

ABSTRACTS BOOK



5th International Conference on New Trends in Chemistry

ICNTC CONFERENCE

INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

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Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of “**5th International Conference on New Trends in Chemistry**”, to be held at Athens, Greece dates between April, 22 – 24 2019

Limited number of Papers and Posters with the below mentioned topics will be accepted for our conference:

- Polymer Chemistry and Applications
- Pharmaceutical Chemistry
- 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 as Oral Presentation will be published as Special Issue Edition of **Journal of Indian Chemical Society**. **Journal of Indian Chemical Society** is indexed by Science Citation Index Expanded (SCI-E). (00194522)

Web site of journal : [http://www. http://indianchemicalsociety.com/journal/index /](http://www.http://indianchemicalsociety.com/journal/index/)

- Selected papers (limited as 5) presented as poster and oral related with material science consisting of microelectronics, photonics and micromachining will be published in **Material Science-Poland** after Material Science-Poland publication reviewing process. **Material Science-Poland is Science Citation Index Expanded Journal (ISSN 2083-1331)**

Web site of journal : <http://www.materialsscience.pwr.wroc.pl>

We kindly wait for your attendance to our congress to be held on 22 –24th of April 2019, with a hope to realize a satisfactory conference with it's social activities as well as the scientific ones and leaving a trace on your memories.

Respectfully Yours,

On Behalf of the Organization Committee of ICNTC Conference

Assoc. Prof. Dr. Dolunay SAKAR DASDAN

5th ICNTC 2019 | Conference Chair

Yildiz Technical University – Istanbul / Turkey

Chemistry Department

This Conference is organized in cooperation with **Smolny Institute of the Russian Academy of Education, St. Petersburg**

22 APRIL 2019 MONDAY

08:30-17:00 : REGISTRATION

MAIN HALL : OPENING CEREMONY

09:30 – 09:40

Welcome Speech : Assoc. Prof. Dr. Dolunay SAKAR DASDAN / Yildiz Technical University
Conference Chair

09:40 – 10:30

KEYNOTE SPEAKER : Prof. Dr. Sotiris HADJIKAKOU

Speech Title : Conjugates of Non Steroidal Anti-inflammatory Drugs or Antibiotics, with metal ions (CoMed's) towards the discovery and development of new therapeutic agents.

10:30 – 10:40	C O F F E E / T E A B R E A K
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HALL 1 / SESSION A (ACID)

SESSION CHAIR	Prof. Dr. Sotiris HADJIKAKOU	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
10:40 – 11:00	CO-Releasing Properties and Local Reactivity Descriptors of New $\text{Re}(\text{CO})_3(\text{benzylbenzimidazole})(\text{bpy})\text{IOTf}$	Elvan USTUN
11:00 – 11:20	Production and <i>In Vitro</i> Characterization of Various Doped and Formed S53p4 Bioactive Glass	Efsun SENTURK, Cem Batuhan CEVLIK, Ali Can OZARSLAN, Burcu KARAKUZU IKIZLER, Yeliz BASARAN ELALMIS, Sevil YÜCEL
11:20 – 11:40	Binary Biomaterials (Inorganic material / Natural resin): Synthesis, Characterization and Performance for Adsorption of Dyes	Sedef SISMANOGLU, Hakan DURAN, Tuba SISMANOGLU
11:40 – 12:00	Effects of The Some Parameters on The Astaxanthin Productivity From <i>Haematococcus Pluvialis</i> Algae	Muharrem BOGOCLU, Ceren KECECİLER, Cem ÖZEL, Bilge Sema TEKEREK, Sevil YÜCEL
12:00 – 12:20	Effects of Flue Gas As a CO_2 Source on The Cultivation of <i>Chlorella Protothecoides</i>	Cem ÖZEL, Muharrem Erdem BOĞOÇLU, Ceren KEÇECİLER, Ecem KAPLAN, Sevil YÜCEL
12:20 – 12:40	Thermoelectric Properties Of Poly (3,4-Ethylene Dioxythiophene)/Titanium Disulphide Composite	Naseer Subhi AHMED, Ferdane KARAMAN

12:40 – 13:40	LUNCH
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HALL 1 / SESSION B (BLOOMING)

SESSION CHAIR	Prof.Dr.Sevil Yücel	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
13:40 – 14:00	Influences of Some 2-Aminothiazole Derivatives on Glutathione Reductase Activity	Hasan KARADAG , Emine EROGLU, Cumhur KIRILMIS
14:00 – 14:20	Preparation and characterization of bismuth oxychloride nanoparticles for the development of Photocatalytic performance	Bilal İbrahim DAN-IYA, G. Selda POZAN SOYLU
14:20 – 14:40	The Influence of Chemical Composition on Peroxidation Kinetics of Palm and Nut Oils	Temel Kan BAKIR
14:40 - 15:00	Kinetics and mechanism of pyridine substitution of $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\text{py})_2]$ (X = Cl, Br; py = pyridine) by 1,10-phenanthroline	Khalil J. ASALI

15:00 – 15:20	C O F F E E / T E A B R E A K
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HALL 1 / SESSION C (CATALYSIS)

SESSION CHAIR	Dr.Esin BOZKURT KOPUZ	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
15:20 – 15:40	Steric and Electronic Requirements for Atropisomerization in Heterocyclic Analogues of Biaryls	Ilknur DOGAN
15:40 – 16:00	Investigation of changes in antioxidant activity of some <i>Pleurotus</i> species by using composts including different metal salts	Mertcan KARADENİZ , Temelkan BAKIR, Sabri UNAL
16:00 – 16:20	Single Enantiomer Thioureas As Chiral Solvating Agents	Sule EROL GUNAL
16:20 – 16:40	Non Linear Phenomena in Cellular Automata Simulations of Metal Corrosion and Passivity	Jan STĘPIEŃ, Janusz STAFIEJ
16:40 – 17:00	Investigation of Sensitivity Precision of Smaller Particles Through The Asymmetric Nanopo	Dürdane YILMAZ , Dila Kaya, Kaan Kececi, Ali DİNLER
17:00 – 17:20	Fabrication, Modification and Sensing Behaviour of Quartz Micro/ Nanopipettes	Dila KAYA , Kaan KECECI, Durdane YILMAZ
17:20 - 17:40	Discrete-Time Controllers For Temperature Control of A Polystyrene Polymerization Reactor	Semin ALTUNTAŞ , Hale HAPOĞLU, Gülay ÖZKAN
18:00 – 18:20	Varying the Granulometric Composition of an Electromelted Corundum Based Ceramic with A Porcelain Binder To Control Its Open Porosity and Strength	Zaw Ye Maw Oo

23 APRIL 2019 TUESDAY

08:30-17:00 : REGISTRATION

HALL 1 / SESSION D (DILUENT)

SESSION CHAIR	Assoc.Prof.Dr.Emel AKYOL	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
09:00 – 09:20	Nanoencapsulation of polar bioactive compound	Flavio MASSIGNAN, Éva KISS
09:20 – 09:40	Removal of Bentazon and Metalaxyl Pesticides From Aqueous Solutions By Almond and Chestnut Shells: Optimization, Kinetics and Isotherm Studies	Barış DİLER, Dilek KILIÇ APAR
09:40 – 10:00	Absorbption of Glyphosate-Ipa Herbicide on Mesoporous Silica Nanoparticules	Birsen Sengul OKSAL, Yunus SENTURK
10:00 – 10:20	Degradation Mechanism of Capsaicin Molecule in gaseous phase: Molecular Modeling and DFT study	Bahar EREN, Yelda YALCIN GURKAN, and Yasemin IYIDOGAN
10:20 - 10:40	Structural and electronic properties of layered semiconductor chalcogenide crystals: TlGaSe ₂ , TlGaS ₂ , and TlInS ₂	Burak GURKAN, Savas BERBER
10:40 – 11:00	Water Quality In Istanbul, Marmara Sea	Esin BOZKURT KOPUZ, Gökberk KARA, Burak DİNÇER, Yeşim GÜRTÜĞ

11:00 – 11:20	C O F F E E / T E A B R E A K
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HALL 1 / SESSION E (ELECTRON)

SESSION CHAIR	Assoc.Prof.Dr.Nuriye AKBAY	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
11:20 – 11:40	Interaction of Insoluble Silica Gel Derivatives With Signaling Nucleotide of Bacteria	Secil TURKSOY, Merve BICER, Gokce MEREY
11:40 – 12:00	The Treatment of Detergent Industry Wastewaters By Supercritical Water Oxidation	Ekin KIPÇAK, Sema ŞENTÜRK, Mesut AKGÜN
12:00 – 12:20	In Situ Synthesis Of Triglyceride Oil Based Polymer Clay Nanocomposite	A. Tuncer ERCIYES, Yagmur BAYRAM, Emel AKYOL
12:20 – 12:40	Biosorption of Remazol Orange Rgb By Kefir Biomass Under Sonication	Hatice MUTLU, Dilek KILIÇ APAR
12:40 – 13:00	Ag Particles Deposition on Polyacrylonitrile Fibers Grafted By Acrylamide, Acrylamide-Itaconic Acid and Acrylamide-Maleic Acid	Zeynep OKAY, Meryem KALKAN ERDOĞAN, Meral KARAKIŞLA and Mehmet SAÇAK

13:00 – 14:00	LUNCH
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HALL 1 / SESSION F (FUNCTION)

SESSION CHAIR	Dr.Flavio MASSIGNAN	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
14:00 – 14:20	Preparation of A Novel Gold Nanocluster-Based Biosensor Using Egg White Protein and Its Application for Measuring Prooxidant Activity	Esin AKYÜZ , Furkan Burak ŞEN, Mustafa BENER, Kevser Sözen BAŞKAN, Esma TÜTEM, Reşat APAK
14:20 – 14:40	Temperature Controlled Infrared Drying Kinetics of Mussels	Sema SEVİM, Emek DERUN, Nurcan TUGRUL, İbrahim DOYMAZ, Azmi Seyhun KIPCAK
14:40 – 15:00	A highly selective non-enzymatic H ₂ O ₂ sensor supported on Eupergit CM decorated with PdMoAg nanoparticles	Hilal ÇELİK KAZICI , Fırat SALMAN, Mehmet Sait İZGİ, Ömer ŞAHİN
15:00 – 15:20	Development of Chitosan-Based Edible Biocomposite Films Incorporated with Kumquat Peels Extract as Food Packaging	Fatmagül ŞAHİN, İlknur KÜÇÜK and İbrahim DOYMAZ
15:20 – 15:40	A Theoretical Study of The Reaction of Dimethyl Phosphoramidate With Hydroxyl Radicals	Seyda AYDOĞDU , Arzu HATİPOĞLU
15:40 – 16:00	Increased Solubility And Efficacy of Water Insoluble Flavonoids With N,N-Dimethylalkyl Groups Carrying Calix[N]Arenes	Serdar KARAKURT , Mehmet OGUZ, Mustafa YILMAZ

16:00 – 16:20	COFFEE / TEA BREAK
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HALL 1 / SESSION G (GRAVITY)

SESSION CHAIR	Prof.Dr.Khalil J. ASALI	
TIME	PAPER TITLE	PRESENTER / CO AUTHOR
16:20 – 16:40	New method for the synthesis of the 1,5-methanoazocino[4,3- <i>b</i>]indole by intramolecular cyclization of -1,2,3,4-tetrahydrocarbazoles mediated by tetrachloro-1,4-benzoquinone	Nesimi ULUDAG , Naki ÇOLAK
16:40 – 17:00	Silver Nanoparticles as a scavenging material for new assay for polyphenols metal scavenging activity	Abdelaziz ELGAMOUZ , Alaa Alsaidi, Rana Alsaidi, Chahlaa Naser Nassab
17:00 – 17:20	Structure/Reactivity Properties of Manganese-Based Imidazole Complexes: A DFT Study	Gaye GÜNGÖR, Dolunay ŞAKAR DAŞDAN , Elvan ÜSTÜN
17:20 – 17:40	Novel carbon quantum dots and their bioimaging applications	Fatima OUANZI , Imre BERTÓTI, Miklós MOHAI, Tamás KOLONITS, Kata HORVÁTI, Szilvia BŐSZE, Gergő GYULAI

HALL 1 / POSTER SESSION H

SESSION CHAIRS	ASSOC.PROF..DR.DİLEK KILIÇ APAR ASSIST.DR.ILKNUR KUCUK Janusz STAFIEJ Abdelaziz ELGAMOUZ Fatima OUANZI	
18:00 – 19:00	PAPER TITLE	PRESENTER / CO AUTHOR
	An Investigation Of Stability And Activity Of Poly(Methyl Vinyl Ether-Alt-Maleic Anhydride) Copolymer In The Different Phs And Simulated Body Fluids	Ata AKSOY, İmren ÇOTUK ULUSOY, Kadir ÇAKIRAL, Dolunay ŞAKAR DAŞDAN
	Effect Of Dopant Localization İn The Micelles On The Formation Of Uniaxial And Biaxial Lyotropic Cholesteric Phases	Esra SAHIN , Baris OKUYAN, Erol AKPINAR
	Development And Optimization Of An Hplc Method For The Simultaneous Analysis Of A Multi Component Drug Product By The Help Of Central Composite Design	Şule DİNÇ-ZOR, Evridiki PİNGO , Özlem AKSU DÖNMEZ, Bürge AŞÇI
	Modeling Particle Size of Polyacrylic Acid-Copper(II)-Bovine Serum Albumin Ternary Complex In Salt Solution	Dolunay ŞAKAR DAŞDAN, MESUT KARAHAN, FATMA NOYAN TEKELİ , GÜLHAYAT GÖLBAŞI ŞİMŞEK
	Synthesis and Thermoelectric Properties of Polythiophene/Poly(3,4-ethylene dioxythiophene) Nanocomposites under Magnetic Field	Keziban HUNER, Ferdane KARAMAN
	Influence of Some Parameters on The Protective Power of Caffeine Against Copper Corrosion	Hiba MESSAOUDI , Mohamed LITIM, Maamar SLIMANE, Djilali BEKHITI
	Adsorption Behavior And Surface Analysis Of Caffeine As A Green Corrosion Inhibitor For Copper	Hiba MESSAOUDI , Bahadır KESKİN
	Catalytic hydrodeoxygenation of bio-oil in a fixed bed reactor	WANG JUNDONG, NOURELHOUDA BOUKAOUS, LOKMANE ABDELOUAHED , CHETNA MOHABEER, LIONEL ESTEL, BECHARA TAOUK
	Detailed modelling of Anaerobic digestion with experimental validation	LOKMANE ABDELOUAHED , ANDRES MARTINEZ, BECHARA TAOUK, LIONEL ESTEL
	Improving of Dye Uptake and Moisture Absorption Abilities of Polyacrylonitrile Fiber By Grafting of Hydroxymethyl Methacrylate	Merve BARUT, Meral KARAKIŞLA and Mehmet SAÇAK
	Lyotropic Uniaxial and Biaxial Cholesteric Phase Properties of Potassium Alkanoate/Decanol/H ₂ O/Brucine Sulfate Mixtures	Nazli UYGUR , Seda UYANIK, Erol AKPINAR
	Functionalized Clinoptilolite For Removal of Soluble Dyes in Aqueous Solution	Neli MINTCHEVA , Gospodinka GICHEVA, Lyubomir

	DJERAHOV, Marinela PANAYOTOVA
Preparation Of Silver Nanoparticles-Zeolite Nanocomposite And Its Potential Application As An Antibacterial Agent In Water Treatment	Neli MINTCHEVA , Gospodinka GICHEVA, Marinela PANAYOTOVA, Lyubomir DJERAHOV
Naproxen Derivative Interaction Properties With CT-DNA	Nuriye AKBAY , Zeynep KOKSAL, Tugba TASKIN-TOK, Ayse UZGOREN-BARAN
Stimuli-responsive polyzwitterionic microgels with tunable UCST – LCST and study of their anti-polyelectrolyte effect in salt solutions	Pabitra SAHA , Nikhil K. SINGHA, Andrij PICH
Micellization properties of some tetradecylalkylammonium bromide surfactants	Sezin CETINKAYA , Emre GUNER, Erol AKPINAR
Evaluation of extraction and HPLC separation of polyphenol compounds in <i>Mallotus oppositifolius</i> (Geisel) Müll. Arg.	Soleya DAGNON , Nikoleta MARGOVA, Dimitar BOJILOV, Kouadio KOUASSI
UHPLC-MS investigation of polyphenol composition in <i>Clinopodium vulgare</i>	Dimitar BOJILOV, Soleya DAGNON , M. KIRILOVA
Hydroxyl Radical Decomposition Reaction of Ciclacillin Molecule	Yelda YALCIN GURKAN , Nilay SAKARYA, Bahar EREN

24 APRIL 2019 WEDNESDAY

12:00 – 18:00	SOCIAL PROGRAM FOR CONFERENCE PARTICIPANTS
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ABSTRACTS

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CONJUGATES OF NON STEROIDAL ANTI-INFLAMMATORY DRUGS OR ANTIBIOTICS, WITH METAL IONS (COMED'S) TOWARDS THE DISCOVERY AND DEVELOPMENT OF NEW THERAPEUTIC AGENTS.

