in the presence of an external trigger (e.g. CO₂). Consequently, its application may facilitate isolation of the product as well as catalyst recycling.

In this work the synthesis of switchable polarity solvents and their application in the reaction of keto- and formyl-steroids has been explored. A guanidine base, used as catalyst and solvent, was converted to an ionic liquid in the presence of an alcohol and by the addition of CO₂. Then the steroidal products were extracted with apolar solvents. By the removal of CO₂, the system could be converted back to the non-polar, molecular state by heating it under reduced pressure and the base catalyst could be recovered and reused.

Firstly, different guanidine derivatives were prepared and were used as solvents and catalysts in the Claisen-Schmidt reaction of steroidal substrates. [2] Efficiencies of the catalysts were compared and the reaction conditions were optimised to produce several new condensation products.

Then the recyclability of the base catalysts was investigated. The parameters necessary for removing carbon-dioxide from the ionic state were determined for several guanidine-alcohol pairs. Claisen Schmidt reactions of different substrates were carried out in the presence of the optimal guanidine base, leading to the steroidal product in good yield and ensuring easy conversion between the ionic and molecular state.

The new compounds were characterised various methods, such as different NMR measurements, FTIR and GC-MS.

The new steroids may have favourable pharmacological effect, as similar compounds can be used as inhibitors of different enzymes, for example 17 β -HSD1, 17 β -HSD3 and aromatase that can cause hormone-dependent tumours. Consequently, the inhibition of these enzymes by appropriate steroidal derivatives can be a solution for the treatment of these diseases. [3]

The elaborated process enables efficient, new and environmentally-friendly synthesis of biologically active compounds.

Key Words: ionic liquid, carbon dioxide, steroid, reversibility, enzyme inhibition

References

- [1] Schuchardt U, Vargas RM, Gelbard G (1995) Journal of Molecular Catalysis A: Chemical 99:2, 65-70.
- [2] Ispán D, Szánti-Pintér E, Papp M, Wouters J, Tumanov N, Zsirka B, Gömöry Á, Kollár L, Skoda-Földes R (2018) European Journal of Organic Chemistry, 24, 3236-3244.
- [3] Marchais-Oberwinkler S, Henn C, Möller G, Klein T, Negri M, Oster A, Spadaro A, Werth R, Wetzel M, Xu K, Frotscher M, Hartmenn RW, Adamski J (2011) Journal of Steroid Biochemistry & Molecular Biology, 125, 66-82.

Acknowledgments

The support of MOL Hungarian Oil and Gas Public Limited Company's (MOL NYRT.) and Foundation of PEREGRINATIO I. (VVE) are acknowledged. This work is supported by Foundation Industry for Education of Engineering in Veszprém (Ipar a veszprémi mérnökképzésért Alapítvány), Association of Hungarian Chemists (Magyar Kémikusok Egyesülete) and the National Research, Development and Innovation Office (OTKA 116727 and 120014).

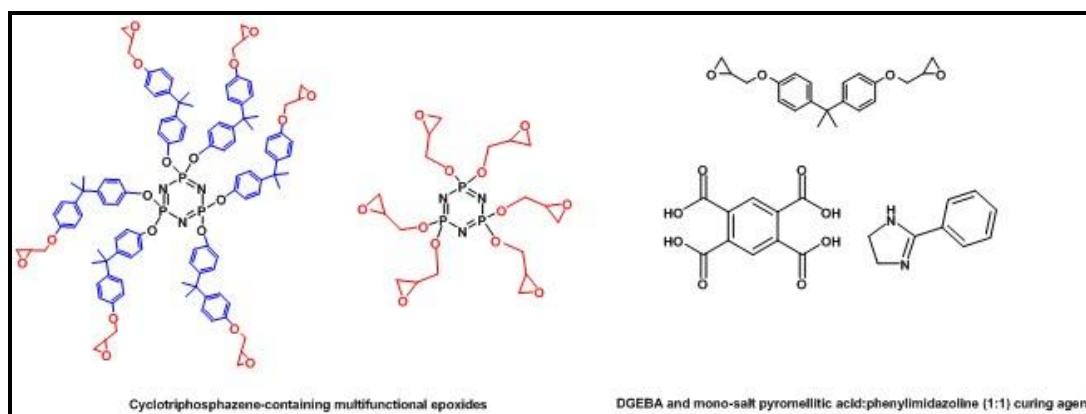
SYNTHESIS AND CHARACTERIZATION OF PHOSPHAZENE-BASED EPOXY BINDERS

Elif Büşra Çelebi, Halil Duyar, Cengiz Ayar, Rûmeysa Baran, Ferda Hacivelioglu

Gebze Technical University Department of Chemistry, 41400, Gebze, Kocaeli, Turkey
bsracelebi@gmail.com

Abstract

Today, mostly halogen-based additives are used to increase the level of non-flammability. The use of polybromo diphenyl ether derivatives, which are halogenated flame retardants, was banned in 2004. Due to the negative effects of halogen-based additives on human and environmental health, alternative flame retardants were needed [1]. Phosphazenes form compounds with different characteristics as a result of nucleophilic substitution reaction with various groups. Because of these properties, they are used in the production of high-tech materials. Phosphazene compounds are frequently used in the preparation of new polymers and in the production of fire resistant materials [2-3]. In this respect, it is very important to determine the synthesis studies and application areas of new phosphazene derivatives. In this study, hybrid compounds obtained by bonding organic groups to hexachlorocyclotriphosphazene (trimer) compound in certain proportions were added to the epoxy binder and the changes in the thermal properties of the resin were investigated. For this purpose, trimer compound first underwent nucleophilic substitution reaction with glycidol, as a result of this reaction, hexaglycidylcyclotriphosphazene (HGCP) hybrid compound was synthesized. Another hybrid compound was synthesized using the bisphenol-A derived epoxide compound, the second hybrid compound, and the structure of the obtained compounds was elucidated using ^1H NMR, ^{13}C NMR, ^{31}P NMR, FT-IR and MALDI techniques. The synthesized hybrid compounds were added to the solid epoxy resin-hardener (R-S) mixture in certain proportions (10%, 20%, 30% w/w) and the glass transition temperature (T_g) and thermal resistance properties of the mixtures were examined by DSC and TGA methods.



Key Words: *Phosphazene; epoxy resin; flame retardant*

References

- [1] Ren H, Sun J, Wu B, Zhou Q (2007) Polym. Degrad. Stab. 92:956–961.
- [2] Diefenbach U, Allcock HR (1994) Inorganic Chemistry 33(20):4562-4565.
- [3] Liu R, Wang X (2009) Polym. Degrad. Stab. 94(4):617-624.

TETRA 7-OXY-4-(PYRIDIN-3-yl)COUMARIN SUBSTITUTED COPPER (II) and COBALT (II) PHTHALOCYANINES: SYNTHESIS, SPECTROSCOPIC PROPERTIES and THEORETICAL STUDY

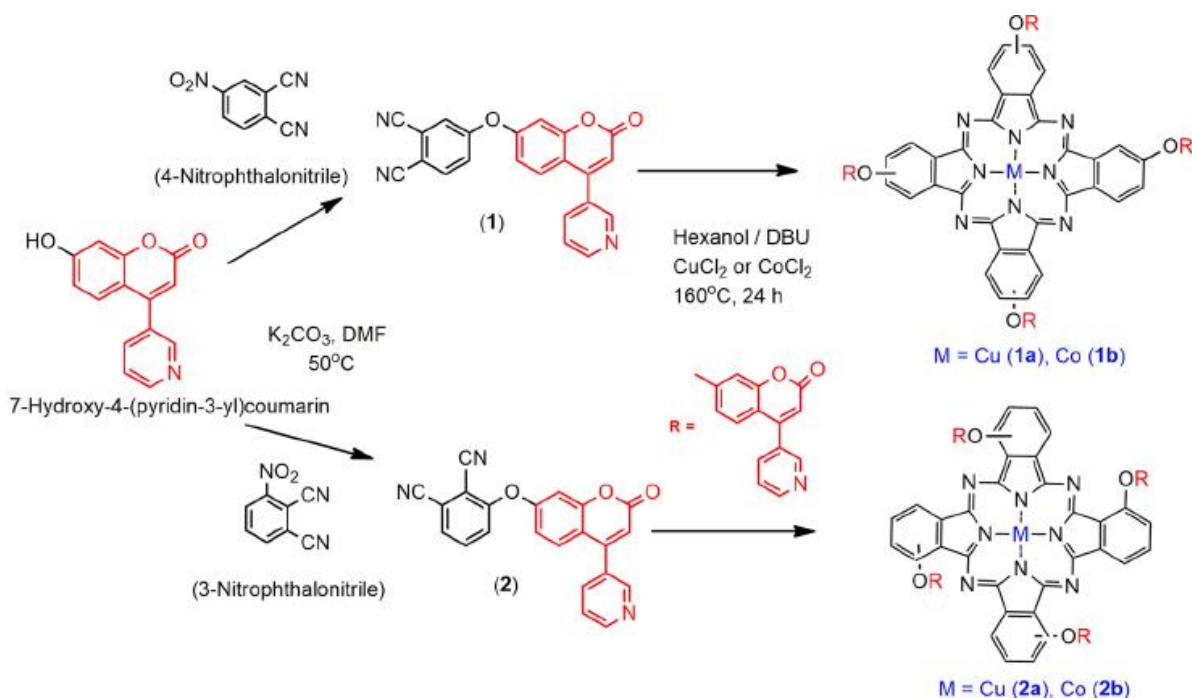
Yelda YALCIN GURKAN¹, Şimal KURUMOĞLU¹, Caner Yahya BOYAR², Yasemin KESKEK KARABULUT¹, Meryem CAMUR²

¹Tekirdag Namik Kemal University, Department of Chemistry, Tekirdag, Turkey, e-mail: yyalcin@nku.edu.tr

²Kirklareli University, Department of Chemistry, Kirklareli, Turkey, e-mail: meryemcamur@klu.edu.tr

Abstract

The original Cu(II) and Co(II) metallo phthalocyanine complexes substituted with 7-oxy-4-(pyridin-3-yl)coumarin moieties both in peripheral and non-peripheral positions were synthesized and their structure characterized. Their electronic absorption spectra and aggregation properties were investigated in DMF and DMSO. The Cu metallo peripheral substituted phthalocyanine complex was exhibited an aggregation band in both DMF and DMSO. On the other phthalocyanine complexes no aggregation band was observed. Optimized geometry of the molecules was drawn using Gauss-View 5 program, and their state at lowest energy was determined using Gaussian 09 program. However, energy-minimized structure, electronic distribution and molecular orbitals were obtained by DFT/B3LYP/6-31G (d,p) calculations which were supported by experimental results.



Scheme 1. Synthesis of phthalonitriles (1, 2) and tetra 7-oxy-4-(pyridin-3-yl)coumarin substituted Pcs (1a-b, 2a-b).

Key Words: Metallo phthalocyanine; 2H-chromen-2-one; UV-vis spectroscopy; DFT.

References

- [1] Lobanov AV, Dmitrieva GS, Sultimova NB, Levin PP (2014) Russ J. Phys. Chem. B 8: 272.