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Conjugation of a metal with drug is the key for the enhancement of the biological activity of the drug. Moreover, a new era was recently opened in the discovery and development of new therapeutic agents, from the combination of two distinct classes of chemical or biological agents into a single entity. This provides the opportunity for synergistic effects, most notably when one of the components acts as a detector agent which scout the targeted intracellular component, cell, tissue etc and the other interacting with the desired biological system. In our laboratory we are examining closely the biological activity of new CoMeD's which we are developing.

Antimicrobial:

New antibacterial compounds have been developed from the conjugation of the salicylic acid (NSAID), the ciprofloxacin (antibiotic) and thionicotinic acid (antimetabolite) with silver(I). Their formulae are $[\text{Ag}_2(\text{SALH})_2]_2$ (AGSAL-1), $[\text{Ag}(\text{CIPH})_2]\text{NO}_3$ (CIPAG) and $\{[\text{Ag}_6(\mu_3\text{-HMNA})_4(\mu_3\text{-MNA})_2]^{2-} \cdot 2[(\text{Et}_3\text{NH})^+]\}$ (AGMNA). The Minimum Inhibitory Concentration (MIC), Minimum Bactericidal Concentration (MBC) and their Inhibition Zone (IZ) against the *Staph. epidermidis*, *Staph. aureus* and *Pseudomonas aeruginosa* were determined. The toxicity of the compounds was evaluated against human immortalized keratinocytes (HaCaT) (AGSAL-1) or corneal epithelial cells (HCECs) (CIPAG, AGMNA). The wound healing epithelialization of AGSAL-1 against HaCaT cells and its anti-inflammatory activity was also investigated.

Oncology:

Clinical trials and epidemiological studies have shown that Non Steroidal Anti-inflammatory Drugs (NSAID's) exhibit protective role against the incidence of mammary cancer. The conjugation of mitochondriotropic ligands "Trojan horse" with specific NSAID's is used for the delivery of the drugs to mitochondria. The low toxicity against humans of silver(I) ions enable their use in the development of new metallotherapeutics.

The synthesis of a series of silver(I) metallotherapeutics of formulae $[\text{Ag}(\text{D})(\text{EAR}_3)_n]$, (D= salicylic acid, aspirin, diclofenac, naproxen, nimesulide etc; E= P, Sb etc; Ar= Ph-, p-tolyl-, m-tolyl, o-tolyl) is reported. The compounds were characterized by spectroscopic (NMR, IR, Raman etc) and X-Ray diffraction techniques. These complexes were *in vitro* evaluated for their activity against human breast cells, MCF-7 (Hormone Depended) and MDA-MB-231 (Hormone Independent). Their toxicity was evaluated against normal human cells (normal human fetal lung fibroblast cells (MRC-5)).

STRUCTURE/REACTIVITY PROPERTIES OF MANGANESE-BASED IMIDAZOLE COMPLEXES: A DFT STUDY

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Carbon monoxide (CO) which is a colorless, odorless gas is produced in the human body through heme oxygenase, present in two forms: the constitutive (HO-2 and HO-3) and inducible (HO-1) isoforms [1]. Recently, it has been discovered that CO gas in small doses exhibits some anti-inflammatory and antimicrobial properties making it useful as a potential therapeutic agent for disease control [2]. Countless transition metal carbonyl complexes are now known, and some of these can release CO within the human body without affecting the level of carboxyhemoglobin produced. These complexes are now referred to as “Carbon Monoxide Releasing Molecules (CORMs)”. Most of the recent research on CORMs has been focused on the CO-releasing properties, and the drug sphere has been essentially ignored. Since the drug sphere is essential for targeting the CORM into a desired area of the body, more research is needed in this area [3].



Fig 1. The structures of $[\text{Mn}(\text{CO})_3(\text{bpy})(\text{imidazole})]\text{PF}_6$ (**1**) and $\text{Mn}(\text{CO})_3(\text{bpy})(\text{methylimidazole})]\text{PF}_6$ (**2**)

In this current work, 2 optimized CORMs containing $\text{Mn}(\text{CO})_3(\text{bpy})$ moiety such as $[\text{Mn}(\text{CO})_3(\text{bpy})(\text{imidazole})]\text{PF}_6$ (**1**) and $\text{Mn}(\text{CO})_3(\text{bpy})(\text{methylimidazole})]\text{PF}_6$ (**2**) showing the anticancer agent property [4] (Fig 1) were analyzed with local/global reactivity descriptors for getting insight about the reactivity/activity properties of the molecules [5].

Key Words: CO-releasing molecules (CORMs); cancer treatment; manganese complexes; imidazole

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INFLUENCES OF SOME 2-AMINOTHIAZOLE DERIVATIVES ON GLUTATHIONE REDUCTASE ACTIVITY

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Abstract

Glutathione reductase (EC 1.8.1.7) converts oxidized glutathione (GSSG) to reduced glutathione (GSH) in the presence of NADPH (β -Nicotinamide adenine dinucleotide 2'-phosphate reduced) [1]. Oxidized glutathione (GSSG) has a disulfide bridge. 4,4'-(disulfanediybis(methylene)) bis(thiazol-2-amine) dihydrochloride is a 2-aminothiazole derivative containing also a disulfide bridge in its structure. 2-amino-4-(chloromethyl)thiazole hydrochloride is the 2-aminothiazole derivative without disulfide bridges. 2-aminothiazole derivatives have antiviral [2], antimicrobial [3], anticancer [4] and anti-inflammatory activities [5].

In this work, glutathione reductase from baker's yeast (*S. cerevisiae*) exposed to 0, 25, 50, 100, 250 and 500 ppm 4,4'-(disulfanediybis(methylene))bis(thiazol-2-amine) dihydrochloride and 2-amino-4-(chloromethyl)thiazole hydrochloride. In case of exposure of 4,4'-(disulfanediybis(methylene))bis(thiazol-2-amine) dihydrochloride slightly decrease was observed in glutathione reductase activities. But, in all tested 2-aminothiazole concentrations, no important statistical differences were observed in glutathione reductase activities ($p > 0.05$, $n=3$) when compared to control groups.

Key Words: *Glutathione Reductase; 4,4'-(Disulfanediybis(methylene))bis(thiazol-2-amine) Dihydrochloride; 2-Amino-4-(Chloromethyl)thiazole Hydrochloride; 2-Aminothiazole; Enzyme.*

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AG PARTICLES DEPOSITION ON POLYACRYLONITRILE FIBERS GRAFTED BY ACRYLAMIDE, ACRYLAMIDE-ITACONIC ACID AND ACRYLAMIDE-MALEIC ACID

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Abstract

Poly(acrylonitrile) (PAN) fibers have drawn much attention due to its excellent mechanical properties and has been one of the most preferred synthetic textile fibers used in many fields. PAN fibers have also been frequently used in textile composites production for conductivity [1,2], sensors [3], antibacterial [4] and adsorbent [5] purposes and etc. However, having a tendency to electrostatic charge deposition, having low humidity absorption and low dye uptake of some dye types limit the use of PAN in related application areas. These obstructions could be resolved with different techniques such as graft copolymerization, by imparting desired properties of different monomers to the PAN fibers using a chemical method. In this study, to gain new functional groups to PAN fiber surface such as $-NH_2$ and $-COOH$ groups, graft copolymerization of acrylamide, acrylamide-itaconic acid and acrylamide-maleic acid monomer mixtures was performed on PAN fibers in aqueous medium using benzoyl peroxide as initiator at 85 °C. The effect polymerization conditions such as concentrations of monomer and mol ratios (%) of monomer mixtures were investigated on graft yield (%) of PAN fibers. Relatively the highest graft yield (%) of PAN fiber (29.3%) was obtained when the mol ratios (%) of acrylamide/itaconic acid mixture was taken as 80/20 in the polymerization. The graft modified-PAN fibers were characterized with different techniques including 1H -NMR, ATR-FTIR and SEM techniques, respectively. After incorporation of new functional groups to PAN fibers, noble Ag particles were deposited on these graft modified-fibers by two steps including (I) adsorption of Ag^+ ions via newly introduced functional groups and then (II) reduction of Ag^+ with $NaBH_4$. The presence of Ag particles on the composite fibers was confirmed with SEM and EDX. These composites have the potential of use in different fields such as antibacterial activity and catalysis.

Keywords: *graft copolymerization; poly(acrylonitrile) fiber; Ag particles deposition*

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BINARY BIOMATERIALS (INORGANIC MATERIAL / NATURAL RESIN): SYNTHESIS, CHARACTERIZATION AND PERFORMANCE FOR ADSORPTION OF DYES

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Abstract

The sol-gel method has been reported a useful techniques for synthesizing inorganic material HSS. In this study, the sol-gel process was used in two stages [1]. In the first step, the hydrolysis of phenyltrimethoxysilane (PTMS) was carried out under acidic conditions. In the second step, the silane condensation proceeded under basic conditions and as a result the HSS were obtained. The obtaining HSS was treated with epichlorohydrin to carry out an epoxidation process (HSEPC). Then, HSEPC was functionalized by treatment with natural resin (gum arabic) and obtained HSEPCGUM. Gum arabic has GA-GP-GA-glycoprotein, hydroxyproline glucuronic acid and polysaccharides groups. Anionic and cationic dyes were adsorbed onto HSEPCGUM and values of absorbance was measurement by UV-visible spectrophotometers. Adsorption isotherm experiments of adsorbed dyes on HSEPCGUM were performed at 35°C with Freundlich, Langmuir and Dubinin–Radushkevich (DR) methods. Adsorption maximum capacity of HSEPCGUM (X_{max}) was obtained 100 mg/g for BB3. Before and after dye adsorption the structure characterization of adsorbent was done by SEM and FTIR analysis.

Key Words: *hollow silica spheres, reactive blue 21, basic blue 3, adsorption, sol-gel method*

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PREPARATION AND CHARACTERIZATION OF BISMUTH OXYCHLORIDE NANOPARTICLES FOR THE DEVELOPMENT OF PHOTOCATALYTIC PERFORMANCE

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Abstract

Bismuth oxychloride (BiOCl) is an important nanocomposite material, which has various applications [1-2]. Bismuth oxychloride nanocomposite was successfully synthesized using bismuth (III) triacetate [Bi (CH₃COO)₃] as starting material. Tetragonal structure and size were characterized by X-ray diffraction whereas SEM shows morphology and dispersion at different magnifications as well as FT-IR spectrum range of 450-4000 cm⁻¹ describes the stretching absorption at different absorption bands. The photocatalytic activity of the BiOCl nanocomposite was evaluated by degradation of bisphenol A (BPA) under different irradiation. The degradation rate of BPA and its mineralization effectiveness were analyzed by HPLC and TOC measurements. The BiOCl nanocomposite showed a total degradation (100%) of BPA and almost wholly TOC removal value (98%) in 60 min.

Key Words: *BiOCl; Characterization; Bisphenol-A; photo-oxidation; UV irradiation*

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STERIC AND ELECTRONIC REQUIREMENTS FOR ATROPISOMERIZATION IN HETEROCYCLIC ANALOGUES OF BIARYLS

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Abstract

Atropisomers are enantiomers or diastereoisomers that result from slow axial rotation that can, in principle, interconvert thermally, but for which the half-life of interconversion is ~1000 s or longer, thus allowing analytical separation [1]. The slow rotation along a bond axis usually results from steric hindrance and/or electronic factors. This work describes the steric and electronic requirements needed to produce stable heterocyclic nonbiaryl atropisomers with an Nsp²-Caryl stereogenic axis. The micropreparative separations and assignment of absolute conformations/configurations of the axially chiral heterocyclic atropisomers described and the reasons for the observation of high barriers to rotation are discussed.

Key Words: *Atropisomers; Axial Chirality; Nonbiaryl Atropisomeric Compounds; micropreparative resolution; HPLC on optically active stationary phases*

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DEGRADATION MECHANISM OF CAPSAICIN MOLECULE IN GASEOUS PHASE: MOLECULAR MODELING AND DFT STUDY

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Abstract

Capsaicin is known as a considerably strong and stable alkaloid, which is formed in nature only in hot pepper as crystal. Capsaicin is a kind of oil, which is the main component obtained from chilli paprika, and is also known as ‘oleoresin capsicum’. In addition to its pharmacological use, it is also widely used as a pepper spray, which is produced through dissolving the oil in organic solvents such as chloroform, alcohol and ether as 1-10% solution.

The known harmful effects of this molecule can be exemplified as irritation and lacrimation in the eye, asthma, various respiratory irritations, and irritating effects on epithelial tissues, although the exposed area is washed up with water.

In this study, in order to eliminate the harmful effects of capsaicin, the reaction of the fragmentation of capsaicin with OH radical was analysed. Quantum chemical calculations of Density Functional Theory (DFT) were used to analyse the structural and physical characteristics of capsaicin and its derivatives.