EFFECT OF N-BUTANOLIC EXTRACT OF A PLANT GROWING SPONTANEOUSLY IN CENTRAL ALGERIA AS AN ADDITIVE IN ELECTRODEPOSITION

Karima HANINI¹, Sameh BOUDIBA², Merzoug BENAHMED¹, Hocine LAOUER³ and Louiza BOUDIBA⁴

¹ Laboratory of active molecules and applications, Tebessa University, Constantine Road, 12002, Tebessa-Algeria - haninikarima@yahoo.com-

² Laboratory of organic materials and heterochemistry, Tebessa University, Constantine road, 12002, Tebessa-Algeria – boudibasameh@gmail.com-

³ Laboratory for the valorization of natural biological resources, Ferhat Abbas University, Setif, 19000, Algeria- hocine_laouer@yahoo.fr-

⁴ Chemistry department, normal higher school, old Kouba, Algiers, Algeria- boudibalouiza@gmail.com-

Abstract

The aim of this work is the evaluation of *n*-butanolic extract obtained from the aerial part of "*Taxus Baccata*" [1] as additive in electrodeposition using potentiodynamics polarization and weight loss measurements. The electrodeposition of the zinc on the steel in chloride solution was performed using a direct current supply [2, 3]. The presence of the *n*-butanolic extract as additive in the electrolytical bath performs the quality of the electrodeposition of the zinc. This constatation was observed through the deposit parameters as the brightness, the adhesion and the thickness [4-6]. It was found that the electrodeposition process changed with additive concentration. In addition their efficiency against corrosion was evaluated indicating that the samples coated in the presence of the extract were more resistant against this phenomenon.

Key Words: Corrosion; *Taxus Baccata*; electrodeposition; extract; additive.

References

- [1] Benahmed M, Akkal S, Louaar S, Laouer H and Duddeck H (2006) Biochemical systematics and ecology 34, 645-647.
- [2] Hanini K, Benahmed M, Boudiba S, Selatnia I, Laouer H and Akkal S (2019) Sustainable Chemistry and Pharmacy, 14, 100189.
- [3] Loto C, Olofinjana A, Oniso J and Popoola A (2015) Can. J. Pure Appl. Sci, 9, 3267-3277.
- [4] Astm, D., 2002. 3359-02: standard test methods for measuring adhesion by tape test. ASTM International, West Conshohocken.
- [5] ASTM, D., 1989. Standard Test Method for Specular gloss 6, 36–40, 523-589.
- [6] ASTM D A879–Steel Sheet. Zinc Coated by the Electrolytic Process for Applications Requiring Designation of the Coating Mass on Each Surface.

DETERMINATION OF HEXANAL AS MARKER OF LIPID OXIDATION IN EDIBLE OILS BY HEADSPACE GAS CHROMATOGRAPHY

Birutė BUGELYTĖ, Gintarė PIPIRAITĖ, Vilius POŠKUS, Vida VIČKAČKAITĖ

Department of Analytical and Environmental Chemistry, Vilnius University, Naugarduko St. 24, LT-03225
Vilnius, Lithuania, e-mail: b.bugelyte@gmail.com

Abstract

Edibles oils constitute an important component of human diet. However, during storage and especially during heating, unsaturated fatty acids of edible oils undergo oxidation [1]. Some oxidated edibles oils products can be toxic and can increase propensities to various cardiovascular and metabolic diseases [2]. Thus there is a great interest on fast and simple detection of lipid oxidation.

The evaluation of the oxidation level can be based on the quantity of secondary oxidation product such as hexanal [3]. In this study, we developed a sensitive, fast, reliable and reproducible technique for hexanal determination in edible oils using static headspace extraction coupled to gas chromatography (SHS-GC). Usually, calibration solutions of hexanal are prepared in fresh corresponding oils or in fresh rapeseed oil [1, 3, 4]. However, most of the edible oils contain significant quantities of unsaturated fatty acids, thus the standard solutions prepared in the oils should be kept at low temperature and are of limited storage, otherwise additional quantity of hexanal can form. In this work, coconut oil as a stable and hexanal-free solvent for standard solutions of hexanal was suggested.

Headspace extraction conditions (sample equilibration temperature, time, weight, injection time) were determined to provide the highest extraction to the headspace efficiency. Quality parameters were determined under the optimized conditions. The calibration curve was linear in the concentration range from 50 µg/kg to 2 g/kg with the correlation coefficient 0.9977. The limit of detection was 30 µg/kg, repeatability of the results was 1.1 % (hexanal concentration 10 mg/kg).

The developed SHS-GC method was applied for hexanal determination in four popular edible oils - olive oil, rapeseed oil, sunflower oil and linseed oil. The biggest quantity of hexanal was observed in sunflower oil but in linseed oil was rather small. Rapeseed oil was the most resistant to the oxidation at elevated temperatures.

Key Words: *edible oils, hexanal, coconut oil, static headspace extraction, gas chromatography*

References

- [1] Sghaier L, Vial J, Sassiati P, Thiebaut D, Watiez M, Breton S, Rutledge DN, Cordella CBY (2016) European Journal of Lipid Science and Technology 118:906-918.
- [2] Gotoh N, Watanabe H, Osato R, Iwasawa A, Inagaki K, Wada (2005) Journal of Oleo Science 54:397-405.
- [3] Azarbad MH, Jeleń H (2015) Food Analytical Methods 8:1727-1733.
- [4] Gromadzka J, Wardencki W (2010) Chromatographia, 7:S81-S86.

Analysis of Molecular Orbital Energies, Global Reactivity Descriptors, and Electronic Transitions of $[\text{Mn}(\text{CO})_3(\text{bpy})(\text{N-benzimidazole})]\text{PF}_6$ Complex by DFT/TDDFT-Based Computational Methods

Dolunay ŞAKAR DAŞDAN^{1*}, Elvan ÜSTÜN²

¹ Department of Chemistry, Faculty of Art and Science, Yıldız Technical University, 34220 Istanbul, Turkey

² Department of Chemistry, Faculty of Art and Science, Ordu University, 52200 Ordu, Turkey

*Presenter email: dolunaykar@yahoo.com

Abstract

Although carbon monoxide is known as toxic, it is a by-product produced endogenously during hemoglobin degradation in the body. Therefore, there is always a certain amount of CO in the tissue and the concentration of carbon monoxide in the body assigns its toxicity level. CO is a transmitter and the studies about biological activity and therapeutic properties of CO give favorable results [1]. Besides various organic molecules have been researched for this purpose; the most important candidates for CO-Releasing Molecules (CORMs) are metal carbonyl complexes that contain CO as a ligand in their structure. Many metal carbonyl complexes have been synthesized and analyzed for their bioactivities, and there are currently used as CO-releaser drugs [2].

Recently, important developments have occurred in the field of theoretical chemistry. The theoretical methods give compatible results with the experimental values and computational chemistry is a frequently used field in optimization and characterization [3]. The properties of the frontier orbitals of molecules provide important data about the reactivity of molecules. The type and location of the frontier molecular orbitals are also remarkable in the analysis of the reactive regions of the molecules [4].

In this study, $[\text{Mn}(\text{CO})_3(\text{bpy})(\text{N-benzimidazole})]\text{PF}_6$ type metal carbonyl complex was analyzed for molecular orbital energies, global reactivity descriptors, and electronic transitions by DFT/TDDFT-based calculation methods and evaluated structure/reactivity correlation.

Key Words: CORMs, Molecular Docking, Benzimidazole, DFT/TDDFT

Acknowledgments: This work was supported by Yıldız Technical University Scientific Project Coordination Department as Project no:FBA-2020-3805 and TÜBİTAK 112T320.

References

- [1] Romão CC, Blättler WA, Seixas JD, Bernardes GJL (2012) Chem. Soc. Rev. 41:3571.
- [2] Johnson TR, Mann BE, Teasdale IP, Adams H, Foresti R, Green CJ, Motterlini R (2007) Dalton Trans. 1500-1508.
- [3] Gonzalez MA, Carrington SJ, Chakraborty I, Olmstead MM, Mascharak PK (2013) Inorg. Chem. 52:11320-11331.
- [4] Tian Z, Zang F, Luo W, Zhao Z, Wang Y, Xu X, Wang C (2015) J. Photochem. Photobiol. B Biol. 142:103-109.

The Effects of Naphthenic Oil, BR, NR and Content of Vinyl in S-SBR on Passenger Tread Compounds

Duygu KABAKOĞLU¹, Sezgin GÖKÇESULAR¹

¹ Brisa Bridgestone Sabanci Tire Company, İzmit/Kocaeli, 41310,
Tel. +90 262 316 5182; emails: d.kabakoglu@brisa.com.tr (D. Kabakoğlu)
Tel. +90 262 316 5150; emails: s.gokcesular@brisa.com.tr (S. Gökçesular)

Abstract

Tire is a part of vehicle that contact to the road. The tire is made up rubber compounds and reinforcement materials. Rubber compounds are categorized as tread compounds and case compounds. The tread compounds are surrounding the area of tire that contact to ground keeping the tire on the road. Also, case compounds function could be summarize as support to tread and transmission of generated energy to the tread part of tire [1]. At that point, the reinforcement materials are used to support case compounds to load. These are classified as textile cord, steel cord and bead wire.

Dynamic property analysis of tire tread compound is interpreted with mechanical loss angle ($\tan\delta$) data. Mechanical loss is a function of time, temperature and strain. In addition to that, it is found as taken ratio of dynamic loss modulus (E'') and dynamic storage modulus (E'). The dynamic property analysis made with using $\tan\delta$ vs. temperature ($^{\circ}\text{C}$) curve. On this curve, $\tan\delta$ at -20, 0, and 60 $^{\circ}\text{C}$ refers to ice traction, wet traction and rolling resistance properties of compounds, respectively [2].

Tread compounds consist of polymers, fillers, vulcanization systems, protectants and various special additives [1]. Polymers could be separated as Styrene Butadiene Rubber (SBR), Butadiene Rubber (BR) and Natural Rubber (NR). Type of rubber contents in tire is changeable for considering load/speed index for groups of vehicles. Mainly, tread compound that belong to passenger group vehicle is consist of high content SBR that gives effective traction properties and also wear resistance to the tread compounds if make comparison with tread compounds that belong to truck group. The main reason of that, passenger group vehicle has lower load/speed ratio regarding truck group [3].

Solution and emulsion polymerization techniques are commonly used in SBR synthesis. The comparison of SBR could be summarized as solution polymerized SBR (S-SBR) give much more rolling resistance and tread wear properties to tire regarding emulsion polymerized SBR (E-SBR) [4].

The expectations of environment protection including decreasing trend of carbon emission, conservation of resources and increasing sensitivity of safety vehicle perception strategy have a big role to force passenger vehicle industry. Also, these reasons directly affect the tire industry to reduce fuel consumption, decrease rolling resistance etc. Therefore, demand of higher performance in passenger tires in worldwide trend direct tire industry to use S-SBR in passenger tire tread compounds [5]. Because of that reasons, this paper focuses on improvement of passenger groups' tread compounds dynamic properties that consist of high amount of S-SBR in tire. The effects of naphthenic oil, BR, NR and content of vinyl in S-SBR are observed.

Key Words: tread compound; dynamic property; styrene butadiene rubber; passenger tire; mechanical loss

References

- [1] Rodgers, B. and A. Halasa. (2016) Compounding and Processing of Rubber/Rubber Blends. (161-201)
- [2] Al-Hartomy O., A.Al-Ghamdi, A., Dishovsky, N., Mihaylov, M., Malinova, P., Said, S.F., Arabia, S., & Ohridski, K. (2015). Comparative Study of the Dynamic Properties of Natural Rubber Based Composites, Containing Carbon-Silica Dual Phase Fillers Obtained by Different Methods
- [3] Puchong Thaptong, Pongdhorn Sae-oui, Chakrit Sirisinha; Influences of Styrene Butadiene Rubber and Silica Types on Performance of Passenger Car Radial Tire Tread. Rubber Chemistry and Technology 1 December 2017; 90 (4)
- [4] Akron, H., & Tallmadge, M., Jr. (2002). U.S. Patent No. US 6455655. Washington,DC: U.S. Patent and Trademark Office.
- [5] Inagaki, K., Hayashi, M., & Imai, A. (2004). Development of the Solution SBRs for High-performance Tires.

Aminocarbonylation in the presence of supported palladium catalyst

Enikő Nagy^{1a}, Bernadett Adamcsik¹, Máté Papp¹, Béla Urbán¹, Rita Skoda-Földes^{1b},

¹Department of Organic Chemistry, Institute of Chemistry, University of Pannonia, P.O. Box 158,
Veszprém, H-8200 Hungary

^anagyencsi6@gmail.com

^bskodane@almos.uni-pannon.hu

Abstract

In the present work carbonylation reactions performed with heterogeneous catalysts were studied. Heterogeneous catalysts have considerable advantages over homogeneous ones. Besides the high yields, the catalyst is reusable and the metal leaching can be minimised, so they have a good perspective in medicinal chemistry. [1]

In the first stage of the research, heterogeneous catalysts were produced and tested. As a first step, ionic liquids (ILs) of different structure were synthesized and then they were grafted on the surface of silica gel. The palladium precursor was immobilised on the IL-modified supports. The new materials were characterised by various methods, such as by solid phase NMR measurements, FTIR and TEM. The supported catalysts were tested first in the aminocarbonylation reactions of simple substrates. Good selectivity, high conversion and yield were measured as the result of the model reactions. Various features of the catalysts were also investigated, such as the palladium content, stability, recyclability and palladium-leaching.

Furthermore, the applicability of the best catalyst was tested in the synthesis of different molecules with pharmaceutical importance, such as nikethamide and steroid derivatives. The target compounds were successfully synthesised in short reaction times, with excellent selectivity, good yield. Under optimised conditions, a low palladium-leaching was observed and the catalyst was reusable in five runs.

The further aim of the work is to investigate the efficiency of the developed heterogeneous catalyst in the synthesis of various heterocyclic derivatives with potential biologically activity.

The support of MOL Hungarian Oil and Gas Public Limited Company's (MOL NYRT.) and Foundation of PEREGRINATIO I. (VVE) are acknowledged. This work is also supported by Foundation Industry for Education of Engineering in Veszprém (Ipar a Veszprémi Mérnökképzésért Alapítvány) and GINOP-2.3.2-15-2016-00049 grant.

Key Words: *heterogeneous catalysis, palladium catalyst, selectivity, reusability, pharmacologically active compounds*

References

[1] Béla Urbán, Máté Papp, Rita Skoda-Földes (2019) Current Green Chemistry 6(2):78-95.

Antioxidant activity of new glycoconjugates containing Selenium

**Luigia SERPICO,¹ Mauro De NISCO,² Flavio CERMOLA,¹
Michele MANFRA,² Claus JACOB,³ Silvana PEDATELLA¹**

¹Dept. of Chemical Sciences, University of Napoli Federico II, Via Cintia 4, I-80126 Napoli, Italy;

²Dept. of Sciences, University of Basilicata, Viale dell'Ateneo Lucano 10, I-85100 Potenza, Italy;

³Dept. of Pharmacy, Saarland State University, D-66123 Saarbruecken, Germany

e-mail: luigia.serpico@unina.it

Abstract

Nowadays Selenium (Se) is recognized as a trace element essential for human health, low Se levels are actually associated with several diseases [1]. Many natural occurring Se compounds show redox and biological capacities, thus stimulated synthesis of new molecules with the aim to spread antioxidant effects in biological systems. Most of these bioactive Se-containing molecules showed a strong therapeutic and biological relevance [2].

Here we propose a new strategy to synthesize glycoconjugates consisting of a seleno-deoxysugar (**1**) bound to a polyphenolic moiety. The methodology was applied for the synthesis of the short library of the new molecules displayed in Chart 1.

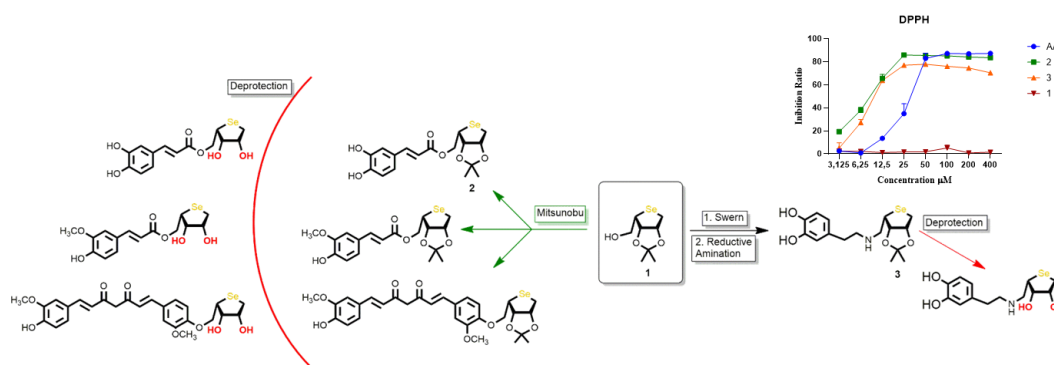


Chart 1. Scheme of seleno-glycoconjugates.

Antioxidant activity of the new glycoconjugates has been investigated by specific tests. Namely, FRAP and DPPH assays were performed to verify the reducing and scavenging abilities, respectively.

Key Words: Selenium, Antioxidants, Oxidative stress, Deoxysugars, Polyphenols

References

[1] Rayman MP (2020) Hormones 19:9–14

[2] Lenardão EJ, Santi C, Sancineto L (2018) New Frontiers in Organoselenium Compounds. Springer, Cham 2:99-143

Acknowledgment. Authors wish to thank European Union (FSE, PON Ricerca e Innovazione 2014-2020, Azione I.1 “Dottorati Innovativi con caratterizzazione Industriale”), for funding a Ph.D. grant to Luigia Serpico.

THE CONTRIBUTION OF ELECTRONEGATIVE GROUPS ON THE SYNTHESIS AND THE ANTIMICROBIAL EFFECTS OF TETRAZOL COMPOUNDS CONTAINING DIFFERENT SUBSTITUTENT GROUPS

Elvan HASANOĞLU ÖZKAN¹, Hatice ÖĞÜTÇÜ², Ali DİŞLİ¹, Nurşen SARI¹

¹Gazi University, Faculty of Science, Department of Chemistry, 06500, Teknikokullar, Ankara

²Ahi Evran University, Faculty of Agriculture, Department of Field Crops, 40200 Kırşehir
ehasanoglu@gazi.edu.tr

Abstract

Tetrazole is an organic heterocyclic compound composed of a carbon and four nitrogen atoms and a five-ring structure containing three unsaturated bonds. A comprehensive study have reported that compounds containing tetrazole ring are frequently used in drug synthesis due to their pharmacological activities including antibacterial, antifungal, antiviral, antiallergic, antiulcer, antihypertensive, anticonvulsant, anti-inflammatory, and antituberculosis[1,2].

In the present study, three new compounds with tetrazole rings containing -H, -F and -Cl substituent groups were synthesized, and the structures of the synthesized compounds were examined by the spectroscopic methods (ATR, ¹H-NMR, ¹³C-NMR and LC-MS). Then, the antimicrobial activities of the synthesized compounds were investigated.

Experimental Method: Following this procedure, 1a-1c in the solution was filtered and placed in a clean beaker, and left to rest for four days. The resulting precipitate was filtered using a filter paper and washed with 10 mL ethyl alcohol, and dried in the oven at 80°C for one day.

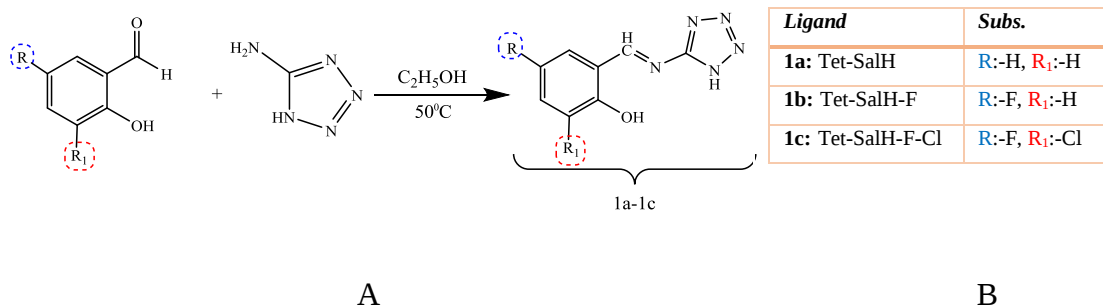


Figure 1. Synthesis pathway of new compounds synthesized (A), changing substituent groups (B)

Antimicrobial Test: The antimicrobial tests were performed using the well method. Solutions of all the synthesized new ligands in the DMSO solvent were prepared at a concentration of 10⁻³ M. As a positive control, the resistance of the studied bacteria and fungal cultures to the antibiotic was tested. As a negative control, the antimicrobial activity of the DMSO solvent against test microorganisms was examined and no effect was observed.

Results & Discussion: Evaluating the antimicrobial test results of the compounds containing tetrazole ring (Table 1), it was found that these compounds were not only effective on *M. luteus*, but were effective on all the other studied species. Among the synthesized compounds, it was seen that only Tet-SalH was effective on *K.pneumonia*, while the structures containing substituents had no effect. However, with the increase in the substituents, the effect on the

fungus *Candida albicans* was also seen in all the studied species. In general, terms, when electronegative groups were attached to the aromatic ring in Schiff bases and the number of these groups increased, it was observed that the effect on all the studied species increased.

Table 1. Antimicrobial test results of the synthesized compounds. (10^{-3} M DMSO)

		Tet-SalH	Tet-SalH-F	Tet-SalH-F-Cl
Gram (+)	<i>M. luteus</i>	-	-	-
	<i>S. epidermis</i>	20.	15.	23.
	<i>S. aureus</i>	20.	-	22.
	<i>B. cereus</i>	16.	16.	13.
Gram (-)	<i>P. putida</i>	20.	18.	19.
	<i>K. pneumonia</i>	10.	-	-
	<i>E. aerogenes</i>	14.	12.	12.
	<i>S. typhi</i>	20.	19.	23.
	<i>E. coli</i>	16.	14.	20.
	<i>P. vulgaris</i>	12.	11.	14.
Yeast	<i>Candida albicans</i>	12.	30.	26.

Positive Control

	<i>M. luteus</i>	<i>S. epidermis</i>	<i>S. aureus</i>	<i>B. cereus</i>	<i>P. putida</i>	<i>K. pneumonia</i>	<i>E. aerogenes</i>	<i>S. typhi H</i>	<i>E. coli</i>	<i>P. vulgaris</i>	<i>Candida albicans</i>
K30	23	25	25	28	14	23	24	20	25	21	nt
SXT25	21	25	24	25	18	20	19	17	18	19	nt
AMP10	22	26	30	23	8	21	21	11	10	17	nt
NYS100	nt	nt	nt	nt	nt	nt	nt	nt	nt	nt	20
AMC30	25	27	30	20	15	21	20	19	14	20	nt

nt: not tested;

Inhibition zone (mm).