The aim of this study is to estimate the degradation mechanism of capsaicin molecule in gaseous phase for each fragmentation and to compare the energy values and stabilities of this molecule and its five stable fragments in solvents, namely water, ethanol, diethyleter, and chloroform. Calculation of the probable reaction path of this molecule was made, and their most stable state in the thermodynamic frame was determined for these phases.

Key Words: *Capsaicin; Pepper Gas; Gaussian 09; DFT, OH radical*

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WATER QUALITY IN ISTANBUL, MARMARA SEA

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Abstract

In Istanbul, where dense industrialization and dense population are located, people can use Marmara Sea for recreational reasons. The beaches in which they interacted with the sea were selected primarily for the determination of heavy metal pollution. In this study, the quality of sea waters used for recreational purposes such as swimming was investigated in terms of human health. Temperature, pH, conductivity, dissolved oxygen were measured in Kucuksu, Fenerbahce and Suadiye beaches in Istanbul Anatolian side. Weekly measurement values were recorded 18 November 2019 to 31 January 2019. The water pollution was investigated with the limit values in the Turkish Water Pollution Control Regulation published by the Ministry of Environment and Urbanization.

Key Words: Marmara Sea, sea water quality, beaches, pH, recreation

Acknowledgments

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CO-RELEASING PROPERTIES AND LOCAL REACTIVITY DESCRIPTORS OF NEW [RE(CO)₃(BENZYLBENZIMIDAZOLE)(BPY)]OTf

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Abstract

The researches about carbon monoxide-based therapy have gone to an exciting point of biomedical fields [1]. It is necessary to release CO in specific tissue with controllable dosages for utilizing the therapeutic properties of CO [2]. Molecules that stored CO in solid form must be triggered endogenously or exogenously for releasing CO. It is known from previous studies that CO-releasing could be done by photo-irradiation, enzyme, pH and thermal change and ligand exchange reactions [3]. Among these methods, particular attention is given to photoactivatable CO-releasing because of better tissue and time control [4, 5].

In this study, [Re(CO)₃(benzylbenzimidazole)(bpy)]OTf (bpy: 2,2'-bipyridyl, OTf: triflate) complex (Fig. 1) was synthesized, characterized, analyzed for CO-releasing properties and investigated global and local reactivity descriptors by DFT/TDDFT calculation methods.

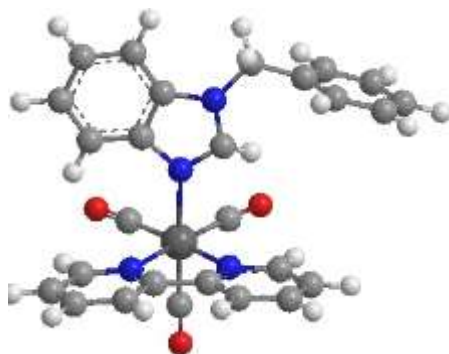


Figure 1. Structure of [Re(CO)₃(benzylbenzimidazole)(bpy)]⁺

Key Words: CO-Releasing Molecules, Rhenium Complexes, DFT/TDDFT, local reactivity descriptors

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PREPARATION OF A NOVEL GOLD NANOCUSTER-BASED BIOSENSOR USING EGG WHITE PROTEIN AND ITS APPLICATION FOR MEASURING PROOXIDANT ACTIVITY

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Abstract

In living organisms, reactive oxygen and nitrogen species (RONS) can be produced during normal cellular metabolism. Oxidative stress occurs when antioxidants and oxidants/prooxidants are not balanced in favour of the latter, which may cause biomacromolecular damage leading to various diseases. Although the main health beneficial effects of natural bioactive compounds originate from their antioxidant properties, they may exhibit prooxidant behavior under certain conditions (such as transition metal ions and O₂). Therefore, understanding the antioxidant/prooxidant behavior of bioactive substances depending on structures and conditions in which they are found is of great importance. In this work, chicken egg white protein (CEW)-protected gold nanoclusters (CEW-AuNCs) were prepared to measure the Cu(II)-induced prooxidant activity of antioxidant compounds such as epicatechin, epigallocatechin gallate, catechin, rosmarinic acid, resveratrol, ascorbic acid, and glutathione [1]. This assay involved the reduction of Cu(II) ions to Cu(I) by antioxidant compounds (simultaneously giving rise to reactive oxygen species) and binding of the formed Cu(I) to the CEW-AuNC structure. The bound Cu(I) may be released with the cuprous-selective ligand neocuproine (Nc), forming the basis of a spectrophotometric method measuring absorbance at 450 nm pertaining to the Cu(I)–Nc chelate. The order of the molar absorption coefficients of the tested compounds with respect to the CEW-AuNC biosensor were: epigallocatechin gallate > epicatechin > catechin > resveratrol > glutathione > ascorbic acid ≥ rosmarinic acid. The developed method involved a one-pot synthesis and determination without tedious separations, and was applied to binary synthetic mixtures of studied antioxidant compounds and to certain herbal plant (green tea, linden, echinacea, and artichoke leaf) extracts to determine the total prooxidant activities. The results were statistically compared with those of a literature Cu(II)–Nc assay using a calcium proteinate-based solid biosensor [2]. The developed biosensor was stable, reliable, easily applicable, of low cost and wide linear range, and could reproducibly determine the prooxidant activities of natural antioxidant samples.

Key Words: *Chicken egg white proteins (CEW); gold nanocluster (AuNC); CEW-AuNC prooxidant biosensor; cuprous-neocuproine; natural antioxidants.*

Acknowledgment

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DISCRETE-TIME CONTROLLERS FOR TEMPERATURE CONTROL OF A POLYSTYRENE POLYMERIZATION REACTOR

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Abstract

Exothermic reactions in various industrial reactors that may have potential safety problems exhibit very interesting behaviour for investigation. Undesirable performances of some controllers applied to control the temperature of reaction medium were reported [1]. The polymerization reactions generate a large amount of heat which must be removed from the reactor to follow the required temperature values. The suitability of controller highly depends on the types of reaction and reactor, the process operating temperature, the processing method, and catalyst [2]. Polystyrene reactors are highly used in industry because of its economic importance. A well-tuned feedback control loop is essential because this process may exhibit unstable dynamic behaviors.

For temperature control, styrene free radical polymerization in a 1.1 l batch reactor was presented with the zero-order hold-equivalent discrete time models which are analogous to its continuous-time version discussed in [3]. Two discrete-time controllers were applied to the reactor. Firstly, a discrete-time controller with three tuning parameters was designed, and its parameters were determined by checking control performance and closed loop pole-placement in z-plane. The sixth order closed loop transfer function between reactor temperature and set point was obtained. The best tuning parameters were determined as -0.1, -0.9 and -0.1. Effect of tuning parameters to stability was investigated. Secondly, the discrete-time proportional integral derivative controller (2 DOF) was employed. Simulink control design was utilized for tuning the six parameters of the controller as -10.75, -1.09, -19.26, 0.689, 0.1686, 4.123e-0.5 respectively. These controller performances were compared to each other for a step decrease in set point. It is noted that a very close matching was achieved and the controllers have made the closed loop system desirable and stable with the best tuned parameters determined.

In order to obtain good quality 52000 g/mole polystyrene, these two different discrete-time controllers were applied theoretically for tracking previously determined optimal temperature profile. The published experimental data in [3] were used for validation. Experimental conventional proportional integral derivative control results in [3] was obtained by using the flow rate of cooling water at a fixed value and applying heat with the help of a module as manipulating variable. In the present study, cooling water flow rate was used as manipulated variable to obtain better control performance with minimum response time and reduced production cost. In the set point tracking cases studied, the best tuned controllers acted to produce non-oscillatory closed loop behavior without offset throughout the length of the batch run.

Key Words: *polymerization; polystyrene; discrete-time model; zero-order hold; discrete-time controllers*

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INTERACTION OF INSOLUBLE SILICA GEL DERIVATIVES WITH SIGNALING NUCLEOTIDE OF BACTERIA

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Abstract

Cyclic nucleotides are ubiquitous second messengers: Intracellular molecules which transmit signals in cells and derived from extracellular signals. In bacteria, cyclic dimeric guanosine 3',5'-monophosphate (c-di-GMP), one of the cyclic nucleotides, have emerged as an important secondary messenger involved in the regulation of major physiological transitions such as transportation, metabolism of lactose [1], virulence, motility and biofilm formation [2].

The relative rotational state of the two bases of this cyclic nucleotide can result in both *cis* and *trans* conformation and *cis* conformation is able to further dimerize to form G-quadruplex structure [3]. Studies show that c-di-GMP forms a stable G-quadruplex structure in the presence of planar aromatic intercalators such as proflavine and acridine derivatives even at very low concentrations [4].

In this study, we synthesized different acridine derivatives attached to amine functionalized silica gel in order to form an insoluble structure which is capable of binding c-di-GMP signalling nucleotide of bacteria. For this purpose, 3-(ethylenediamino)propyl-functionalized silica gel was reacted with different acridine derivatives and the samples were analyzed with IR spectroscopy. After the confirmation of the acridine derived silica gel, UV and HPLC analysis were performed to observe if the synthesized structure interacts with the aromatic groups of the GMP nucleotide.

UV and HPLC analysis confirmed a slight interaction between GMP and synthesized acridine derivatives. Then it was investigated whether the acridine derivatives interact with c-di-GMP of the *Bacillus subtilis* strain which has the ability to form biofilm.

After this study, our group may propose a new and beneficial method to capture c-di-GMP nucleotide of bacteria which is responsible from its virulence and biofilm formation. Thus, the basic functions of bacteria can be blocked by this method and level of bacteria be measured by regaining the captured c-di-GMP from the insoluble acridine derived silica gel structure.

Key Words: *Biofilm formation, virulence, c-di-GMP, G-quadruplex, acridine.*

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FABRICATION, MODIFICATION AND SENSING BEHAVIOUR OF QUARTZ MICRO/ NANOPIPETTES

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Abstract

Resistive-pulse sensing is a method for detecting particles by measuring ionic current flowing through a micro/nano opening. Various materials either biological or synthetic can be used to generate micro/nanopores for resistive-pulse sensing. These pores can be grouped as solid-state (i.e. nanoporous polymers, carbon nanotubes) and biological nanopores (i.e. α -hemolysin) [1]. In this work, we use glass/quartz as a material in the capillary form to fabricate micro/nano pipettes as a sensing tool for micro/nanoparticles detection.

Micro/nanopipettes are simply defined as capillary pipettes with micro/nano-sized openings and in the recent years they have gained importance in many applications. Especially in nanoscience, micro/nanopipettes are used in a number of areas such as probes in atomic force microscopy (AFM), scanning electrochemical microscopy (SECM), tip-enhanced Raman spectroscopy (TERS) and many others, due to their small tip size, needle-like structure and easy fabrication properties [2]. Additionally, quartz nanopipettes can be integrated in sensor applications as DNA sensor, renewable nanosensor and allergen sensor.

We have used a laser-based pipette puller system for the production of micro/nanopipettes from quartz capillaries (I.D.: 0.7 mm; O.D.: 1.0 mm). The pipettes were characterized via optical microscopy and SEM. We have studied the translocation events of polystyrene micro/nanoparticles at different concentration ($0.1 \times 10^8 - 1 \times 10^8$ number of particles per mL) and potential (0 – 1000 mV) values to investigate the resistive-pulse sensing behaviour and performance of the obtained pipettes. The focus of this study was to understand the effect of surface charge on detection/translocation phenomenon. For this purpose, we used silane chemistry and modified the inner surface of the micro/nanopipette with (3-aminopropyl) triethoxysilane. We have recorded current-potential (I-V) measurements and observed the ionic current rectification (ICR). ICR, which is the characteristic of asymmetric pores, is known to be directly related to the pore surface charge and can be used to verify the modification process. Therefore the modification of the pipette surface was confirmed using electrochemical measurements. We think modification of the inner surface of the micro/ nanopipettes can entail selective and enhanced transport of analytes of interest and holds promise for future studies.

Key Words: Resistive-pulse sensing, quartz nanopipettes, surface modification, nanopore sensor, nanopore fabrication

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VARYING THE GRANULOMETRIC COMPOSITION OF AN ELECTROMELTED CORUNDUM BASED CERAMIC WITH A PORCELAIN BINDER TO CONTROL ITS OPEN POROSITY AND STRENGTH

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Abstract

Porous permeable ceramics is mainly used as elements for ceramic membranes, catalyst supports in the processes of oxidation, hydrogenation and dehydrogenation at high temperature, corrosion in feed processing - corrosive environments at endothermic and exothermic reactions [1]. As the filler used corundum (0.5 mm) and (2--3 mm) and as the bunch used powder porcelain. The quantity of granular filler in all the mass was 95 wt. %, the bunch - 5 wt. %. And then to obtain a porous permeable ceramic products with sufficient for the operating conditions of the superior strength and filtering characteristics altered the ratio of the grain aggregate of large and small fractions of 2--3mm / 0.5 mm: 0 / 95, 35 / 60, 40 / 55, 45 / 50, 50 / 45 and 95 / 0. In the experiment, the pressing pressure was 25, 50 and 100 MPa (for compounds 0 / 95 95 / 0 applied pressure of 25 and 50 MPa), the maximum firing temperature of the ceramic preforms was 1350 and 1450 °C. The obtained samples were studied by open porosity, density and mechanical strength in accordance with the techniques described in [2]. There was obtained a highly porous ceramic of alumina carriers for catalysts. The filler used to be electro corundum, as reinforcing filler, forming on fire a bundle used porcelain. The samples were prepared by pressing, followed by drying and calcining at 1450 °C. The porosity after firing was 20 - 25 %, the compressive strength of 150-155 MPa.

Keywords: ceramics, porosity, strength, electro corundum, porcelain

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TEMPERATURE CONTROLLED INFRARED DRYING KINETICS OF MUSSELS

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Abstract

Mussel has impressive nutritional values, which contains many vitamin, mineral and protein by comparison with other shellfish. It is a sustainable, common and cheap seafood that supports your immune system and brain [1]. In order to increase its preservation, many drying methods can be used in mussel drying. Among these techniques infrared drying has gained popularity in the food industry due to its rapid drying rate/response time and superior thermal efficiency compared to traditional drying methods for the recent years. By subjecting the material to infrared radiation, heating power produced penetrate into the products [2]. In this study, various temperatures (60, 70 and 80°C) were applied to mussels via infrared dryer to investigate the temperature effect on drying characteristics, effective moisture diffusivity and activation energy. The drying times were detected as 405, 255 and 165 min for 60, 70 and 80°C, respectively. The results showed that rate of evaporation increased with temperature rise and consequently structural properties of mussel was affected from this increment. It can be expressed as the fat, which is been in mussel, turns into to peroxides throughout the drying process. Therefore, fat oxidation leads to spoilage in quality and taste of products so this causes to reduce of product nutritional value and shelf life. When the drying time decreases with temperature increases, the fats are degraded less [3]. Hence, drying temperature at 80°C was given optimum temperature in the experiments for quality of mussel and also energy consumption. To identify the drying kinetic of mussel, seven mathematical models Aghbashlo et al., Alibas, Hendersen and Pabis, Lewis, Midilli and Kucuk, Parabolic and Wang and Singh were applied to the experimental results. As a result of the modelling, Alibas model provided to best estimation for each temperature according to drying data. The results are 0.999886, 0.999916, 0.999964 for coefficient of determination (R^2); 0.000011, 0.000009, 0.000006 for reduced chi-square (χ^2) and 0.002946, 0.002614, 0.001854 for root mean square error (RMSE) drying at 60, 70 and 80°C, respectively. Effective moisture diffusivity values were found as 4.23×10^{-9} , 7×10^{-9} and 1.17×10^{-8} m²/s at 60, 70 and 80°C, respectively. It is obviously clear that the effective moisture diffusivity values were increased with temperature the increase. The effect of temperature on the moisture diffusivity depends on Arrhenius equation. According to the relationship 49.67 kJ/mol was calculated as an activation energy of mussel.