K30, Kanamycin 30µg; SXT25, Sulphamethoxazol 25µg; AMP10, Ampicillin 10µg; CIP5, Ciprofloxacin 5µg; AMC30, Amoxycillin 30µg; NYS100, Nystatin 100µg.

*C: Control (DMSO)

Therefore, it can be argued that these newly synthesized compounds containing the tetrazole ring are good candidates for the synthesis of oral and vaginal fungicides.

Key Words: Tetrazole; *Candida albicans*; Antimicrobial agents

References

- [1] Malik MA, Wani MY, Al-Thabaiti, SA, Shiekh, RA (2014) Journal of Inclusion Phenomena and Macrocyclic Chemistry 78: 15-37.
- [2] Ostrovskaya, VM, Shpigun, LK, Shushenachev, YV, Buryak, AK, Peregodov, AS (2015) Russian Journal of General Chemistry 85:2048-2057.

INTERACTIONS OF NEW TETRAZOLATO COMPLEXES CONTAINING VIII B GROUP TRANSITION METALS WITH DNA

Elvan HASANOĞLU ÖZKAN¹, Süheyla ÇELİK², Leyla AÇIK², Ali DİŞLİ¹, Nurşen SARI¹

¹Gazi University, Faculty of Science, Department of Chemistry, 06500, Teknikokullar, Ankara

²Gazi University, Faculty of Science, Department of Biology, 06500, Teknikokullar, Ankara, Turkey

ehasanoglu@gazi.edu.tr

Abstract

Tetrazole compounds are widely used in various industries including medicine, pharmaceutical chemistry, chemistry, and agriculture, and studies on various uses of these compounds such as drugs, explosives, dyestuffs, inhibitors, and gas-production compounds are found in the literature. The fact that these compounds are used in many practical applications makes them the focus of research each passing day [1].

Tetrazoles are easily adaptable ligands to different bonding modes. Also, since they are more stable in the body than bioactive carboxylic acid groups, it has been seen that they replace carboxylic acid groups in novel drugs. Therefore, tetrazole compounds have gained importance in the pharmaceutical industry recently and they have been used in the synthesis of anticancer, antimicrobial, antihypertensive, and antiallergic agents [2,3].

In the present study, a new compound containing 5-substituent 1*H*-tetrazole and -CH₃ substituent group and three new tetrazolato complexes formed by Ni²⁺, Pd²⁺, Pt²⁺, metal ions were synthesized and spectroscopic methods including ATR, ¹H-NMR, ¹³C-NMR, LC-MS, elemental analysis, and TGA were used in the characterization of these structures. Then, the interactions of the synthesized compounds containing tetrazole with DNA were investigated.

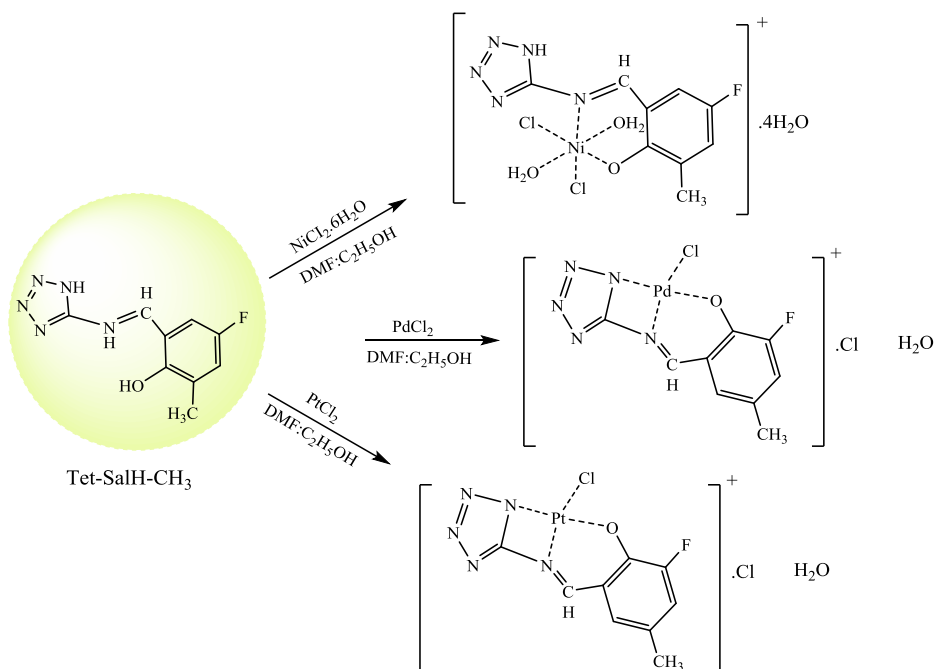


Figure 1. Synthesis pathway of new tetrazolato complexes synthesized

Experimental Method; The compound-DNA mixtures were first incubated for 24 h at 37°C and then subjected to *HindIII* and *BamHI* digestion. The mixtures were incubated at 37°C for

another 1 h. confirmation of restriction digest was determined by electrophoresis by 1% (w/v) agarose gel. the gel was visualised under UV light with a biometra UV imager and photographed.

HindIII/BamH1 restriction enzymes digestion; *HindIII* and *BamH1* are restriction endonuclease that hydrolyses the phosphodiester bonds by binding to the recognition sequence 5¹-AAGCTT-3¹ and 5¹-GGATCC-3¹ respectively, and cut these sequences just after the 5¹- adenine and 5¹ guanine on each strand (Maniatis). The plasmid DNA has a single restriction site for both enzymes that convert the supercoiled form I and singly nicked circular form II to linear form III DNA.

Results & Discussion; The Plasmid DNA interacted with tetrazolato complexes [Ni(Tet-SalH-F-CH₃), Pd(Tet-SalH-F-CH₃), Pt(Tet-SalH-F-CH₃) were studied by Agarose Gel Electrophoresis. When the DNA interacted with decreasing concentrations of tetrazolato complexes, generally two DNA bands corresponding to forms I and II were observed in both untreated and treated plasmid DNA. Pt(Tet-SalH-F-CH₃) no band was observed in lane 1 corresponding 1000-250 μM.

The changes in mobility of the bands indicated changes in DNA conformation brought about by binding of the compounds with the DNA.

Electrophoretograms applying to the incubated mixtures of plasmid DNA and compounds: 4; (Tet-SalH-F-CH₃, 5; [Ni(Tet-SalH-F-CH₃), 6; [Pd(Tet-SalH-F-CH₃) followed by digestion with *BamH1* and *HindIII*. Lane P corresponds to the untreated plasmid DNA and undigested with enzyme, lane P/B and P/H apply to untreated but digestion with *BamH1* and *HindIII*. Lanes 1 to 6 apply to plasmid DNA interacted with tetrazolato complexes followed by enzyme digestion.

Key Words: DNA interacted; Tetrazolato complexes; Transition metal

References

- [1] Uemura M, Yoshikawa Y, Yoshikawa K, Sato T, Mino Y, Chikuma M, Komeda S (2013) Journal of Inorganic Biochemistry 127:169-174.
- [2] Malviya N, Mandal P, Das M, Ganguly R, Mukhopadhyay S (2017) Journal of Coordination Chemistry, 70: 261-278.
- [3] Abdnoor ZM, Alabdali AJ (2019) J Chin Chem Soc. 66:1474-1483.

A SPECTROPHOTOMETRIC INVESTIGATION OF THE INTERACTION BETWEEN DNA AND THE ANTICANCER DRUG CANDIDATE SCHIFF BASES AND THEIR Pt (II) COMPLEXES

Elvan HASANOĞLU ÖZKAN¹, Süheyla Pınar ÇELİK², Leyla AÇIK², Ali DİŞLİ¹, Nurşen SARI¹

¹Gazi University, Faculty of Science, Department of Chemistry, 06500, Teknikokullar, Ankara, Türkiye

²Gazi University, Faculty of Science, Department of Biology, 06500, Teknikokullar, Ankara, Türkiye
nursens@gazi.edu.tr

Abstract

The human body has developed protective and repair systems against the DNA damage. When the function of these systems decreases, the damages in DNA cannot be repaired. This leads the cell to divide and multiply uncontrollably. When cells multiply and metastasize uncontrollably, a disease occurs, defined as cancer. The toxic properties of anticancer drugs also damage healthy tissues and cells. Therefore, researchers tend to develop specific molecules that are less toxic or non-toxic.

DNA is a polymer made up of units called nucleotides. Purines and pyrimidines form the organic base part of the nucleotide [1]. If we can determine the interaction between the nucleotides and the anticancer drug candidate using plasmid DNA interaction and the UV-GB spectra, we can evaluate whether the synthesized molecules can interact with DNA. Accordingly, whether the newly synthesized Schiff bases including tetrazole and their Pt (II) complexes would interact with DNA was investigated with agarose gel electrophoresis and the UV-GB spectrophotometer instrument. Compound-Plasmid DNA interaction studies showed that when DNA was interacted with decreasing concentrations of compounds there was an increase in intensity of DNA bands and change in mobility indicating change in DNA conformation in case of Tet-SalH-F, Tet-SalH-Pt(II), Tet-SalH-F-Pt(II). The separation between the bands increased a single coalesced band was observed corresponding to 1000 µM concentration of Tet-SalH-Pt(II) and Tet-SalH-F-Pt(II) indicating DNA damage. This research was conducted in the 220-280 nm wavelength range [2]. Measurements were made in Tris-EDTA buffer solution. Evaluating the spectra, it was suggested that the new peak at 267 nm wavelength might be the result of the interaction between the studied molecules and nucleotides.

Key Words: Schiff bases; Guanine; Tetrazole; Pt(II) complexes; DNA

References

- [1] Asron J-J, Trajkovska S (2005) Encyclopedia of Analytical Science (Second Edition), pg 393-402.
- [2] Chandraboss V.L, Karthikeyan B, Senthilvelan S (2015) Physical Chemistry Chemical Physics, 17, 12100-12114.

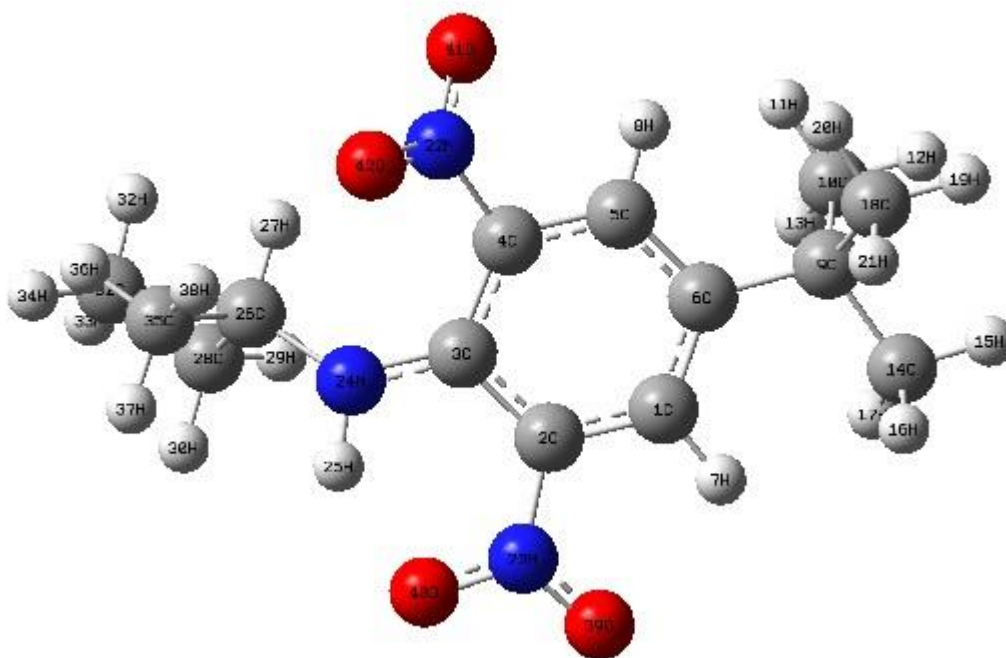
COMPUTATIONAL EXAMINATION OF DEGRADATION REACTIONS OF BUTRALIN

Simal KURUMOGLU¹, Yelda YALCIN GURKAN¹

¹Tekirdag Namik Kemal University, Department of Chemistry, Tekirdag, Turkey, e-mail:
simalsencan@hotmail.com

Abstract

Degradation reactions of molecules to be investigated will be examined by molecular modeling methods and theoretical approaches will be proposed for reaction pathways. For this purpose, possible reactions were calculated using Gaussian09 package program. DFT method was used in the theoretical study. In this study, possible reaction paths in the reaction between herbicide substances and OH radical were determined. Fragmentation reaction requires energy. OH radicals are used to degrade herbicide substances. The lowest energy molecule has the most stable structure. According to this, when we list the herbicide substances and fragments from the most stable to most unstable, they are Butralin, F1, F2, F3. These results will guide experimental workers and determine the mechanism of fragmentation.



The geometric shapes of molecule obtained because of optimization

Key Words: Gaussian09; DFT.

Synthesis of 16 α -substituted-pregnenolone derivatives via ionic liquid-catalyzed aza-Michael and thio-Michael addition

Lilla MAKSO¹, Rita SKODA-FÖLDES²,

¹University of Pannonia, Institute of Chemistry, Department of Organic Chemistry, Egyetem u. 10 (P.O. Box 158), H-8200 Veszprém, Hungary, E-mail address: lillamakso@gmail.com

²University of Pannonia, Institute of Chemistry, Department of Organic Chemistry, Egyetem u. 10 (P.O. Box 158), H-8200 Veszprém, Hungary, E-mail address: skodane@almos.uni-pannon.hu

Abstract

Michael addition of electron deficient steroidal alkenes, e.g. 16-dehydropregnenolone provides an efficient route for the introduction of heteroatoms into the side chain of steroids and often leads to compounds with pharmacological effect. Michael adducts of 16-dehydropregnenolone with different alcohols showed anti-oxidant and antidyslipidemic activity [1]. 16 α -Heteroaryl-pregnenolone derivatives were found to be effective in vitro against cervical HeLa, prostate DU 205 and breast cancer MCF-7 cell lines [2]. Others are potential DPP-4 inhibitors, which can be used for the treatment of diabetes mellitus type 2 [3].

In this work, the catalytic activity of ionic liquids in aza-Michael and thio-Michael addition of 16-dehydropregnenolone was studied. Ionic liquids have several advantages: the products can be separated from the ionic liquid using apolar organic solvents, and they can be reused. They have high thermal stability and are not corrosive.

The addition reactions were carried out using different amines and thiols as reaction partners in basic ionic liquids serving both as solvents and catalysts. After extraction of the products, the ionic liquid phase was recycled. With a careful optimization of the reaction conditions as well as the extraction procedure, the products were obtained in moderate to good yields and were characterized by ¹H- and ¹³C NMR, MS and IR. The reusability of the ionic liquid ([DBU][Ac] was also studied. It was found to be an efficient and recyclable catalyst that was reused five times. The aza-Michael addition products were investigated for the inhibition of in vitro C17,20-lyase activity and displayed moderate inhibitory effect [4].

The support of MOL Hungarian Oil and Gas Public Limited Company's (MOL NYRT.) and Foundation of PEREGRINATIO I. (VVE) are acknowledged. This work is also supported by Foundation Industry for Education of Engineering in Veszprém (Ipar a Veszprémi Mérnökképzésért Alapítvány) and GINOP-2.3.2-15-2016-00049 grant.

Key Words: 16-Dehydropregnenolone, Ionic liquid, Michael addition, P45017 α inhibitors

References

- [1] A. Sethi, G. Bhatia, A.K. Khanna, M.M. Khan, A. Bishnoi, A.K. Pandey, A. Maurya, Expedient synthesis of some novel pregnane derivatives and their evaluation as anti-oxidant and anti-dyslipidemic agents, *Med. Chem. Res.* 20 (2011) 36–46.
- [2] S. Gogoi, R.C. Boruah, P. Saikia, A. Addlagatta, V. Saddanapu, 16 α -Heteroaryl pregnenolone acetate and a process for preparation thereof, WO 170336, 2015.
- [3] M. Kumar, P. Rawat, M.F. Khan, A.K. Rawat, A.K. Srivastava, R. Maurya, Azaannulation on the 16-dehydropregnenolone, via tandem intermolecular Aldol process and intramolecular Michael addition, *Bioorg. Med. Chem. Lett.* 21 (2011) 2232–2237.
- [4] Szánti-Pintér, E.; Maksó, L.; Gömöry, Á.; Wouters, J.; Herman, B.E.; Szécsi, M.; Mikle G.; Kollár, L.; Skoda-Földes, R. *Steroids*. 2017, 123, 61.

INVESTIGATION OF STRUCTURAL AND MAGNETIC PROPERTIES OF NICKEL DOPED IRON OXIDE NANOPARTICLES DEPENDING ON THE AMOUNT OF DOPE VALUES

Nurcan DOGAN¹, Namık DİKTAS², Ceren ERŞEN³, Ayhan BINGOLBALI⁴

¹ Gebze Technical University, Department of Physics Kocaeli/Turkey
ndogan@gtu.edu.tr

² Gebze Technical University, Department of Physics Kocaeli/Turkey
namik.diktas2016@gtu.edu.tr

³ Gebze Technical University, Department of Physics Kocaeli/Turkey
ceren.ersen2016@gtu.edu.tr

⁴ Yıldız Technical University, Department of Bioengineering İstanbul/Turkey
ab1353@gmail.com

Abstract

In today's technology, the importance of the production of nanoparticles containing less toxic substances is increasing for biomedical applications, especially in intra-body medical applications. Magnetic nanoparticles are widely used in biomedical applications today because they can be directed to the target by magnetic field.

Magnetization, which is the strength of the response of magnetic nanoparticles to the magnetic field, is a very important parameter in this sense. The magnitude of magnetization determines the magnetic field strength that should be used in magnetic-based medical imaging devices. Therefore, it is important to produce nanoparticles with high magnetization in a low magnetic field [1].

Nanoparticles were synthesized by the production method using hydrothermal synthesis and co-precipitation methods together. With these methods, nickel iron oxide nanoparticles were synthesized with different dope ratios [2]. $\text{Ni}_x\text{Fe}_{3-x}\text{O}_4$: $x = 0, 0.05, 0.1$ doping ratios were produced to investigate the structural and magnetic properties of nanoparticles by XRD, SEM and FTIR analysis [3].

Key Words: *Nanoparticle synthesis, Nickel doped iron oxide, Hydrothermal synthesis and co-precipitation method, Magnetic field*

References

- [1] Kamellia Nejati and Rezvanh Zabihi, "Preparation and magnetic properties of nano size nickel ferrite particles using hydrothermal method", Chemistry Central Journal. 2012, 6:23
- [2] A. H. Lu, E. L. Salabas, F.Schüth, "Magnetic Nanoparticles: Synthesis, Protection, Functionalization, and Application", Angewandte Chemie, 46, 1222-1244, 2007.
- [3] S.Sivakumar, D. Anusuya, C. P. Khatiwada, J. Sivasubramanian, A. Venkatesan, P. Soundhirarajan, "Characterizations of diverse mole of pure and Ni-doped α -Fe₂O₃ synthesized nanoparticles through chemical precipitation route", Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 128, 69-75, 2014.

CO₂ METHANATION WITH Ce PROMOTED Ni CATALYST SUPPORTED ON MIXED MATERIALS OF Al₂O₃ AND Y₂O₃

Nyamsuren Battumur, Enkhsaruul Byambajav

Department of Chemistry, School of Arts & Sciences, National University of Mongolia, Ulaanbaatar, 14201, Mongolia, bbnyamsuren@gmail.com, enkhsaruul_b@num.edu.mn

The activity of the 15%Ni catalyst supported on γ -Al₂O₃, the 15%Ni catalysts supported on a mixture of γ -Al₂O₃ and Y₂O₃ (Ni/Al-yY; y=5-25%) and the Ce promoted Ni catalysts supported on the mixture of γ -Al₂O₃ and Y₂O₃ (Ni-xCe/Al-yY; x=1-5%, y=15%) were investigated for CO₂ methanation. Reactions were performed at the temperature of 350°C in the ambient pressure of CO₂+H₂ (molar ratio of 1:4) feed gas with the GHSV of 3000h⁻¹. All catalysts were prepared by the method of impregnation - co-precipitation. Contents of Y₂O₃ additive (y) in the main catalyst support of γ -Al₂O₃ were 5%, 15%, and 25%. It was determined that the addition of Y₂O₃ in the main support material improved the distribution of nickel catalyst, consequently increased the reaction activity of methanation. However, the most convenient content of the Y₂O₃ additive in Ni/Al-yY was 15%. Then, an effect of Ce promoter on Ni-xCe/Al-15Y was investigated for CO₂ methanation. It was concluded that the Ni-2Ce/Al-15Y catalyst gave the highest CO₂ conversion of 92.5% and the largest CH₄ yield of 92.2% at the present reaction conditions.

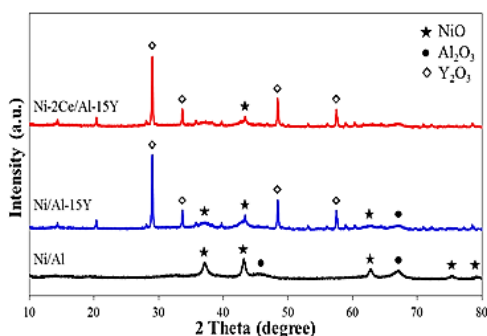


Fig. 1. XRD profiles of the selected catalysts

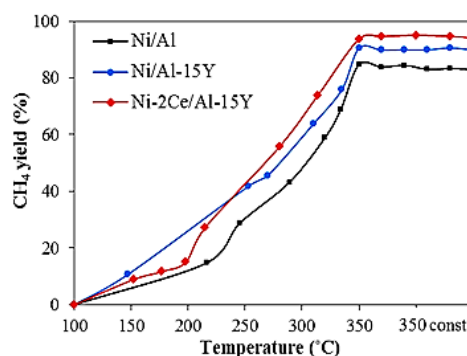


Fig. 2. CH₄ yield in CO₂ methanation with the catalysts

Key words: CO₂ hydrogenation; Ceria, Al₂O₃-Y₂O₃ mixed support; promoter

References

- [1] Jaffar, M. M., Nahil, M. A., & Williams, P. T (2019) Energy Technology 1900795:1-12.
- [2] Rahmani, S., Meshkani, F., & Rezaei, M (2018) Environmental Progress & Sustainable Energy 118-226.
- [3] Buyan-Ulzii Battulga, Tungalagtamir Bold, Enkhsaruul Byambajav (2020) International Journal of Chemical Reaction Engineering 18(5-6):20200076.
- [4] B.Buyan-ulzii, O.Daariimaa, Ch.Munkhdelger, G.Oyunbileg and B.Enkhsaruul (2018) Mongolian Journal of Chemistry 19(45):12-18.