Key Words: Mussel; infrared radiation; drying kinetic; mathematical modelling; activation energy

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NANOENCAPSULATION OF POLAR BIOACTIVE COMPOUND

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Abstract

The nanostructural drug delivery and targeting systems got an increasing interest in present and future pharmaceutical practice. The convenient administration, enhanced bioavailability, controlled release is among the main benefits of colloidal type carriers, such as liposomes, nanoparticles, nanogels or other. Besides the high degree of dispersion of the bioactive component the drug carrier surface can be functionalized to achieve the selective accumulation of the certain parts of the human body.

Once a rarely used class of therapeutic agents, pharmaceutical proteins have increased remarkably in number and frequency of use. With more than 130 FDA (2012) approved products and many more in development, protein therapeutics have gained a significant role in almost every field of medicine [1].

The present nanoencapsulation system is designed mainly for hydrophobic drug materials with limited solubility in aqueous environment. The development of efficient and stable carrier systems for proteinous or peptide type drugs presents a challenge and requires a different approach. More complex nanoparticles are thought to fulfill these requirements which include the protection of the bioactive molecule in the various parts of the body, high enough encapsulation efficiency, and particle size lower than 200-300 nm in diameter [2].

The aim of this work is to build a carrier system containing drug with high degree of dispersion, using material like reverse Pluronic and AOT, and solvents like chloroform, hexane.

Phenylalanine, as a simple model of hydrophilic/peptide-like API, was encapsulated in the system AOT/hexane/water, producing droplets with size from 6 to 12 nm. This system was prepared using shaking and sonication techniques, giving similar results.

In a second system, AOT/chloroform/water, a higher amount of Phenylalanine was managed to encapsulate comparing to the hexane system. That composition allowed the application of AOT at higher concentration leading to smaller droplets size (possibly microemulsion).

The formation of nano- or microemulsion is spontaneous, resulting in drug carrier system with significant colloidal stability for a long time.

Key words: *drug delivery; proteins; nanoemulsions; nanoencapsulation; bioactive compound.*

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NOVEL CARBON QUANTUM DOTS AND THEIR BIOIMAGING APPLICATIONS

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Abstract

The importance of nanoparticle systems has become an intense topic in the field of materials science and nanotechnology. This interest is manifested in different fields ranging from structural materials, optics, energy research to biomedical applications.

Carbon quantum dots which are novel members of carbon-based, have been shown to be suitable alternatives to molecular labeling in chemical analysis, molecular imaging and biomedical diagnostics due to their superior properties. These particular systems are highly fluorescents with tunable spectral properties, non-toxic and biocompatible [1]. In addition, they have an excellent physicochemical and photochemical stability [2].



Figure: Photograph of CQD sample dispersions under normal light (left) and UV light illumination(right)

In this work, we prepared Carbon Quantum Dots using simple, economic methods based on bottom up techniques, and we have investigated the effect of the preparation methods on the chemical composition and fluorescence properties. *In vitro* cellular internalization experiments have also been carried out. The quantum dots have been found to be ideal fluorescent labels with excellent biocompatibility.

Key Words: Carbon Quantum Dots; Fluorescence; Chemical Structure; Biocompatibility; Cellular Imaging.

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KINETICS AND MECHANISM OF PYRIDINE SUBSTITUTION OF $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\text{PY})_2]$ (X = CL, BR; PY = PYRIDINE) BY 1,10-PHENANTHROLINE

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Abstract

Reactions of $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\text{py})_2]$ (X= Cl (1), Br (2); py= pyridine) with 1,10-phenanthroline (= phen) in toluene solution resulted in replacement of the py ligands and the formation of $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\kappa^2\text{-N,N-phen})]$. Thermal kinetics of these substitution reactions, under *pseudo*-first-order reaction conditions, indicated that these reactions proceed by a rate law that is first-order in the concentration of the metal complex and zero order in phen concentration. A mechanism which describes such ligand substitution reaction is proposed and suggests initial replacement of one py through reversible Mo-py bond fission, as rate limiting, followed by rapid (irreversible) attack of one N-atom of phen at the resulting coordinatively unsaturated $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\text{py})]$ intermediate to give initially $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\text{py})(\kappa^1\text{-N-phen})]$. The latter complex undergoes fast ring closure, entropy controlled, with extrusion of the second py to give $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\kappa^2\text{-N,N-phen})]$. Rate constants and activation parameters for these reactions have been determined and discussed. Competition studies for the $[(\eta^3\text{-C}_3\text{H}_5)\text{Mo}(\text{CO})_2(\text{X})(\text{py})]$ intermediates show that these transients are highly reactive and react almost indiscriminately with both py and phen.

Key Words: *Molybdenum hexacarbonyl ; kinetics; allyl ; competition ratios*

INVESTIGATION OF SENSITIVITY PRECISION of SMALLER PARTICLES THROUGH THE ASYMMETRIC NANOPORES

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Abstract

Resistive pulse sensing, based on the Coulter Counter principle, is an important assay for sensing and separation processes to detect/discriminate several types of particles in various mediums. It has been used to reveal the characteristics and translocational behaviours of biomolecules such as DNA, proteins and viruses[1-3]. It can also be implemented for observing drug delivery or desalination. Parameters the system is built on are applied potential, pressure, ionic density, surface charge density and pore geometry which are constructed for simulation by coupling of the PNP (Poisson-Nernst-Planck) and Navier-Stokes equations.

Particle detection by using the nanopore system can be difficult as attaining signal from the smaller particles can be hard among larger particles. In this work, we focus on the critical role of pore shape on signal precision. We have simulated hourglass and cigar shaped nanopores to exhibit the smallest particle sensitivity based on our previous study[4, 5, 6]. We have considered the translocation of 120 nm diameter particle by altering the surface charge as -0.001 C/m^2 , -0.007 C/m^2 and -0.015 C/m^2 under the applied potential between -0.1 V and -1 V with 0.1 increments to show the sensitivity variations corresponding to applied potential. Comparison of pulse magnitudes and normalized current changes yielded from each pore shape shows the cigar shaped pore yields larger signal values for smaller sized particles than the hourglass pore with the increasing potential. However signal differences are stronger from hourglass pore than cigar shape. Namely, our results state that the hourglass pore has higher sensitivity than cigar shape and more preferable asymmetric nanopore geometry option to detect the smaller particles than cigar shaped pores.

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INCREASED SOLUBILITY AND EFFICACY OF WATER INSOLUBLE FLAVONOIDS WITH N,N-DIMETHYLALKYL GROUPS CARRYING CALIX[N]ARENES

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Calixarenes are synthesized through base catalyzed electrophilic aromatic substitutions via condensation of *p*-substituted phenols with formaldehyde an important class of building blocks. These cyclic compounds are readily available on a large scale and have almost limitless possibilities for chemical modification. Moreover, in recent years, supramolecular chemistry has gained large attention in drug delivery system and enhancement of solubility of the water insoluble drugs [1,2]. Flavonoids are micronutrients that are widely identified in foods of plant origin and have been recognized potent antioxidants, possessing bioactive potential to reduce cancer risk, prevent cardiovascular disease, and neurodegenerative disorders. Because of poor water solubility of these flavanones make it less bioactive. The aim of this study is to synthesis new water soluble calixarene derivatives using N,N-dimethylalkyl groups carrying calix[n]arenes and investigate their cytotoxic potential on human carcinoma cells. Besides, water solubility of naturally occurring flavonoid compound; quercetin was also increased and tried to increase its stability. The mechanism of cell death and cell cycle were also clarified. Due to host-guest interaction with, N,N-dimethyl group carrying *p*-sulfocalix[n]arenes stability and efficacy of quercetin against human cervical cell (HeLa) were increased. Quercetin was loaded in physiologic pH (pH 7,4) and released at acidic pH (cancerous cells have pH at 5-6). The IC₅₀ values of quercetin, *p*-sulfocalix[4]arenes and *p*-sulfocalix[8]arenes were calculated as 27.45μM, 219 μM and 298.4 μM, respectively. On the other hand, the cytotoxicity of quercetin-*p*-sulfocalix[n]arene complexes significantly increased to 13.85 μM (1.98-fold) and 8.97 μM (3.06-fold). In conclusions, *p*-sulfocalix[n]arene derivatives may be an important candidate for stability and efficacy of water insoluble compounds. It is also be evaluated as drug carrier molecules.

Key Words: Calixarenes, flavonoids, cervical cancer, Apoptosis, Cytotoxicity

Acknowledgement: This project was supported by TUBITAK (116Z933).

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THE INFLUENCE OF CHEMICAL COMPOSITION ON PEROXIDATION KINETICS OF PALM AND NUT OILS

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Abstract

Knowing the fatty-acid content of vegetable oils is important for industrial use in terms of determining their lipid-oxidation time and food quality [1]. In this study, the fatty-acid content of peanut, hazelnut, coconut and palm oils were determined by gas chromatography (GS-MS), and correlated to the kinetics of lipid oxidation. The peroxidation of oil emulsions was performed at in a ventilated incubation environment at 37 °C and pH 7. Primary products (hydroperoxides) were monitored by ferric thiocyanate method, and the secondary products (malondialdehyde) were analysed by thiobarbituric acid reactive substances (TBARS) analytical methods. Pseudo-first-order kinetics of hydroperoxides and aldehydes were observed in copper-catalysed oil emulsions, and the absorbance values obtained as a function of the incubation period resulted in sigmoidal curves. The rate constants found via the ferric thiocyanate method were calculated to be in the following decending order: peanut oil > hazelnut oil > palm oil > coconut oil, whereas that via TBARS method yeilded peanut oil > hazelnut oil > coconut oil > palm oil. This study demonstrated that it is possible to use foods that have a long shelf life by evaluating the fatty-acid content and the peroxidation kinetic data together.

Key Words: *Ferric Thiocyanate Method, Palm oil, Coconut oil, Lipid Peroxidation, Fatty Acids*

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NON LINEAR PHENOMENA IN CELLULAR AUTOMATA SIMULATIONS OF METAL CORROSION AND PASSIVITY.

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Abstract

We review our simulation results for the passivation and corrosion processes for most valve metal interfaces with an electrolyte and oxidant solution. Our approach is based on a cellular automata methodology both in 2D and 3D. The simulation results give qualitatively correct description of three groups of phenomena occurring on the surface of valve metal electrodes in contact with electrolyte: spontaneous microcell structure (MCSF) formation at a corrosion potential [1,2], nanopore formation (NPF) on anodized alumina [3,4], electric potential (V) or electric current (I) oscillations (VIO) in passivating systems [5,6]. We show that these phenomena emerge from simple and well understood phenomenology that can be effectively coded at a mesoscopic level as a cellular automaton model. In such an approach we can efficiently handle the inherent nonlinearity of the problems. We argue that the common feature of these systems is a characteristic length at which the surface structures appear both in the transient and stationary regimes. This is best understood for the MCSF in terms of the competition between pair creation and pair annihilation processes that take place at the corroding surface for acidic anodic and basic cathodic solutions appearing at the corroding surface. However, our recent study in a 2D system reveals a somewhat more complex mechanism occurring at different length scales for stationary regime [2]. The appearance of the length scales in NPF and VIO is less clear but still some tentative propositions can be formulated. Future developments in this type of modelling for the three phenomena MCSF, NPF and VIO are also outlined.

Key Words: *Corrosion and passivation; microcell structure; nanopore formation; electrochemical oscillations; cellular automata based simulations.*

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IN SITU SYNTHESIS OF TRIGLYCERIDE OIL BASED POLYMER CLAY NANOCOMPOSITE

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Abstract

Polymer-clay nanocomposites have been attracted a great deal of attention due to their excellent properties such as high dimensional stability, thermal resistance, gas barrier performance, optical clarity, flame retardancy, and enhanced mechanical properties [1-5]. In this study, oil based polymer-clay nanocomposites (OBPCNs) were synthesized by in-situ polymerization of oil based vinyl macromonomer with styrene in the presence of clay. The macromonomer was obtained by combining 2-hydroxyethyl methacrylate (HEMA) with partial glycerides. Then, the obtained macromonomer was copolymerized with styrene in the presence of organically modified clay. For the modification of clay, hexadecyltrimethylammonium (HDTMA) was used. Various amounts of clay were studied to determine the effect of clay content on nanocomposite properties. In order to facilitate the clay dispersion mixing was carried out by sonication besides classical mixing. The structure of the oil based polymer clay nanocomposites were characterized by transmission electron microscopy (TEM), X-ray diffraction spectroscopy (XRD), and Fourier transform infrared spectroscopy (FTIR). Thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC) analysis were also applied for determination of the thermal characteristics. It was understood that triglyceride oil could be used for the preparation of nanocomposite product.

Key Words: *Oil based polymer-clay nanocomposites, in-situ polymerization, sonication, renewable source.*

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NEW METHOD FOR THE SYNTHESIS OF THE 1,5-METHANOAZOCINO[4,3-B]INDOLE BY INTRAMOLECULAR CYCLIZATION OF -1,2,3,4-TETRAHYDROCARBAZOLES MEDIATED BY TETRACHLORO-1,4-BENZOQUINONE

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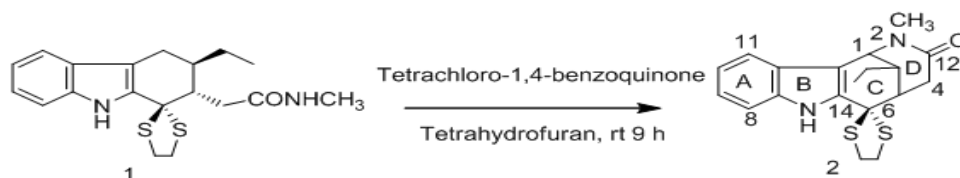
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Abstract

The 1,5-methanoazocino[4,3-b]indole is one of the most-important biological subgroup of the Strychnos alkaloids.¹ It is present in the unique structural features of their methanoazocino[4,3-b]indole tetracyclic ring system (ABCD rings). For these reason, it has been primary target molecules toward strychnos alkaloids such as tubifolidine,² aspidosperimidine,³ uleine,⁴ and epidaycarpidone.⁵

In this study, 12-Ethyl-2-methyl-6,6-ethylenedithio-1,2,3,4,5,6-hexahydro-1,5-methanoazocino[4,3-b]indole-3-one (2) was synthesized in a one-pot reaction of (N-methyl){3-β-ethyl-2,3,4,9-tetrahydro[1H-carbazole-1,2' (1,3)dithiolane]2-yl}-acetamide (1) using tetrachloro-1,4-benzoquinone and tetrafluoro-1,4-benzoquinone. This new reaction represents an improved alternative to the previously reported through a dehydrogenation activating of tetrahydrocarbazoles mediated by tetrachloro-1,4-benzoquinone and tetrafluoro-1,4-benzoquinone for a new cyclization procedure.



Key Words: *alkaloids; indole; uleine; strychnos alkaloids; dasycarpidone*

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INVESTIGATION OF CHANGES IN ANTIOXIDANT ACTIVITY OF SOME *PLEUROTUS* SPECIES BY USING COMPOSTS INCLUDING DIFFERENT METAL SALTS

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Abstract

Nowadays, high content of antioxidants in plants and mushrooms is the reason for choosing a healthy life. Is the change in antioxidant activity in mushroom cultivation related to the metal values found in the compost? [1] In order to find out the answer to this question, antioxidant activities of *Pleurotus ostreatus* and *Pleurotus citrinopileatus* grown with the addition of different metal salts to cotton compost media were determined by using DPPH method and total phenolic content was determined using Folin Ciocalteu method. In addition, metal analyzes of mushroom samples were determined using ICP-OES. Results showed that *P. citrinopileatus* had higher antioxidant activity than *P. ostreatus*. In both fungus species, IC₅₀ values antioxidant activities were found to be Fe> Ca> Pure Water> Na> K in terms of DPPH damping. In the same way, the total phenolic values were followed by Fe> Ca> Pure Water> Na> K order for both mushroom species. These results showed that divalent Fe and Ca metals are important for the development of antioxidant activities in mushroom cultivation.

Key Words: *Pleurotus ostreatus*, *Pleurotus citrinopileatus*, antioxidant activity, total phenolics

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A THEORETICAL STUDY OF THE REACTION OF DIMETHYL PHOSPHORAMIDATE WITH HYDROXYL RADICALS

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Phosphoramidates are important class of organophosphorus compounds with a wide range of biological activity [1]. They find extensive usage areas in medicine as anticancer, inhibitors antihepatitis C virus, in industry as flame retardants, oil additives and in agriculture as pesticides [2, 3]. However the increasing usage over time has led to serious environmental problems. Because of their toxic character the persistence of them in aqueous environment have a public concern. [4,5]. Hence, removal of these compounds from the environment is important task.

In this study, the kinetics of the reactions of OH radicals with dimethyl phosphoramidate have been investigated theoretically. The geometry optimization of the reactants, product radicals, pre-reactive and transition state complexes were performed with the DFT method within the Gaussian 09 package. The DFT calculations were carried out by the hybrid B3LYP functional with 6-31G (d) basis set. The solvation effect was computed using CPCM as the solvation model. The rate constants of all the possible reaction paths have been calculated by means of the Transition State Theory.

Based on the results of the quantum mechanical calculations, the most probable route, branching ratios and the product distributions of all the possible reaction paths were determined.

Key Words: *Phosphoramidates, OH radicals, DFT, solvation effect, kinetics.*

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SINGLE ENANTIOMER THIOUREAS AS CHIRAL SOLVATING AGENTS

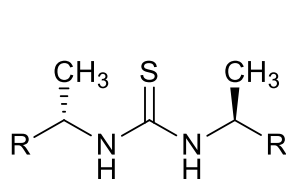
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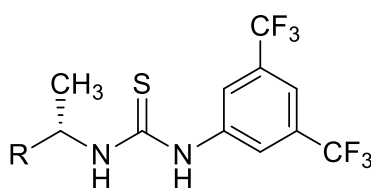
Abstract

Chirality plays an essential role in synthetic and medicinal chemistry. Therefore, assignment of the chirality of molecules is very important and has been an extensively studied area. NMR spectroscopy using chiral solvating agents (CSAs) is one of the most convenient methods because the enantiomeric purity can be determined easily and rapidly.

In recent years, chiral thioureas received considerable interest for their use in various asymmetric reactions as organocatalysts [1]. However, there are few reports on their use as CSAs [2]. In this work, structurally simple chiral thioureas [3] have been investigated as CSAs for the enantiodiscrimination of carboxylic acids in the presence of DMAP. Furthermore, the effect of structure of the thioureas on the discriminating ability has been examined.



R= naphthyl; phenyl; cyclohexyl



R= naphthyl; cyclohexyl

Key Words: *Chiral Solvating agents; chirality; thioureas; enantiodiscrimination; carboxylic acids*

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THE TREATMENT OF DETERGENT INDUSTRY WASTEWATERS BY SUPERCRITICAL WATER OXIDATION

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Abstract

Synthetic household detergents, whose production and consumption have increased dramatically nowadays, are one of the most hazardous environmental pollution sources. When the wastewaters of this industry are discharged to the environment without being subjected to adequate treatment, they cause undesired conditions such as the decrease of oxygen in aquatic media, eutrophication and contamination of drinking water [1]. In the recent years, environmental regulations have begun to be stricter due to the increased sensitivity towards ecological risks and health regarding environmental pollution. Therefore, advanced treatment technologies have been developed to meet these rules, for the treatment of wastewaters containing difficult-to-decompose and/or toxic contaminants [2]. One of these promising technologies is supercritical water oxidation. During the process, organic matter reacts with oxygen at conditions exceeding the critical point of water (374°C and 22.1 MPa). Under these circumstances, water behaves as solvent with a low polarity, in which molecular oxygen and organic compounds are completely miscible. Its diffusivity increases and viscosity decreases, causing increased thermal reaction rates. Hence, supercritical water oxidation can rapidly and efficiently decompose organic substances into carbon dioxide and water, in very short reaction times [3-5]. This study presents the results of our research regarding the treatment of detergent industry wastewaters by supercritical water oxidation. Hydrogen peroxide was used as the oxygen source. The experiments were carried out in the temperature range of 400-600°C and for the reaction time range of 60-150 s, at a constant pressure of 25 MPa. The effects of temperature, reaction time and oxidant use on the total organic carbon, inorganic carbon and total nitrogen contents of the liquid effluents were examined. As a result, it was seen that supercritical water oxidation was a very effective method for the treatment of detergent industry wastewater. Treatment efficiencies up to 97% in terms of total organic carbon conversion, 99.5% in terms of inorganic carbon conversion and 99.7% in terms of total nitrogen conversion were achieved, in very short reaction times.

Key Words: *Detergent industry; Oxidation; Supercritical water; Treatment; Wastewater*

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REMOVAL OF BENTAZON AND METALAXYL PESTICIDES FROM AQUEOUS SOLUTIONS BY ALMOND AND CHESTNUT SHELLS: OPTIMIZATION, KINETICS AND ISOTHERM STUDIES

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Abstract

Pesticides are chemicals that have been used since 1940s for raising the food quality and minimize the loss of agricultural products against some of the problems in the agricultural industry such as weeds, insects and funguses. Due to its easy application and effectiveness in a short period of time, the usage of pesticides has been increased with the increase of world population which leads to nutritional requirements. Because of intensive and insensible usage of pesticides, they contaminate to the water resources in the consequences of run-off and percolation from agriculture field and also that careless and insensible disposal of wastewaters to environment by pesticide producers. Pesticide concentrations of wastewaters from those industries can sometimes reach up to high and dangerous levels such as almost 500 mg/L [1-3].

In the present study, the usability of agricultural wastes almond and chestnut shells as adsorbents for the removal of Bentazon and Metalaxyl pesticides from aqueous solutions were investigated. By using Box-Behnken experimental design, effects of pH (2.0, 3.5 and 5.0), adsorbent concentration (1.0, 2.0 and 3.0 g/50 ml), pesticide concentration (25, 50 and 75 mg/L) and processing time (40, 80 and 120 minutes) on adsorption were investigated and optimizations of the adsorption processes were performed. At the determined optimum conditions 70.3% and 85.1 % Bentazon and 33.3% and 66.1% Metalaxyl removals were obtained with almond and chestnut shells respectively. Also model equations that shows the effects of process parameters and the interactions between them on adsorption were obtained. As a result of the analysing the data obtained from the kinetics and equilibrium studies it was determined that the adsorption of Bentazon and Metalaxyl with almond and chestnut shells could be represented with pseudo-second kinetic and Freundlich isotherm models. The results obtained from this study suggested that the agricultural wastes almond and chestnut shells could be used as cheap and easily accessible adsorbents for the removal of pesticides from waste waters.

Key Words: *Bentazon, metalaxyl, adsorption, experimental design, modelling*

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BIOSORPTION OF REMAZOL ORANGE RGB BY KEFIR BIOMASS UNDER SONICATION

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Abstract

Synthetic dyes are highly stable chemical compounds discharge into naturel water bodies by textile industries. Worldwide annual production of dyes are approximately 700 000 tons and due to inefficiencies of the colouring processes around 10-15% of dyes are lost directly on the wastewater. The pollution by dyes leads to reduction of sunlight penetration that adversely affect the aquatic life. Moreover, most of dyes and their breakdown products are toxic, carcinogenic and harmful to public health. Hence they have to be treated properly before they are discharged to the receiving waters. Several physical or chemical treatment processes have been used with varying degree of success for the removal of dyes from wastewater. Recently, studies have focused on microbial biomass as the treatment by microorganisms is cost effective and environmentally friendly [1- 5].

In the present study, the biosorption of reactive dye Remazol Orange RGB by kefir biomass under sonication was studied. The effects of pH, initial dye concentration and temperature on biosorption were evaluated. Also modelling studies were performed in order to determine the most appropriate kinetic and isotherm models to represent the dye biosorption by kefir biomass. It is determined that the sonication significantly increased the biosorption performance of kefir biomass.

Keywords: *Biosorption, kefir biomass, Remazol Orange RGB, sonication, modelling*

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DEVELOPMENT OF CHITOSAN-BASED EDIBLE BIOCOMPOSITE FILMS INCORPORATED WITH KUMQUAT PEELS EXTRACT AS FOOD PACKAGING

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Abstract

This work focused, the potential of being edible and biodegradable film with properties that can be used as food packaging with chitosan biopolymer of peel extract of kumquat fruit of the family of citrus fruits, especially rich in vitamin C, which is known to have many benefits for human health has been investigated. Edible films incorporate with various ratio of kumquat peel extract were prepared by using solvent casting techniques. In order to determine the effect of kumquat peel concentration, the biofilms have been characterized by physical properties such as moisture content, swelling degree, water solubility, water vapour permeability, colour and transparency as their structures were confirmed by FTIR and SEM. In addition, the mechanical properties have been determined with the tensile strength and elongation in terms of breakage of the prepared films.

It has been observed that the amount of moisture, swelling, and solubility of the films changed between (30.95-22.05%), (177.96-24.8%) and (34.58-54.47%) respectively. It has been observed that the amount of moisture and the degree of swelling of the films decreased and the solubility values increased with the increase of kumquat peel extract. The water vapour permeability, thickness and density values of the films have been as follows: ($1.039 \text{ g H}_2\text{O Pa}^{-1}\text{s}^{-1}\text{m}^{-1}$ and $0.989 \text{ g H}_2\text{O Pa}^{-1}\text{s}^{-1}\text{m}^{-1}$), respectively. It has been determined that the ratio of kumquat bark extract does not cause a significant change on the water vapour permeability, thickness and density values of the films. With the increasing of the concentration of the Kumquat peel extract in the film structure, it has been observed that the films exhibit a more flexible property and the tensile strength at 33.28-13.5 MPa has been observed to vary between 7.74% and 20.57. Results indicate that the chitosan-based films incorporated with kumquat peel extract can be an alternative for food packaging.

Key Words: *Chitosan, kumquat, edible film, biopolymer, food packaging*

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PRODUCTION and *IN VITRO* CHARACTERIZATION of VARIOUSLY DOPED and FORMED S53P4 BIOACTIVE GLASS

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Abstract

Cause of various diseases and increasing age-related damages, the bones are suffering from disorders that cannot be treated by natural means. Artificial bone materials are used to supporting physically, chemically and biologically damaged zones or replacing them for ensure continuance of performance in the treatment of disorders such as fractures and physical changes caused by natural processes or due to certain diseases [1]. One of the studies carried out to restore the specific functions of the zone in terms of biological and mechanical aspects of the damaged region with various approaches is the use of bioactive glass with functions similar to the damaged bone tissue. Bioactive glasses are silicate glasses with sodium, calcium and phosphate in their composition. These materials in the ceramic class of biomaterials show inorganic properties [2]. They are also designed to be used for medical purposes, and they have a strong bond with bone tissue thanks to their bioactive properties. Bioactive glasses have biocompatible, bioactive, and osteoconductive because of these properties they perform perfectly in bone tissue regeneration [3]. These materials are able to bind to the bone through the formation of the hydroxyapatite layer on their surfaces when placed in the human body. Some elements such as Mg, Zn, K etc. can be used chemical composition of bioactive glass as additives in order to improve bone production properties of these materials [4].

In this study, it was aimed to produce by melt-quenching method non-additive ($\text{SiO}_2\text{-Na}_2\text{O-P}_2\text{O}_5\text{-CaO}$) and additive ($\text{SiO}_2\text{-Na}_2\text{O-P}_2\text{O}_5\text{-CaO-MgO-Zn}_2\text{O-K}_2\text{O-CuO}$) bioactive glasses (different forms; powder and granule). Vickers Hardness analysis of doped and undoped bioactive glasses were carried out. In additional, Brunauer-Emmett-Teller (BET) surface areas, pore sizes of powder bioactive glasses were determined with N_2 adsorption-desorption analysis. *In vitro* bioactivity properties of bioactive glasses in different forms (granule and powder) were examined with Simulated Body Fluid (SBF) and TRIS-HCl analyses and compared with each other. Chemical bonds structures and surface morphology analysis of bioactive glasses (both additive and non-additive) were performed with FT-IR and SEM-EDS before and after SBF immersion, respectively. Vickers Hardness analysis shows that doped bioactive glasses (~499 HV) have better Vickers Hardness than undoped bioactive glass (~387 HV). As a results of TRIS-HCl studies, *in vitro* bioactivity of bioactive glasses in powder forms are better than bioactive glasses in granule forms because of rapid raise of its pH value in TRIS-HCl.