Electroanalytical determination of progesterone hormone using Boron-Doped Diamond Electrode

Muhlis UÇAR*, Abdulkadir LEVENT

*Batman University, Faculty of Sciences and arts, Department of Chemistry, 72100, Batman, Turkey
muhlisucar@hotmail.com

Batman University, Faculty of Sciences and arts, Department of Chemistry, 72100, Batman, Turkey
leventkadir@hotmail.com

Abstract

Progesterone is synthesized from pregnenolone, a derivative of cholesterol like other steroids. It is a steroid hormone that has a vital importance in human and animal health. In case of progesterone imbalance, it causes problems such as fertility and infertility. In this study, electrochemical properties of Progesterone hormone Boron doped diamond (BDD) on electrode surface were investigated in strongly acidic environment (HClO₄ and H₂SO₄). A fast, sensitive, selective and simple electroanalytical method was developed for cathodically pre-treated BDD electrodes. A good linear analytical curve in the concentration range of 10 µM to 100 µM at a voltage value of +1.51 V (vs. Ag / AgCl) (after 120 s deposition at +0.1 V voltage) in 0.5 M HClO₄ using the square wave stripping technique for the quantification of progesterone hormone obtained. The observability limit is 0.012 µM (3.77 µg L⁻¹); The relative standard deviation value (RSD) for the concentration of 3.1 µM (n = 11) was calculated to be 4.87%. In addition, the developed voltammetric method has been successfully applied to drug and blood serum.

Keywords: Progesterone, Boron-doped diamond electrode, voltammetry, serum

References

- [1] Christian M.S, Brent R.L, Calda P, Senger P.L., (2007) *Mat-fet. eonat. Med.* 20: 89–112.

THE PROPERTIES OF PHBV/CaCO₃ COMPOSITES PREPARED BY MELT PROCESSING

Semra KIRBOGA, Mualla ÖNER

Yıldız Technical University, Chemical-Metallurgical Faculty, Chemical Engineering Department, 34210,
Istanbul, Turkey

skirboga@yildiz.edu.tr; muallaoner@gmail.com

Abstract

Bio-based polymers can be obtained entirely or partially from natural resources. Polyhydroxyalkanoates (PHA), bio-based thermoplastic polymer, are produced by a wide variety of bacteria. Poly(3-hydroxybutyrate) (PHB), a member of PHA family, is a linear bacterial polyester. It is a very fragile polyester with high crystallinity and the biodegradation rate is very low due to its high crystallinity. The addition of 3-hydroxyvalerate (HV) monomers to poly(3-hydroxybutyrate) (PHB) can be a good solution to this problem. The major application of bioplastics is packaging industry. In the packaging industry, it may be necessary to add additives to the polymer to avoid microbial activity and prevent the formation of biofilms or contamination. The additives/fillers can be used to increase the mechanical, thermal and/or barrier performances of the composites [1,2]. Many low-cost fillers, such as calcium carbonate, are available with different particle properties. Calcium carbonate (CaCO₃) is one of the most important and abundant mineral fillers used in the plastic industry over the years [3]. CaCO₃ can be used to enhance the properties of composites. Nanometer-scale calcium carbonate particles caused to higher tensile and flexural strength of polypropylene. With the addition of calcium carbonate, the nanocomposite module increased by 85%, while ultimate stress and strain, yield stress and strain were not affected much [4,5]. Similarly, the mechanical and tear resistance of Polybutadiene rubber (PBR) increased with the addition of CaCO₃ [6]. Although the incorporation of CaCO₃ into polymers has been carried out, to the best of our knowledge from a thorough survey of the literature, calcium carbonate filled PHBV related research has been limited.

This study aimed to prepare Poly (3-hydroxybutyrate-co-3-hydroxyvalerate, PHBV), biocomposites with incorporating various percentages calcium carbonate (CaCO₃) using extrusion processing. A twin screw extruder was used to prepare the composites. PHBV was kindly supplied by ADMajoris Company, France under the trade name MAJ'ECO FN000HA in a pelletized form suitable for melt extrusion. Uncoated CaCO₃ and stearic acid coated CaCO₃ were supplied from OMYA-Turkey. A twin-screw extruder (Rondol Microlab, England) with L/D ratio 20 was used for preparing composites. CaCO₃ percentages in PHBV/CaCO₃ composites were 0.1 wt%, 0.5 wt%, and 1 wt%. The influence of filler contents on the properties of PHBV composites was studied. The structure of PHBV/CaCO₃ biocomposites was investigated by XRD, TG, and SEM. Dynamic mechanical analysis (DMA), differential scanning calorimetry (DSC), and thermogravimetric analysis (TGA) were used to determine the thermal and thermo-mechanical properties of biocomposites. DMA measurements showed that considerable improvements in storage modulus and viscose damping by incorporating calcium carbonate particles. The storage modulus of the PHBV at 25 °C in the dynamic mechanical analysis (DMA) was increased up to 76% when composite prepared 0.1wt% coated calcium carbonate particle. Oxygen permeability of PHBV composites were determined by SYSTECH oxygen permeation analyser. Mocon equipment was used to test water vapor barrier properties of the samples. Biocomposites exhibited smaller oxygen transmission rate (OTR) and water vapour transmission rate (WVTR) due to the increase of crystallinity and tortuosity of the composite samples.

Key Words: *Poly (3-hydroxybutyrate-co-3-hydroxyvalerate); biocomposite; calcium carbonate; thermos-mechanical properties; barrier properties.*

References

- [1] Oner M, Kizil G, Keskin G, Pochat-Bohatier C, Bechelany M (2018) *Nanomaterials* 8:940
- [2] Oner M, Col AA, Pochat-Bohatier C, Bechelany M (2016) *Rsc Advances* 6: 90973-90981.
- [3] Kirboga S, Oner M (2017) *Powder Technology* 308:442-450.
- [4] Li Y, Fang QF, Yi ZG, Zheng K (2004) *Materials Science and Engineering A* 370:268-272.
- [5] Mishra S, Sonawane SH, Badgujar N, Gurav K, Patil D (2005)96:6-9.
- [6] Chan CM, Wu JS, Li JX, Cheung YK (2002) *Polymer* 43:2981-2992.

Different response of a 2-ureido-4-ferrocenyl pyrimidine sensor to $\text{CF}_3\text{SO}_3\text{H}$ and $\text{CF}_3\text{CO}_2\text{H}$ guests

Soma J. Keszei¹, Szabolcs Balogh², Csaba Fehér¹, Livia Nagy³, Nikolay Tumanov⁴, Johan Wouters⁴, György Lendvai^{5,6} and Rita Skoda-Földes¹

²Department of Organic Chemistry, Institute of Chemistry, University of Pannonia, P.O. Box 158, Veszprém, H-8200 Hungary

E-mail: keszei.soma@mk.uni-pannon.hu

bagira@almos.uni-pannon.hu

skodane@almos.uni-pannon.hu

²Institute of Chemistry, NMR Laboratory, University of Pannonia, Egyetem u. 10. H-8200 Veszprém, Hungary

³János Szentágothai Research Center, University of Pécs, Ifjúság útja 20, H-7624 Pécs, Hungary

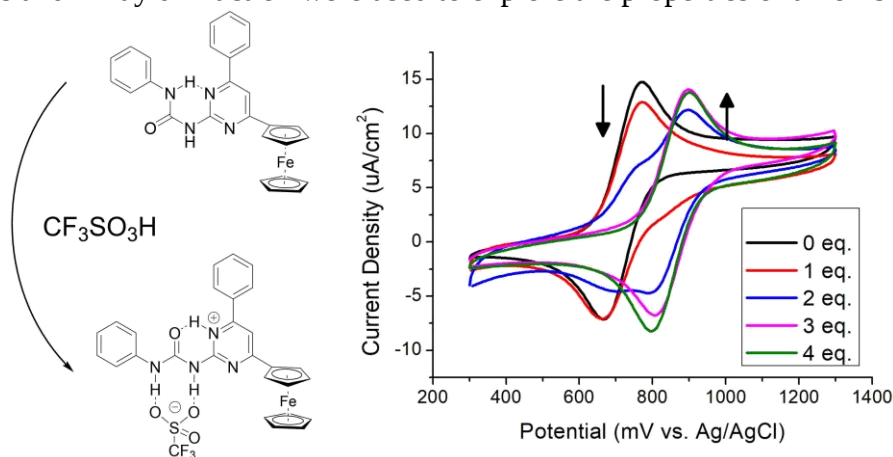
⁴Department of Chemistry, University of Namur, B-5000 Namur, Belgium

⁵Institute of Chemistry, Department of General and Inorganic Chemistry, University of Pannonia, H-8200 Veszprém, Hungary

⁶Institute of Materials and Environmental Chemistry, Research Center for Natural Sciences, Hungarian Academy of Sciences, P.O. Box 17, H-1525 Budapest, Hungary

Abstract

The properties of a ferrocenyl ureidopyrimidine derivative, a potential electrochemical sensor for trifluoromethanesulfonic acid and trifluoroacetic acid, were investigated using UV/Vis, NMR and CV measurements. Upon protonation a structural change was found to take place leading to the formation of a proper binding site for the anion of the acid. Anion binding has been proved for both CF_3SO_3^- and CF_3CO_2^- as well as for the BF_4^- anion by ^1H NMR measurements. Moreover, titration experiments carried out with $\text{CF}_3\text{SO}_3\text{H}$ and $\text{CF}_3\text{CO}_2\text{H}$ resulted in different responses in the NMR spectra of the pyrimidine host. Cyclic voltammetry was found to be suitable to follow the addition of the acids to the host molecule. DFT calculations and X-ray diffraction were used to explore the properties of anion binding.



Acknowledgement:

The support of MOL Hungarian Oil and Gas Public Limited Company's (MOL NYRT.) and Foundation of PEREGRINATIO I. (VVE) are acknowledged. This work is supported by Foundation Industry for Education of Engineering in Veszprém (Ipar a veszprémi mérnökképzésért Alapítvány) and Association of Hungarian Chemists (Magyar Kémikusok Egyesülete) by the GINOP-2.3.2-15-2016-00049 grant.