Key Words: *Bioactive glass, doped, melt-quenching method, various forms, simulated body fluid*

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ABSORPTION OF GLYPHOSATE-IPA HERBICIDE ON MESOPOROUS SILICA NANOPARTICLES

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Abstract

Mesoporous silica nanoparticles (MSNs) have attracted more attention for their uniform pore size, large surface area, tailored mesoporous structure, non-toxicity and biocompatibility, and their important application areas such as targeted drug delivery, controlled release, absorption of organic and inorganic substances and heterogeneous catalyst in the past two decades [1]. Glyphosate (N-(phosphonomethyl) glycine) was introduced by Monsanto (USA) to the world around 1975. Glyphosate and its derivatives is the most frequently used herbicide in both agricultural and non-agricultural areas all over the world. It was entered to soil, groundwater and under groundwater via various route during its manufacture and applications. Many cases of its poisoning in humans, with a variety of symptoms including eye and skin irritation, contact dermatitis, eczema, cardiac and respiratory problems and allergic reactions, increased the concern of its health impacts [2]. In addition, glyphosate is highly water soluble and could be mobile in aquatic systems. Recently, soil contamination with a glyphosate derivative was detected in the concentration range of 12.00-45.2 μmgL^{-1} in natural soil of Eastern black sea region of Turkey [3]. More recently, four different “Round up” formulations of the glyphosate manufactured by Monsanto were found highly toxic to human cells at concentrations far below the recommended agricultural use levels [4].

In the present study, one of ordered MSNs, SBA-15 was synthesized by sol-gel method and named as bare-SBA-15. It was modified 3-aminopropyl triethoxysilane (APTES) and named as APTES-SBA-15. Structures of synthesized bare-SBA-15 and APTES-SBA-15 were identified by BET (N_2 adsorption-desorption), XRD, FTIR and TGA techniques. After that, absorption of glyphosate isopropylamine (Gly-IPA) on bare-SBA-15 and APTES-SBA-15 were investigated. According to the TGA results, amount of the adsorbed Gly-IPA by bare-SBA-15 and APTES-SBA-15 were found to be about %72 and % 62, respectively. The results also indicate that glyphosate-ipa herbicide can be absorbed by a type of ordered mesoporous silica nanoparticle SBA-15 and surface modified APTES-SBA-15 and they can be progressed as adsorbent to remove residual pesticides from aquatic systems.

Key Words: *Mesoporous silica nanoparticle; SBA-15; APTES-SBA-15; Sol-gel method; 3-aminopropyl triethoxysilan(APTES); Glyphosate; Herbicide.*

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STRUCTURAL AND ELECTRONIC PROPERTIES OF LAYERED SEMICONDUCTOR CHALCOGENIDE CRYSTALS: TlGaSe₂, TlGaS₂, AND TlInS₂

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Abstract

We report the density functional theory structure optimization and electronic structure calculations of TlGaSe₂, TlGaS₂, and TlInS₂ compounds. We find that there is a weak bonding between Tl and the chalcogen while Ga and In make covalent bonds with the chalcogen. The s orbitals of the chalcogen hybridize with the d orbitals of Tl, bringing additional directionality to the Tl-chalcogen interaction. There is no direct Tl-Tl bond. Although these three compounds are extremely similar, the band structures exhibit quantitative and qualitative differences. The optimized TlGaSe₂ and TlInS₂ crystals have direct band gaps while TlGaS₂ has an indirect gap. The lowest unoccupied states have a bonding character between the p orbitals of the adjacent Tl atoms. These states form conduction channels along the Tl chains. The valence band maximum originates from Tl-s orbitals and its position in the Brillouin zone is robust. Almost degenerate Tl-p related bands are affected differently by the inter-layer interaction. Therefore, minute changes in the structure may shuffle their energy levels, resulting in qualitatively and quantitatively different band gaps in these extremely similar compounds. External pressure and defects may initiate the same type of electronic structure changes resulting in contradicting results in experiments. A small downshifting of the unoccupied parabolic bands lead to several valleys in the conduction band of TlGaSe₂.

Key Words: Ternary semiconductor chalcogenides, Layered crystal, Electronic structure

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EFFECTS OF FLUE GAS AS A CO₂ SOURCE ON THE CULTIVATION OF *CHLORELLA PROTOTHECOIDES*

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Abstract

Nowadays, the interest in the cultivation of microalgae found in a group of aquacultures is increasing. The first reason of this interest is that microalgae, can be evaluated in different fields as food supplements due to being rich in carbohydrates, proteins and especially high fatty acids contents [1]. Microalgae can also be used as fertilizer, biomass, forage and source of pigment thanks to their rich content of important components. The second reason is that microalgae reduces CO₂ emissions via photosynthesis like plants do. Increasing concerns about global warming and greenhouse gas emissions have led scientists to find new alternative ways to minimise the release of CO₂ gas, which has a share of approximately 70% in greenhouse gas emissions, as a result of industrial processes. The Kyoto protocol also calls attention to this issue [2].

In recent years, fossil-based fuels have been used in order to supply the energy needs of the constantly increased population of the World. The global climate change, which is caused by the accumulation of CO₂ gas in the atmosphere caused by these fossil fuels, makes the use of renewable energy resources inevitable. Microalgae are one of the organisms capable of absorbing air pollutants such as CO₂, NO₂, and SO₂ [2]. They have an incontrovertible potential for biodiesel production thanks to their fatty acids composition. However, researches have shown that biodiesel from microalgal biomass can be more economic by using CO₂ in fossil fuel-based flue gas and solar energy as a natural light source [3].

In this study, the effect of flue gas on cell growth and lipid content of *Chlorella protothecoides* were investigated. Microalgae grown on different nutrient media was produced in the flue gas ambient. In addition, dry matter, optical density, cell count analysis was performed daily, and growth kinetics were examined. Temperature and pH values were fixed to the optimum level (28°C, 7.2-7.5) to ensure high algal populations. Further, the experiments were repeated with air and pure CO₂, the comparison was investigated with the kinetics of microalgae which grown with pure CO₂. The results of cultures fed with flue gas showed similarities with those fed with pure CO₂ gas. When CO₂ free medium compared with the mediums containing 10% and 15% CO₂, it was seen that algae culture containing 15% CO₂ reached the highest density with 3.42 optical density at the end of 12th day. The lipid content of cultures fed with flue gas and CO₂ were, 44% and 45% respectively. All these results showed that direct flue gas can be used as a carbon source and *Chlorella Protothecoides* has great potential of reducing CO₂ emission.

Key Words: *Chlorella Protothecoides*, microalgae, CO₂ emission, flue gas, oil

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EFFECTS OF THE SOME PARAMETERS ON THE ASTAXANTHIN PRODUCTIVITY FROM *HAEMATOCOCCUS PLUVIALIS* ALGAE

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Abstract

Microalgae are microorganisms that grow in water and are generally rich in carbohydrates, proteins, lipids and vitamins. Microalgae are used in many different fields such as food industry, cosmetics, health, animal feeds, fertilizer and water treatment. It is also a good source of pigment used in coloring [1]. Microalgae commonly used in recent studies; *Chlorella vulgaris*, *Spirulina platensis*, *Haematococcus pluvialis*, etc. Astaxanthin is a high antioxidant red carotenoid pigment obtained from many marine organisms (crustacean) and some microalgae. It is an important preservative of the immune system and it is used in the treatment of cancer, skin and heart diseases. For these reasons, the importance of astaxanthin has increased. The most efficient source of astaxanthin is *Haematococcus pluvialis* microalgae [2].

In this study, the efficiency of the production of astaxanthin in microalgae of *Haematococcus pluvialis* was investigated. Many different parameters are effective for the production of astaxanthin, such as culture species, medium, light, and nitrogen effect. The growth conditions of *Haematococcus pluvialis* microalgae has been achieved primarily with Bold Basal media and Bristol media under specific light intensity (36W) at 27±2°C [3]. Firstly, algae was produced on solid culture media and then culture was transferred to liquid medium after 15 days. Moreover, stress conditions were applied to the culture medium and the increase of astaxanthin production from *Haematococcus pluvialis* microalgae was measured. The stress conditions were addition of tap water and iron, application of light and also nitrogen deficiency in both Bold Basal medium and Bristol medium. The effect of stress conditions on the production efficiency of nitrogen deficiency media and tap water; OD measurements and cell counts were evaluated by measurement of the amount of dry matter and the amount of astaxanthin. The results in this study; the *Haematococcus pluvialis* microalgae in Bold Basal medium was found to be more efficient than Bristol media. When the yield of astaxanthin accumulation in stress conditions was examined, nitrogen deficiency of Bristol media was found to be advantageous. Using tap water has been also found advantageous in terms of cost but accumulation of astaxanthin was similar in Bold nitrogen-free basal medium. In a stress environment nitrogen deficiency Bristol environment, the light intensity was doubled, and a comparative experiment was performed. After 12 days, these two experiments showed the same result. As a conclusion, doubling the light intensity did not show an advantage. In addition, more efficient results have been achieved by applying agitation in both feed media.

Key Words: Algae, *Haematococcus pluvialis*, astaxanthin production, stress, medium.

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SILVER NANOPARTICLES AS A SCAVENGING MATERIAL FOR NEW ASSAY FOR POLYPHENOLS METAL SCAVENGING ACTIVITY

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Abstract: Polyphenols are widely used in numerous applications they are synthesized in plants as secondary major metabolites, their structures are exceedingly varied, they have many roles and functions in the plants, they are also very useful in many practical applications [1]. The common in the structure of polyphenols is they have aromatic rings with several hydroxyl groups attached to them. Their role includes their participation in self-defense external pathogens and extreme conditions such as UV light. They can be classified into four categories: (i) phenolic acids, (ii) flavonoids, (iii) stilbenes, and (iv) lignans. The classification is based on the number of phenolic rings they contain as well as the structural elements that binds these phenolic rings [2]. Antioxidant and anti-inflammatory activities are very old identified character of polyphenols, many other biological functions have been identified and they have been attributed to a particular structure of the polyphenols. Namely the wide resonance structure they have with attached hydroxyl groups make them very good electron donors or acceptors, scavenging radicals and other reactive oxygen species (ROS) [3]. The antioxidant activity was widely studied by using different assays, namely H_2O_2 , OH^\cdot , iron scavenging activity, 2,2-diphenyl-1-picrylhydrazyl (DPPH), reducing antioxidant power (FRAP), oxygen radical absorbance capacity (ORAC) and photochemiluminescence (PCL). However, none of these in vitro methods, individually or collectively are relevant to the actual physiology of the human body [3]. This paper attempts to establish a correlation between the polyphenols content of natural antioxidant and ability to form silver nanoparticles without using reducing agent. Moreover, silver nanoparticles formation was assessed by their surface plasmon resonance, optimization experiments were also conducted for the kinetic, the concentration of plant extract and pH. Extracts of Turmeric, ginger, garlic, cinnamon and henna were used as natural antioxidants for the preparation of silver nanoparticles.

Biography

Dr Abdelaziz Elgamouz is bioanalytical chemist in the department of chemistry, University of Sharjah, Prior to joining the University of Sharjah in UAE, Dr Abdelaziz was an associate researcher in the University of Surrey UK, where he spends more than 5 years working on Coordination chemistry of macrocyclic ligands. He is expert in designing new macrocyclic ligands that stem mainly from their use as models for protein-metal binding sites in a substantial array of metalloprotein in biological systems. Recently he has shifted his interest to bioassays such as synthesis of nanoparticles for hydrogen peroxide detection.

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Category: (Oral presentation)

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THERMOELECTRIC PROPERTIES OF POLY (3,4-ETHYLENE DIOXYTHIOPHENE)/TITANIUM DISULPHIDE COMPOSITES

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Abstract

Thermoelectric (TE) generators can directly produce electricity by harvesting thermal energy from solar heat, radioactive decay, body heat, thermal springs and industrial waste heat, etc. for practical applications [1]. Among the renewable energy technologies, TE process is the simplest and easy to maintain without pollutants and noise. The state-of-the-art TE materials which are alloys such as bismuth-telluride and lead-telluride cannot be used widely for large-scale applications due to their high toxicity and high production costs. The production of novel cheap and environmentally benign TE materials is very attractive research area, nowadays.

The studies conducted so far have shown that poly (3,4-ethylenedioxy thiophene) (PEDOT) is the most promising candidate for a conductive polymer that is non-toxic and has a low processing cost [2,3]. However, since the efficiency of pristine PEDOT is not high enough, research has now focused on the production of efficient TE materials from its composites [4].

TE properties of PEDOT:PSSA/titanium disulfide composites were studied in the present study. At first, PEDOT was synthesized by chemical oxidation of 3,4-ethylene dioxy thiophene with hydrogen peroxide at room temperature in the presence of polystyrene sulfonic acid (PSSA). Then, titanium disulfide was introduced into the PEDOT:PSSA dispersion in various ratios. The TE efficiency of the composites was estimated by measuring their electrical conductivity and Seebeck coefficient. It was found that the synthesized PEDOT:PSSA/titanium disulfide composites displayed an enhanced TE performance compared to that of pristine PEDOT:PSSA. To the best of our knowledge, this is the first study on the thermoelectric behavior of PEDOT:PSSA/ titanium disulfide composites.

Key Words: *poly (3,4-ethylene dioxythiophene)(PEDOT); titanium disulfide; thermoelectric; composite; thermopower*

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A HIGHLY SELECTIVE NON-ENZYMATIC H₂O₂ SENSOR SUPPORTED ON EUPERGIT CM DECORATED WITH PDMOAG NANOPARTICLES

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Abstract

At present, Pd, Mo and Ag multimetallic nanoparticles were synthesized by the chemical reduction method based on the dissolution of metal salts and the reduction of these metal salts to zero valence [1]. Novel Eupergit CM supported Pd, Mo, and Ag multimetallic nanoparticles were characterized with X-ray Diffraction (XRD), Energy Dispersive X-ray Spectroscopy (EDS) and Scanning Electron Microscopy (SEM) technics. The electrochemical behaviour of the modified electrode was investigated by Cyclic Voltammetry (CV) and Chronoamperometry (CA). The effect of third metal addition was examined through electrochemical Hydrogen peroxide (H₂O₂) sensing ability. The resulting sensor exhibits high sensitivity, good reproducibility, and long-term storage stability. Several milk samples were analyzed for their H₂O₂ contents using a PdMoAg/ Eupergit CM sensor system. The contents were determined using the standard addition method. As could be seen, there was a close relationship between the values found for the H₂O₂ measurements in the sensor and those real values on the sample. The resulting PdMoAg/ Eupergit CM nanocatalysts offer new features for electrochemical devices due to the synergistic effect of trimetallic nanoparticles.

Key Words: Multimetallic, Hydrogen peroxide, Eupergit CM, Milk

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LYOTROPIC UNIAXIAL AND BIAxIAL CHOLESTERIC PHASE PROPERTIES OF POTASSIUM ALKANOATE/DECANOL/H₂O/BRUCINE SULFATE MIXTURES

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Abstract

Cholesteric phases are one of the most common structures of the lyotropic liquid crystals. They can be prepared by adding a chiral dopant to a lyotropic mixture, presenting a nematic phase, using a chiral surfactant and dissolving the constituents in a chiral solvent [1]. The main property of the cholesteric phases is that the local directors of the micelles, which are the structural units of lyotropic liquid crystals, turn around a certain axis, so-called “helix axis”, to form a helical structure. The distance traveled by the rotation of the local directors to complete 2π -rotation is known as ‘helical pitch (P)’. Thus, the helical structure and the pitch are two important parameters to describe the lyotropic cholesteric phases.