Key Words: host-guest systems; molecular recognition; cyclic voltammetry; DFT; ferrocene

PREPARATION OF CALCIUM POLYPHOSPHATE POWDER CONTAINING AMORPHOUS CARBON

**Tatiana SAFRONOVA¹, Yanis PAIANIDI², Tatiana SHATALOVA³,
Yaroslav FILIPPOV⁴, Gilyana KAZAKOVA⁵, Umarali UMIROV⁶, Otabek TOSHEV⁷**

¹Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, t3470641@yandex.ru

²Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, paianidi@mail.ru

³Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, shatalovab@gmail.com

⁴Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, filippovya@gmail.com

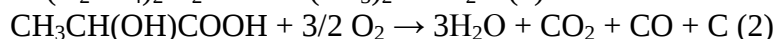
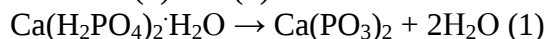
⁵Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, gilyanak@gmail.com

⁶Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, umarjonumirov@mail.ru

⁷Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1,
otabektoshev0995@mail.ru

Abstract

As a dye, carbon-coloured powders can be used in the production of porous ceramics with given geometry of porous space based on calcium phosphates using 3D printing of semi-finished items from light-cured suspensions loaded with highly dispersed powders. Dark grey powders of calcium polyphosphate $\text{Ca}(\text{PO}_3)_2$ was prepared via heat treatment of monocalcium phosphate monohydrate (MCPM) $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ after treating in water solution of lactic acid under mechanical activation using planetary mill. Powder of MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ was dissolved in water solution of lactic acid during treatment under mechanical activation using planetary mill. According to XRD analysis data the phase composition of powder after crystallisation from solution, containing MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ and lactic acid, and drying at room temperature was the same as a phase composition of the starting powder. Particle dimensions of MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ after mill treatment, crystallisation in presence of lactic acid and drying changed from 100-300 μm to 10-50 μm . So, lactic acid acted as surface active agent during crystallisation of particles of MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ from the solution. Then powder of MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ containing lactic acid was heat treated at 500 °C. According to XRD analysis data powder after heat treatment consisted of $\beta\text{-Ca}(\text{PO}_3)_2$. The reactions (1) and (2) reflect the chemical transformation taking place during heat treatment.



The total mass loss for powder of MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ after treatment in lactic acid at 1000°C was 37,5% according to thermal analysis data. The mass loss of powder under investigation was due to decomposition of both inorganic and organic components. According to mass-spectroscopy data there were two intervals of CO_2 evolving: 100-400 °C and 900-1000 °C. It means that amorphous carbon can be kept in the powder of calcium polyphosphate up to the quite high temperatures. Uniform dark grey colored calcium polyphosphate powder with fine particles (2-4 μm) was prepared using heat treatment of MCPM $\text{Ca}(\text{H}_2\text{PO}_4)_2 \cdot \text{H}_2\text{O}$ modified with lactic acid.

Dark grey coloured powders of calcium polyphosphate can be used as a multifunctional additive in technology of porous calcium phosphate ceramics. Due to dark grey colour it can be an agent improving lateral resolution of 3D stereolithographic printing of semi-finished items with given geometry of porous space. And due to the melting point (964 °C) it can be an additive making the firing temperature of calcium phosphate ceramics lower.

Acknowledgements: The financial support of RFBR project # 18-29-11079.

Key Words: monocalcium phosphate monohydrate, lactic acid, calcium polyphosphate powder

Electrochemical Oxidation of Vildagliptin on Pencil Graphite Electrode: Extremely sensitive determination in drugs and human urine with square wave voltammetry

Yalçın ALTUNKAYNAK¹, Ömer YAVUZ², Abdulkadir LEVENT³

¹Department of Chemistry, Science Institute, Dicle University, 21280 Diyarbakir, Turkey
altunkaynak4772@gmail.com.tr

¹Batman University, Vocational School of Technical Sciences, 72100 Batman, Turkey
yalcin.altunkaynak@batman.edu.tr

²Department of Chemistry, Faculty of Science, Dicle University, 21280 Diyarbakir, Turkey
omeryavuz@gmail.com.tr

³Batman University, Faculty of Sciences and arts, Department of Chemistry, 72100, Batman, Turkey
leventkadir@hotmail.com

Abstract

Vildagliptin (VLDG), one of the antidiabetic agents, is a dipeptidyl peptidase 4 inhibitor. It is a drug developed for oral administration[1]. In the literature, there is only one study in which electrochemical methods were used for the analysis of Vildagliptin in biological fluid and drug forms[2]. In this study, the electrochemical properties of VLDG, which is one of the drugs used as an antidiabetic agent, were determined by using pencil graphite electrode in phosphate buffer solution (PBS/pH 9.0). The irreversible and diffusion controlled adsorption oxidation peak was measured by cyclic voltammetry at approximately +1.13 V for this compound. Using square wave stripping voltammetry, the current showed a linear correlation in PBS buffer at pH 9.0, with a concentration range of 2.94 to 49.98 μM . At a concentration of 2.94 μM ($n=9$), the limit of detection of 8.20 nM (2.48 ng mL⁻¹) and a relative standard deviation of 2.95 % were calculated. This method was successfully applied for VLDG analysis without any separation in pharmaceutical preparations and urine samples.

Key words: Vildagliptin; Pencil Graphite Electrode; Voltammetry; Drug; Urine

References

- [1] Turan E, Kulaksızoğlu M (2015) Okmeydanı Tıp Dergisi 31(Ek sayı):86-94.
- [2] Fadr M, Amro A.N, Aoun S.B (2018) Tropical Journal of Pharmaceutical Research. 17: 1847-1852.

BITTER VETCH SEED OIL (*VICIA ERVILIA* L.) – A NEW SOURCE OF BIOACTIVE COMPONENTS

Zhana PETKOVA¹, Ginka ANTOVA¹, Olga TENEVA¹, Maria ANGELOVA-ROMOVA¹

¹University of Plovdiv 'Paisii Hilendarski', Department of Chemical Technology,
24 Tzar Asen Str., 4000 Plovdiv, Bulgaria, e-mail: zhanapetkova@uni-plovdiv.net

Abstract

Nowadays, the demand of underused plants which may be a new sources of bioactive compounds is constantly growing. For that reason, the lipid composition of bitter vetch seed oil (*Vicia ervilia* L.) has been examined. The plant has Russian origin but has been introduced in southern Bulgaria. The oil content of the seeds is rather low (1.4%), but the lipids are rich in unsaponifiable matter (39.7%) – phytosterols (4.7%), tocopherols (4010 mg/kg) and carotenoids (684 mg/kg). Fatty acid and sterol composition were determined by gas chromatography with flame ionization detector and tocopherols – with high performance liquid chromatography and fluorescent detection. Unsaturated fatty acids (73.4%) predominate in the glyceride oil and the main ones are oleic (52.0%) and linoleic (20.4%) acids. The major saturated fatty acid is palmitic with amount of 20.8%. The quantity of monounsaturated fatty acids (52.6%) is higher than that of polyunsaturated (20.8%) ones. β -Sitosterol (83.3%) is the main component in the sterol fraction, followed by campesterol (12.1%). Only two tocopherols (α - and γ -) are identified in the tocopherol fraction, in which γ -tocopherol predominates (87.6%). Total phospholipids in bitter vetch seeds are 0.7% and the major component is phosphatidylinositol (28.9%). Fatty acid composition of three classes of the phospholipids (phosphatidylinositol, phosphatidylcholine and phosphatidylethanolamine) in the seeds has also been examined. Oleic acid is the main fatty acid in the last two phospholipids (61.1 and 48.2%, respectively), while palmitic acid (46.8%) predominates in phosphatidylinositol.

These results depict that the oil from bitter vetch seeds is a promising source of bioactive components and can be successfully implemented in different functional food ingredients.

Key Words: *Bitter vetch; Lipid composition; Fatty acids; Biologically active components*

Acknowledgments

This work was supported by the Bulgarian National Science Fund (BNSF), Ministry of Education and Science, projects of junior basic researchers and postdocs – 2018 [grant number KP-06-M29/2, 01.12.2018].

CHEMICAL REACTION IN POWDER MIXTURES OF CALCIUM HYDROXYAPATITE AND POTASSIUM HYDROSULFATE UNDER MECHANICAL ACTIVATION IN ACETONE MEDIUM

Tatiana SAFRONOVA¹, Marat AKHMEDOV², Tatiana SHATALOVA³,
Snezhana TIKHONOVA⁴, Gilyana KAZAKOVA⁵

¹Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, t3470641@yandex.ru

²A.N. Kosygin State University of Russia (Technology. Design. Art), 117997, Russia, Moscow, Sadovnicheskaya str., 33, p. 1, akhmedov.mm@yandex.ru

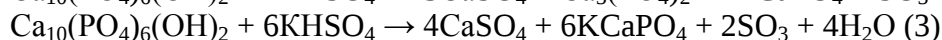
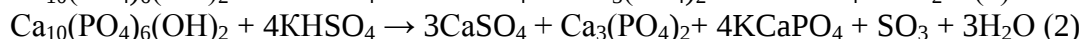
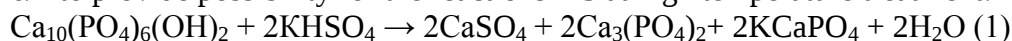
³Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, shatalovatb@gmail.com

⁴Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, kurbatova.snezhana@yandex.ru

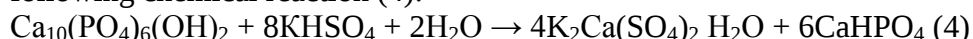
⁵Lomonosov Moscow State University, 119991, Russia, Moscow, Leninskie Gory, 1, gilyanak@gmail.com

Abstract

Powder mixtures of hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ and potassium hydrosulfate KHSO_4 were investigated to confirm possibility of creating ceramic composites with biocompatible and bioresorbable phases of tricalcium phosphate $\text{Ca}_3(\text{PO}_4)_2$, potassium rhenanite KCaPO_4 , potassium-substituted tricalcium phosphate $\text{Ca}_{10}\text{K}(\text{PO}_4)_7$ and calcium sulfate anhydrite CaSO_4 . Powder mixtures of calcium hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ and potassium hydrosulfate KHSO_4 were homogenized in acetone medium in planetary mill. Powder mixtures were made with molar ratio of $\text{KHSO}_4/\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ established as 2/1, 4/1 and 6/1 to provide possibility for the reactions 1-3 at high temperature treatment.



According to XRD analysis data the phase composition of powder mixtures after treatment in planetary mill in acetone media consisted of syngenite $\text{K}_2\text{Ca}(\text{SO}_4)_2 \cdot \text{H}_2\text{O}$, monetite CaHPO_4 and calcium hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$. So, the formation of phase composition of powder mixtures during treatment in planetary mill in acetone media can be reflected with following chemical reaction (4):



The potassium hydrosulfate KHSO_4 was taken in insufficient quantity according to reaction (4) in all prepared powder mixtures. Additional water necessary for reaction (4) could come from an acetone available on the market as a commercial reagent which were used in these experiments.

XRD analysis was carried out for ceramic samples made of these powder mixtures after firing at temperature range of 700-900°C. The following phases were found in samples after firing in interval of 700-900°C: potassium calcium phosphate $\text{Ca}_{10}\text{K}(\text{PO}_4)_7$ and calcium langbeinite (potassium calcium double sulfate) $\text{K}_2\text{Ca}_2(\text{SO}_4)_3$ for $\text{KHSO}_4/\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ established as 2/1 and potassium calcium phosphate $\text{Ca}_{10}\text{K}(\text{PO}_4)_7$, calcium langbeinite (potassium calcium double sulfate) $\text{K}_2\text{Ca}_2(\text{SO}_4)_3$, potassium sulfate K_2SO_4 and calcium sulfate for $\text{KHSO}_4/\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ established as 6/1.

The results of present investigation can be taken into account when creating a resorbable ceramic materials in the $\text{K}_2\text{O}-\text{CaO}-\text{SO}_3-\text{P}_2\text{O}_5$ system for bone defect treating.

Acknowledgements: The financial support of RFBR project # 20-03-00550.