Three types of lyotropic cholesterics were identified as being cholesteric discotic (Ch_D), cholesteric biaxial (Ch_B) and cholesteric calamitic (Ch_C) [2]. Cholesteric-to-cholesteric phase transitions in the lyotropic mixtures were widely discussed in the literature [3,4] and, experimentally, the Ch_D–Ch_B phase transition was shown to be continuous in their phase diagrams [5]. In a recent study, first order uniaxial-to-uniaxial phase transition has been also reported as proposed in an early theoretical study [6]. In all the phase diagrams, the Ch_B phase domain is located in between the Ch_D and the Ch_C domains.

In the present study, we examined the uniaxial and biaxial cholesteric phase properties of potassium alkanoate/decanol (DeOH)/water/brucine sulfate lyotropic mixtures as a function of surfactant alkyl chain length by polarizing optical microscopy. The lyotropic mixtures were composed of potassium alkanoates/decanol (DeOH)/water/brucine sulfate. Potassium alkanoate surfactants were potassium undecanoate (KC11), potassium dodecanoate (KC12) and potassium tridecanoate (KC13). The reference mixture was chosen as KC12/DeOH/water/brucine sulfate. The lyotropic mixtures were prepared by replacing some amount of KC12 with the same amount of KC11 and KC13, separately, in mole fraction, i.e. the total surfactant concentration was kept constant in each lyotropic mixture. The results indicated that the surfactant alkyl chain length is a very important parameter for the formation of different lyotropic cholesteric phases.

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EFFECT OF DOPANT LOCALIZATION IN THE MICELLES ON THE FORMATION OF UNIAXIAL AND BIAxIAL LYOTROPIC CHOLESTERIC PHASES

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Abstract

Lyotropic liquid crystals (LLCs) are obtained by dissolution of surfactant molecules in a suitable solvent under appropriate conditions of temperature, pressure and relative concentrations of the constituents of the mixtures [1]. Depending on the shape of the micelles, which are the building units of LLCs, the orientations of the local director of the micelles and arrangement of the micelles in the sample, different LLC phases are observed in the phase diagrams. From this respect, the understanding the physicochemical properties of LLC phases and the transitions between LLC phases provide new insights for researchers from their biotechnological applications point of view [2].

In the lyotropic cholesteric phases, the micelles are spatially arranged to form a helicoidal structure, where the local directors of the micelles complete 360°-turn around a certain axis, so-called “helix axis”. In terms of the micelle symmetry and orientation of the helix axis with respect to the magnetic field direction, three types of lyotropic cholesterics are identified in the literature, which are cholesteric discotic (Ch_D), cholesteric biaxial (Ch_B) and cholesteric calamitic (Ch_C) [3]. For the lyotropic mixtures including the surfactants with hydrocarbon chains, while helical axes of Ch_D and Ch_B align parallel to the magnetic field direction, the helicoidal structure in Ch_C phase is unwound by the effect of the magnetic field. From the phase transitions point of view, the Ch_D – Ch_B phase transition was shown to be continuous in their phase diagrams [4]. In addition, first order uniaxial-to-uniaxial phase transition has been also recently reported [5] as proposed theoretically [6]. In all the phase diagrams, the Ch_B phase domain exists between the Ch_D and the Ch_C domains.

In the present study, we studied the effect of dopant localization in the micelles on both the formation of the uniaxial and biaxial cholesteric phases and the phase transitions. Some specific dopant molecules were chosen and added in the lyotropic host mixture potassium laurate/undecanol/water. Some of the dopant molecules were located within the micelles, however, others at the micelle surfaces. The results indicated that the localization of the dopant molecules in the different part of the micelles affect not only the formation of the uniaxial/biaxial cholesteric phases and the phase transitions but also the induction of the cholesteric phases.

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MICELLIZATION PROPERTIES OF SOME TETRADECYLALKYLAMMONIUM BROMIDE SURFACTANTS

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Abstract

Surfactants are surface-active compounds and they are assumed to be one of the most versatile products of the chemical industry. They have applications in oil, food, soap, drug, cosmetic, mining, textile etc. industries and in high-technology fields such as electronic printing, magnetic recording, and microelectronics [1,2]. Surfactants consist of hydrophobic (water-hating) and hydrophilic (water-loving) parts [3,4]. When they are dissolved in water, they form a superstructure, so-called ‘micelle’ [5]. In that structure, the hydrophobic parts fill up the interior of the micelle, its surface is covered by the hydrophilic ones. Because the surfactants are important for the industry and biotechnology, the studies on the micellization properties of the surfactants make contributions to their applications.

In the present study, we examined the micellization properties of some tetradecylalkylammonium bromides in terms of the symmetric and asymmetric head group growth of those surfactants. For this purpose, some micellization parameters such as critical micelle concentration (cmc), degree of counterion ionization from the micelle (α), degree of counterion binding to the micelle and micellization Gibbs free energy ($\Delta_{mic}G$) were evaluated from the electrical conductivity measurements at constant temperature as a function of the additional CH₂ group in their head groups. The results indicated that the head group growth of the surfactant exhibited very important role on the micellization properties of the surfactants and the greater the head group growth after a critical point results in the penetration of some CH₂ group through the interior of the micelle.

Acknowledgment: We would like to thank The Scientific and Technological Research Council of Turkey (TUBITAK) [grant number: 217Z079] for supporting the present study.

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IMPROVING OF DYE UPTAKE AND MOISTURE ABSORPTION ABILITIES OF POLYACRYLONITRILE FIBER BY GRAFTING OF HYDROXYMETHYL METHACRYLATE

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Polyacrylonitrile (PAN) fiber among the synthetic fibers has a prominent place in the textile industry. It shows superior properties such as good thermal stability, high abrasion resistance, compatibility with polar materials because of its nitrile groups. But also, it has undesired properties such as low moisture absorption, low dyeability with different types of dyes and poor antistatic properties limit their further usage. Therefore, surface modification is needed for PAN fiber/fabric materials. So, chemically initiated grafting has been frequently considered and used for improving synthetic or natural fiber properties [1-3]. After hydroxy functional groups with the grafting of hydroxy methylmethacrylate is also incorporated to PAN structure chemically by this method, it was investigated moisture absorption and dye uptake abilities by using direct black dye of fibers having various percent graft yields. While its moisture absorption and dye uptake values increase with the increasing graft yield, dye uptake values also changed both depend on the pH of the medium. Color strength measurements were evaluated according to K/S, L*, a*, b* values and these of dyed samples were compared to washed PAN fibers of five times after dyeing.

Keywords: *poly(acrylonitrile) fiber; graft copolymerization; dye uptake, moisture absorption*

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EVALUATION OF EXTRACTION AND HPLC SEPARATION OF POLYPHENOL COMPOUNDS IN MALLOTUS OPPOSITIFOLIUS (GEISEL) MÜLL. ARG.

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Abstract

Mallotus oppositifolius (Geisler) Müll. Arg. family Euphorbiaceae is a shrub or small tree to 13 m high, widespread across tropical Africa to Madagascar. *M. oppositifolius* is traditionally used against headache, febrile pain, venereal diseases, infantile diarrhea and dysentery. The leaves mixed in an ointment with shea butter are used in wounds and ulcers healing. *M. oppositifolius* leaves are known for their richness in natural bioactive compounds, emphasizing phloroglucinol derivatives in the polyphenol complex. This class comprises compounds having two phloroglucinol units joined either through a methylene linkage or by the formation of a chroman ring. Phloroglucinol dimers (methylene-bis-aspidinol AB, mallopposinol, together with aspidinol B and methylene-bis-aspidinol) have been isolated from *M. oppositifolius*, but only *Mallotus japonicus* is examined thoroughly. At this point we found as necessary to evaluate proper extraction and chromatographic conditions for adequate analysis of polyphenol complex in *M. oppositifolius*. The extraction yield of main polyphenol components using several solvents was studied. Separation optimization was performed with different columns, mobile phases and gradients. Extraction yield, peak shape, resolution and UV spectra were monitor in order to develop HPLC-PDA fingerprint profile of polyphenol complex. The highest yield of polyphenols was obtained by ultrasound-assisted extraction using 60% aqueous methanol in ratio to the sample 50:1 or 100:1. Best resolution and peaks shape were achieved on Kromasil column in two scale gradient for 40min up to 40% phase B (2% formic acid in water and 2% formic acid in AcN used in ratio 10:90). All major components showed λ_{max} between 272nm and 288nm corresponding to the absorption of phloroglucinols. The developed extraction and chromatographic conditions would be very useful tool for researching and analyzing the polyphenol compounds in *M. oppositifolius*.

Key Words: *Mallotus oppositifolius*, extraction, polyphenols, HPLC-PDA method

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UHPLC-MS INVESTIGATION OF POLYPHENOL COMPOSITION IN *CLINOPODIUM VULGARE*

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Abstract

The present investigation was conducted to analyze and characterize the polyphenol compounds in *Clinopodium vulgare* L. herb traditional used in Bulgarian medicine as an anti-inflammatory drug. The polyphenol complex comprises mainly from representatives of the three groups of compounds: phenolic acids, flavonoid glycosides and aglycones. In this study ultrasound-assisted extraction of polyphenols with methanol was performed. The resulted extract was evaporated to dryness, resolved in 95 % methanol and divided into chloroform fraction and ethyl acetate fraction. Both fractions were subjected to Orbitrap UHPLC-mass spectrometry analysis. In the chloroform fraction the presence of flavonoid aglycones quercetin, luteolin, naringenin and apigenin was established. In the ethyl acetate fraction seven flavonoid glycosides and twelve phenolic acids were identified, some of them for the first time. They refer to rutin, quercetin-3-*O*-glucoside, luteolin-7-*O*-glucoside, luteolin-4'-*O*-glucoside, apigenin-7-*O*-rutinoside, apigenin-7-*O*-glucoside, apigenin -7-*O*-glucuronide, rosmarinic acid, o-,m-,p-coumaric acids, ferulic acid, caffeic acid, protocatechuic acid, 3,4-dihydroxyphenylpropionic acid, feruloylquinic acid, mono- and di-caffeoylquinic acids. The characteristic pattern of polyphenol complex of *Clinopodium vulgare* is due to phenolic acids as main compounds with rosmarinic acid in largest percent. It is evident, that the high antioxidant and anti-inflammatory properties of *Clinopodium vulgare* preparations could refer to the synergistic effect of the highly bioactive flavonoid glycosides and phenolic acids.

Key Words: *Clinopodium vulgare*, polyphenols, UHPLC-mass spectrometry analysis

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HYDROXYL RADICAL DECOMPOSITION REACTION OF CICLACILLIN MOLECULE

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Abstract

Today, antibiotics are the most widely used drugs are powerful drugs used to combat bacterial infections. Antibiotics can be lifesaving when used correctly. However, in the wrong bacteria or excessive use of antibiotics leads to the formation resistivity. In particular drugs used in veterinary medicine and antibiotics it may be provided both cheap and easy. This poses problems from an environmental perspective. Human and animal health in order to use drugs, particularly antibiotics, is to find the environment in several ways.

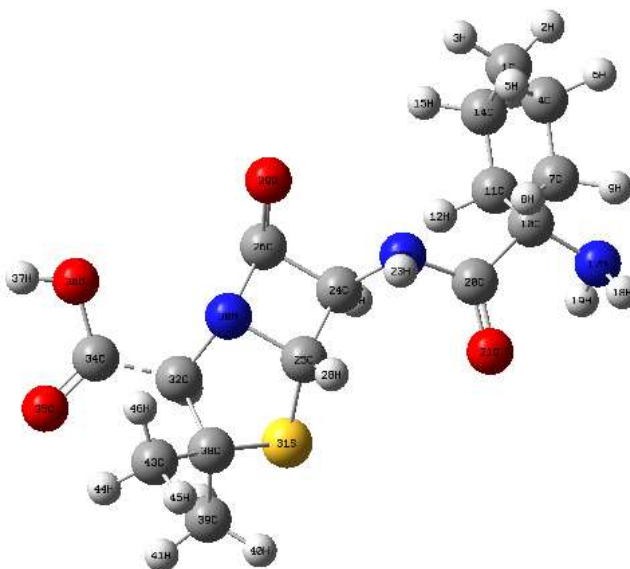


Fig. 1. Optimized structure of cyclacillin

This study examined theoretically possible reaction paths of cyclacillin toxic and water-soluble high. Optimized geometries draw with Gaussian calculations were made in Gaussian09 View 5 software package. DFT method is used in the program. Geometric structures have been analyzed and the bond lengths and bond angles are calculated. In this way, thanks to this program, which will be analyzed in greater costs in terms of material and experimental as more power is intended to calculate the theoretical.

Key Words: DFT, cyclacillin, antibiotics

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NAPROXEN DERIVATIVE INTERACTION PROPERTIES WITH CT-DNA

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Abstract

Development of the tumor cell targeted drugs is a highly motivated subject because of the DNA damaging effects of most anticancer chemotherapeutic drugs and the limited number of DNA targeted drugs relatively to the protein targeted drugs [1]. It is important to clarify the type of interaction of possible drug molecules with DNA, to provide guidance for applications as well as to understand the reaction mechanism and to design new drugs. Three main interaction modes used to characterize the organic molecule binding to DNA are electrostatic interactions, minor and major groove binding and intercalation [2-5].

Naproxen is a commonly used nonsteroidal anti-inflammatory drug (NSAID) of the propionic acid class. New generation of naproxen derivatives attract attention because of naproxen's various side effects in long term use. When the studies in the literature were examined, it was observed that the side effects were reduced in the naproxen structures where the acid group was protected [6].

In this study, microwave irradiation method, inspired by recent studies and the latest trends in the use of environmentally friendly techniques, was used as a green method in the synthesis of naproxen hydrazide. ct-DNA interactions of this synthesized naproxen derivative were systematically studied by molecular docking technique, UV-Vis absorption spectroscopy and fluorescence spectroscopy. The experimental results revealed the static quenching as a result of groove binding between the naproxen derivative and ct-DNA. Computational studies were carried out to deeper understanding of the interactions. Molecular docking calculations shown that the interaction between NH and ct-DNA is resulted by groove binding. Beside spectral data, docking studies elicited that NH-A_DNA and NH-B_DNA complexes have different interaction and conformation trends to each DNA isomer.

Key Words: *Quenching, ct-DNA, Naproxen, Stern-Volmer, Groove binding*

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FUNCTIONALIZED CLINOPTILOLITE FOR REMOVAL OF SOLUBLE DYES IN AQUEOUS SOLUTION

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Abstract

Among organic pollutants in water soluble dyes are considered as stable, persistent and harmful substances for the environment that require multiple steps treatment. Various methods have been applied for removal of dyes from wastewater such as adsorption, membrane ultrafiltration, electrochemical oxidation, photocatalysis, etc.