Key Words: calcium hydroxyapatite; potassium hydrosulfate; syngenite; monetite; powder

STABILIZATION AND HARVESTING OF HESPERETIN MICRORODS FROM THE HESPERETIN STABILISED VIA PLANTACARE 2000 SOLUTION BY USING TEMPLATE-ASSISTED PARTICLE INFILTRATION METHOD

Yesim KARAHAHAN¹, Marcel POURASGHAR², Marc SCHNEIDER², Cornelia M. KECK³,
Dolunay SAKAR DASDAN¹

¹Yıldız Technical University, Faculty of Art and Science, Chemistry Department, 34210, İstanbul, Turkey
44yesim@gmail.com dsakar@yildiz.edu.tr

²Saarland University, Institute of Biopharmaceutics and Pharmaceutical Technology, 66123, Saarbrücken, Germany marc.schneider@uni-saarland.de marcel.pourasghar@uni-saarland.de

³Marburg University, Pharmaceutical Technology and Biopharmacy, 35037, Marburg, Germany cornelia.keck@pharmazie.uni-marburg.de

Abstract

Recent studies have shown that the particle properties of drugs play a major role for drug delivery systems. One of the most important factors is the shape of particles for uptake of the carrier systems by phagocytes in pulmonary drug delivery. Cylindrical rods have highest particle acquisition and binding efficiency. [1,2] Hesperetin, [(2S)-5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)-2,3-dihydrochromen-4-one] has pharmacological properties such as anti-inflammatory, anti-carcinogenic, anti-hypertensive, antioxidant, antiallergic, etc. and it is found in Citrus Fruits [3,4]. Nevertheless, it slightly dissolves in aqueous media [5]. It is necessary to use a stabilizer to increase its dispersability in water, particle stability and bioavailability in the final formulation via interactions with cells and cell layers. Plantacare2000, which is a non-ionic surfactant made from 100% renewable and plant-derived feedstocks, is used as a base surfactant or a co-surfactant in cosmetic surfactant cleansing preparations.

In order to prepare cylindrical microrods of Hesperetin, a template-assisted method with particle infiltration approach can be used. This method has three steps: infiltration, stabilization and harvest. In this study, microrods inside the pores which are obtained by hesperetin-plantacare 2000 solution infiltrating into pores of track-etched polycarbonate membranes, were stabilized by using different polymers and harvested.

Key Words: *Hesperetin, Plantacare2000, microrods, Template-assisted method, Polycarbonate track-etched membranes.*

FUNDING: *100/2000 PhD Scholarship by the Turkish Council of Higher Education (YÖK) ; Erasmus+ by the Yildiz Technical University Erasmus Department and This work was supported by Research Fund of the Yildiz Technical University. Project Number: FDK-2020-3853.*

References

- [1] Barua S, Yoo JW, Kolhar P, Wakankar A, Gokarn, R Y, Mitragotri S (2013) PNAS, 110: 3270-3275.
- [2] Champion J A, Mitragotri S (2005) PNAS 103: 4930–4934.
- [3] Garg A, Garg S, Zaneveld L J, Singla A K (2001) Chemistry and pharmacology of the citrus bioflavonoid hesperidin, Phytother Res 15: 655–669.
- [4] Cai Y Z, Luo Q, Sun M, Corke H, Antioxidant activity and phenolic compounds of 112 traditional Chinese medicinal plants associated with anticancer, (2004) Life Sci 74: 2157–2184.
- [5] Kanaze F, Kokkalou E, Niopas I, Georgarakis M, Stergiou A, Bikiaris D, Dissolution enhancement of flavonoids by solid dispersion in PVP and PEG matrixes: A comparative study, (2006) J. Appl. Polym. Sci. :102, 460–47.

EFFECT OF INCORPORATION OF ZINC OXIDE ON THE PROPERTIES OF PHBV

Semra KIRBOGA

Yıldız Technical University, Chemical-Metallurgical Faculty, Chemical Engineering Department, 34210,
Istanbul, Turkey
skirboga@yildiz.edu.tr

Abstract

Over the last decades, polymer nanocomposites have attracted attention in both academic and industrial areas. The environmental effect of polymer waste has become a major global problem because of the increase in the application of plastics. Therefore, biological based and /or biodegradable polymers with a suitable life cycle and suitable properties have become important as an alternative to conventional synthetic polymers [1]. Biodegradability is essential for many applications, such as food packaging, drug delivery, bioabsorbable materials. Poly (3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV), a microbial bio-based polyester copolymer, is a member of the group of polyhydroxyalkanoates. By incorporation the 3-hydroxyvalerate to the poly (3-hydroxybutyrate) polymer, while the mechanical properties of the polymer improve, the melting point decreases. Thus, distortion is reduced during processing and ease of processing is provided. There are limitations in the use of PHBV due to its low mechanical, thermal and barrier properties and its fragility. It is reported that the introduction of functional additives to the polymer, the properties of PHBV can be improved and the application area of the polymer can be customized [1,2]. Inorganic materials, such as TiO₂, ZnO and MgO can be used in antimicrobial applications. They are regarded as safe for human beings and animals relative to organic compounds. In addition they are stable under the high temperatures and pressures. Zinc oxide (ZnO), a promising material for a variety of applications, attracts a lot of scientific attention. It is known that zinc oxide affect not only the optical and electrical properties of polymer composites but also thermal and mechanical properties of composites [3,4].

The aim of this study is the investigation of the effect of zinc oxide on the properties of PHBV composites. Composites of poly(3-hydroxybutyrate-co-3-hydroxyvalerate) (PHBV) and zinc oxide nanoparticles (nZnO) were prepared by melt mixing method. A twin screw extruder was used to prepare the composites. Since solvent is not used in this method, it can be considered environmentally friendly. PHBV was kindly supplied by ADMajoris Company, France under the trade name MAJ'ECO FN000HA in a pelletized form suitable for melt extrusion. The valerate content of the PHBV reported by the company is 8% by weight. ZnO was purchased from Aldrich. A twin-screw extruder (Rondol Microlab, England) with L/D ratio 20 was used for preparing composites. ZnO percentages in PHBV/ZnO composites were 0.1 wt%, 0.5 wt%, and 1 wt%.

Barrier properties of PHBV composites were determined by SYSTECH oxygen permeation analyzer. The addition of 0.5 wt% of zinc oxide increased the barrier properties by 19% compared to neat polymer. Dynamic mechanical measurements were performed on neat PHBV and composite samples to investigate the effect of the zinc oxide on their thermo-mechanical properties. DMA analysis informed an improvement in storage modulus and loss modulus in the presence of ZnO.

Key Words: Poly (3-hydroxybutyrate-co-3-hydroxyvalerate); biocomposite; zinc oxide; thermo-mechanical properties; barrier properties.

References

- [1] Oner M, Col AA, Pochat-Bohatier C, Bechelany M (2016) Rsc Advances 6: 90973-90981.
- [2] MAlmir S, Barral L, Bouza R, Esperanza M, Seoane M, Feijoo-Bandin S, Lago F (2019) Cellulose 26:2333-2348.
- [3] Atayev P, Oner M (2014) Journal of Plastic Film & Sheeting 30:248-265.
- [4] Castro-Mayorga JL, Fabra MJ, Pourrahimi AM, Oisson RT, Lagaron JM (2017) Food and Bioproducts Processing 101:32-44.

Susceptibility of ^{99m}Tc -ciprofloxacin for common infection causing bacterial strains isolated from clinical samples: an in vitro and in vivo study

Syed Ali Raza NAQVI, Aysha AZIZ, Hassina SABIR

Department of Chemistry, Government College University, Faisalabad-38000, Pakistan

Abstract

^{99m}Tc -ciprofloxacin scintigraphy is useful in the detection of gram positive and gram negative bacterial infections and also for differentiating the infection from aseptic inflammation. However, due to growing bacterial resistance to antibiotics, the ^{99m}Tc -ciprofloxacin no longer can be effective in broad spectrum infection imaging as it is gradually losing specificity. In this study we are presenting our findings regarding the in vitro and in vivo susceptibility of ^{99m}Tc -ciprofloxacin for *S. aureus*, *E. coli*, and *P. aeruginosa* bacterial strains which was isolated from clinical samples. The results of radiosynthesis of ^{99m}Tc -ciprofloxacin showed more the 95% radiochemical purity and less than 5% radioactive impurities. In vitro ^{99m}Tc -ciprofloxacin susceptibility test showed that *E. coli* is more resistant to ^{99m}Tc -ciprofloxacin binding as compared to *S. aureus* and *P. aeruginosa*. The biodistribution study revealed lowest up take by *E. coli* lesion. The T/NT values were obtained 1.96 ± 0.15 in case of *E. coli*; 2.81 ± 0.51 in case of *S. aureus* and 2.32 ± 0.66 in case of *P. aeruginosa* at 4 hours post injection. The SPECT infection imaging of *S. aureus*, *E. coli*, and *P. aeruginosa* bacterial infection induced rabbit models also indicated the clear accumulation in *S. aureus* and *P. aeruginosa* lesions while negligible uptake by *E. coli* lesion which verify the in vitro and in vivo (biodistribution) bacterial susceptibility data. As a conclusion, the ^{99m}Tc -ciprofloxacin no longer can be used as an agent for infection imaging with affordable susceptibility, sensitivity and specificity.

Key Words: ^{99m}Tc -antibiotics, ^{99m}Tc -ciprofloxacin, infection, scintigraphy, radiopharmaceuticals

EXPERIMENTAL AND THEORETICAL ANALYSIS OF A REFRIGERATION SYSTEM WITH PHASE CHANGE MATERIAL (PCM) INTEGRATION

Tuğçe NOYA¹, Berçem KIRAN YILDIRIM², Ebru MANÇUHAN³, Sibel TİTİZ SARGUT⁴,

¹Marmara University, Faculty of Engineering, Chemical Engineering Department, İsatnbul/ TURKEY,
tugcenoya@marun.edu.tr

²Marmara University, Faculty of Engineering, Chemical Engineering Department, İsatnbul/ TURKEY,
emancuhan@marmara.edu.tr

³Marmara University, Faculty of Engineering, Chemical Engineering Department, İsatnbul/ TURKEY,
sibel.sargut@marmara.edu.tr

⁴Marmara University, Faculty of Engineering, Chemical Engineering Department, İsatnbul/ TURKEY,
bercem.kiran@marmara.edu.tr

Abstract

A review of the literature indicates that the research into improvement, both financially and environmentally, of all refrigeration systems has only been conducted within the last twenty years, and that a great deal of research remains to be done. The need for further research of Phase Change Materials (PCMs) on the performance of refrigeration systems is obvious when considering the reported results of refrigeration systems with PCMs versus refrigeration systems without PCMs. Also, the number of PCM integrated cooling system model studies is very limited in terms of the type and quantity of PCMs used. Therefore, the extensive modelling and experimental investigation based on usage of PCMs integrated to the evaporator surface for a refrigeration system is very important.

This study aims to improve the performance of a refrigeration system by increasing its compressor off time and in that way minimizing the electrical energy used, by integrating the PCMs to the evaporator's exterior surface. The experiments were done in a test room using the laboratory scale refrigeration system to investigate the PCM charge and discharge rate and corresponding compressor on-off cycle duration. The test room air temperature was maintained at around 25°C by means of an air conditioner. The distilled water was chosen as PCM material. The theoretical results from improved model were compared with experimental for the same operating conditions. Therefore, the advantages of integrating different quantity of PCM to the refrigeration system experimentally and theoretically were determined.

Keywords: Energy Saving; Refrigeration System; PCM