Recently we have aimed to prepare a low-cost and eco-friendly materials based on natural sources that can be used in water treatment. Clinoptilolite itself is well known adsorbent for many heavy metal cations, while the functionalized clinoptilolites are promising for removal of organic compounds. We have prepared new composites consisting of ZnO nanoparticles supported onto the zeolite and examined their properties in decolorization and photodegradation of methylene blue (MB). The nanocomposites were synthesized by precipitation of zinc oxalate onto zeolite followed by thermal decomposition of oxalate to nanosized ZnO loaded on the clinoptilolite. The phase composition, morphology, surface area and surface chemistry were studied by set of methods XRD, SEM, FT-IR, XPS, BET. Additionally, we have evaluated the decolorization of MB as a model of water-soluble dye and examined several experimental conditions such as dye concentration, treatment time, temperature, adsorbent doses for efficient dye removal. Adsorption and photocatalysis of MB over nanocomposites were investigated for comparison of materials and evaluation of their properties. Desorption of the dye and/or its photocatalytic degradation onto ZnO incorporated in nanocomposites were studied in order to minimize the adsorbent waste and to test its reusability.

Key Words: *clinoptilolite; ZnO-Zeolite nanocomposites; dye removal; adsorption; photocatalysis*

PREPARATION OF SILVER NANOPARTICLES-ZEOLITE NANOCOMPOSITE AND ITS POTENTIAL APPLICATION AS AN ANTIBACTERIAL AGENT IN WATER TREATMENT

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Abstract

Silver have been long known for its antibacterial activity and silver nanoparticles, AgNPs, are widely used in many modern fields of nanotechnology – catalysis, microbiology, electronics, and environmental protection. They possess unique physical and optical properties. In order to improve their stability and make them more accessible they're often immobilized onto some support – natural (zeolite, clay, silica) or synthetic (polymers matrix, beads and fibres), thus forming a nanocomposite material. This way their application in environmental protection is much more convenient, long-lasting and cost effective.

In this study we present a method for synthesis of composite material consisting of AgNPs and natural zeolite. The method involves sorption of silver ions onto zeolite followed by chemical reduction of ions to silver nanoparticles. The reduction is conducted at room temperature using sodium citrate as a green reagent. The reaction is catalysed by two type of amines, monoethanolamine (MEA) and triethanolamine (TEA) which lowers the reaction temperature. Using this modified citrate method, we have obtained AgNPs - zeolite nanocomposite materials. The TEM images show that the AgNPs are uniformly distributed onto zeolite surface and have approximate size of 50 nm in diameter. Thus prepared AgNPs -zeolite nanocomposites have been tested against *E. coli* as a potential antibacterial material and its activity has been compared to the activity of AgNPs in solution.

Key Words: *nanotechnology; silver nanoparticles; environmental protection; AgNPs –zeolite; nanocomposite*

CATALYTIC HYDRODEOXYGENATION OF BIO-OIL IN A FIXED BED REACTOR

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Abstract

Biomass pyrolysis results in the formation of bio-oils, which can be used as bio-combustibles or bio-fuels, if their physical and chemical properties (e.g. oxygen content, viscosity, stability...) are improved. Indeed, bio-oil has a different chemical composition than that of petroleum oils and does present some drawbacks [1] such as low heating value, high viscosity, low thermal and chemical stability and high pH. The most attractive route for the improvement of bio-oil is catalytic de-oxygenation at atmospheric pressure. De-oxygenation is based on decarboxylation, decarbonylation and dehydration reactions. (Ni₂P/hzsm-5 and Ni₂P/SiO₂) appear to be the best catalysts for the hydrodeoxygenation of bio-oils.

During this study, a detailed behavior of the de-oxygenation of bio-oil and model molecules were studied. Also, a detailed analysis of the carbon deposit on the catalyst was studied. The de-activation of the catalyst was considered as one of the major problems of the catalytic de-oxygenation reaction of bio-oils. Also, the de-activation of the catalyst often involved the clogging of the installation.

Key Words: *bio-oil, biomass, pyrolysis, FeHZSM-5*

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DETAILED MODELLING OF ANAEROBIC DIGESTION WITH EXPERIMENTAL VALIDATION

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Abstract

Anaerobic digestion

Anaerobic digestion is defined as a complex process where organic matter is transformed, by the action of microorganisms in the absence of oxygen, to biogas (a rich mixture of methane (CH_4) and carbon dioxide (CO_2)) and others energetic compounds [1]. Fats, proteins, and carbohydrates are reduced into smaller compounds (acetic acid, butyrate, propionate, hydrogen, etc.) to produce biogas, a fuel that can be used to produce electricity, heat and as a vehicle fuel. A digestate is produced as a secondary product of the process; it could be used, after upgrading it, as a fertilizer [2].

The anaerobic digestion is held by a sequence of four different reactions: hydrolysis, acidogenesis, acetogenesis and methanogenesis. Hydrolysis phase is characterised by turning complex biopolymers (fats, proteins and carbohydrates) into smaller compounds (long chain fatty acids, aminoacids, sugars...), this reaction is held by the enzymes produced by microorganisms. During the second phase, acidogenesis, products of the hydrolysis are degraded to short chain fatty acids, hydrogen, carbon dioxide and acetate. In the third phase, acetogenesis, short chain fatty acids are converted into hydrogen, carbon dioxide and acetate. For the final phase, methanogenesis, hydrogen and carbon dioxide are used by the CO_2 methanogens to produce methane; and acetate is transformed, by the action of acetoclastic methanogens, into methane and carbon dioxide.

The anaerobic digestion process is affected by the temperature, the organic load rate, the hydraulic retention time, the characteristic of the raw material, the pH, and most importantly the microorganisms' dynamics; as these microorganisms are responsible for the transformation of the organic matter [3].

Biodigesters

Several types of digesters are in use today and their design depends on the material that is going to be digested. They are classified in terms of the type of flow (batch, continuous), number of process stages (one stage or multistage), solid content ("wet-<16% of TS", dry-22-30 % TS) and temperature (mesophilic or thermophilic). The different combination of these characteristics in the digester will lead to different levels of methane production. The best design of anaerobic reactor offers a high continuous production of biogas with the shortest possible time.

Modelling of the anaerobic process

Different models have been developed to describe the anaerobic digestion process. Some of them rely on algebraic equations to determine methane yield (stoichiometric method), and others take into account the biochemical reactions and the external parameters affecting the process. Models that simulate biochemical reactions are very complex and they rely on empirical formulas, most of them derived from Monod's kinetics and its extensions for products inhibition.

Key Words: *biodigesters, anaerobic, digestion*

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INFLUENCE OF SOME PARAMETERS ON THE PROTECTIVE POWER OF CAFFEIN AGAINST COPPER CORROSION

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Abstract:

The possibility of using green corrosion inhibitors has now become an attractive alternative to other methods of protection[1]. This work consists of studying the effect of some parameters (sulfide ions, oxygen) on the protective power of caffeine against copper corrosion in chloride medium (NaCl. wt 3.5%), as well as the contribution of the Cu (II) -Caféine complex to the formation of the protective film. It should be noted that previous work [1] has been carried out to determine the protective effect of caffeine a natural product against the corrosion of copper. The addition of sulfides accelerates the corrosion of copper in chloride medium, while the presence of oxygen and caffeine has a synergistic effect on the effectiveness of the protection of copper in chloride medium.

Caffeine is physically adsorbed on the surface of the copper [1] forming a single-molecule layer of a complex as a result of the interaction between the copper ions and the inhibitor molecules thus protecting the metal from corrosion.

Key words: *Copper, Corrosion, 3.5% NaCl, caffeine, sulfide ions.*

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ADSORPTION BEHAVIOR AND SURFACE ANALYSIS OF CAFFEINE AS A GREEN CORROSION INHIBITOR FOR COPPER

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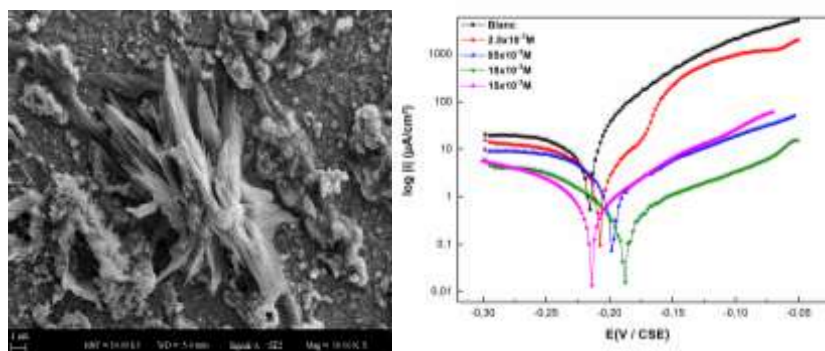
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Abstract

Many organic molecules are recognized as corrosion inhibitors for metals and alloys. The adsorption of organic compounds onto the surface of corroding metals markedly modifies the properties of the metal/solution interface, such as the double layer capacitance and the kinetics of the interfacial electron transfer process [1]. Copper-based materials have widespread application in industry due to their excellent chemical, physical, electrical and mechanical properties, which has led to copper and its alloys lying in third position in terms of the most-used materials [2]. Caffeine (1,3,7-trimethylxanthine) in particular is an organic molecule that shows several of the desirable characteristics of a good organic corrosion inhibitor; it features π -electrons, oxygen and nitrogen hetero-atoms, and polar functions that are typical reaction centers for adsorption.

Electrochemical experiments were carried out to evaluate the corrosion behavior of copper in aerated 3.5wt.% NaCl solutions in the presence of caffeine. The corrosion rate of copper was found to decrease in the presence of caffeine. The adsorption of caffeine was confirmed by cyclic voltammetry (CV), polarization curves and electrochemical impedance spectroscopy (EIS). The formation of a protective film and the presence of organic compounds on the copper surface were further confirmed by SEM imaging and EDS composition analysis, respectively [3].

Key Words: Surface analysis, Organic coatings, Polarization, Neutral inhibition, Caffeine



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AN INVESTIGATION OF STABILITY AND ACTIVITY OF POLY(METHYL VINYL ETHER-ALT-MALEIC ANHYDRIDE) COPOLYMER IN THE DIFFERENT pHs AND SIMULATED BODY FLUIDS

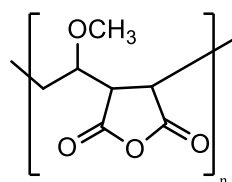
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The poly(methyl vinyl ether-alt-maleic anhydride) (PMVEMA) (Schema 1) copolymer is biocompatible, biodegradable and has a low toxicity [1]. Maleic anhydride copolymers can also be conjugated with molecules containing the amino group (HN-) [2]. Because of these reasons, PMVEMA copolymer promises to be used in drug delivery and controlled drug delivery systems. The stability and activity of drug delivery systems are very important in vivo. The zeta potential is a scientific term for the electrokinetic potential that has a great impact on the various properties of nano-drug delivery systems in colloidal systems. Particle size and charge are the two main factors that play a key role in this regard. Zeta potential, mobility and particle size measurements are investigated by using Zeta Potential Analyzer. [3,4].

In this study, the stability and activity of PMVEMA were determined as a function of time in simulated physiological body fluids such as dextrose, PBS and isotonic NaCl solutions and different pHs. PMVEMA's activity at different pH levels and simulated physiological body fluids were analyzed by UV-VIS.



Poly(methyl vinyl ether
-alt-maleic anhydride)

Mn ~80,000

Mw ~216,000

Schema 1 Chemical structure of PMVEMA

Key Words: *poly(methyl vinyl ether-alt-maleic anhydride) copolymer; polymer-drug delivery, zeta potential; particle size; bioconjugate*

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STIMULI-RESPONSIVE POLYZWITTERIONIC MICROGELS WITH TUNABLE UCST – LCST AND STUDY OF THEIR ANTI-POLYELECTROLYTE EFFECT IN SALT SOLUTIONS

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Abstract

Microgel, a smart class of material has drawn attention in a past few decades due to its response to external stimuli like temperature, pH and ionic strength of the solution [1]. Among them one type of polymer becomes soluble and the other becomes insoluble in water upon heating displaying upper critical solution temperature (UCST) (e.g. polysulfobetaine, PSB) and lower critical solution temperature (LCST) (e.g. poly(*N*-vinylcaprolactam, PVCL)) respectively. Polyzwitterions, electrically neutral polymers are biocompatible, biodegradable and non-cytotoxic in nature and presence of zwitterionic pendant group in the main backbone makes them stable against temperature and pH variations and strong hydration capability in salt solution promotes them to be used as interfacial bio-adhesion resistance material [2]. Majority of zwitterionic microgels have been synthesized in mini- emulsion technique using free radical polymerization approach [3]. Here, a new route to synthesize dual thermo-responsive PVCL microgels decorated with appreciable amount of zwitterionic PSB chains was developed by a purely water-based surfactant-free reversible addition–fragmentation chain transfer (RAFT) precipitation polymerization. PSB macro-RAFTs having different molecular weights were synthesized and utilized for surface-grafting with PVCL microgels varying the macro-RAFT concentration using *N,N'*-Methylenebis(acrylamide) (BIS) as cross-linker. Increasing the PSB concentration in the PVCL microgels resulted in a linear increase in UCST but decrease in hydrodynamic radius due to strong intrachain coulombic attraction forces acting between the opposite charges present in the zwitterionic groups [4]. However, increasing the molecular chain length of the zwitterionic macro-RAFT resulted in shifting of LCST towards lower temperatures. Microgels are also sensitive to ionic strength of electrolyte. They exhibited anti-polyelectrolyte effect on addition of monovalent salt solution up to a certain concentration by swelling their hydrodynamic radii followed by intermolecular ionic or dynamic crosslinking. As a result, UCST disappeared after a critical salt concentration but LCST still existed.

Key Words: RAFT; macro-RAFT; zwitterionic; UCST; anti- polyelectrolyte effect

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SYNTHESIS AND THERMOELECTRIC PROPERTIES OF POLYTHIOPHENE/POLY(3,4-ETHYLENE DIOXYTHIOPHENE) NANOCOMPOSITES UNDER MAGNETIC FIELD

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Abstract

Thermoelectric materials can convert the temperature difference at both ends to a potential difference of electricity. The thermoelectric polymer materials have been attractive than inorganic thermoelectric materials due to their low cost, non-toxicity, high mechanical elasticity, easy processability and intrinsically weak thermal conductivity. Among the conductive polymers investigated for this purpose, poly(3,4-ethylene dioxythiophene) (PEDOT) is seen as a promising alternative. However, its thermoelectric properties alone are not sufficient and their thermoelectric properties can be increased by incorporating inorganic, organic or polymeric nanoparticles into the conductive polymers [1]. On the other hand, an increase in the electrical conductivity is expected due to the increasing electron mobility as the molar mass and branching of the polymer chains increases. It has been shown that the chains become longer and more oriented in the conventional polymers when they are synthesized under magnetic field [2]. Therefore, if conductive polymers are synthesized under the magnetic field, it is expected an increase of the power factor due to increasing electrical conductivity because of more oriented and longer chains.

In this study, polythiophene (PTh) nanoparticles was synthesized in the presence of poly (sulfonic acid diphenyl aniline) in the presence and absence of magnetic field. Then PTh/PEDOT nanocomposites were synthesized by *in situ* synthesis of PEDOT on the PTh nanoparticles in the presence and absence of magnetic field. The power factor of the samples were calculated by measuring their Seebeck coefficients and electrical conductivities from the thin films on the glass substrate. UV-visible, FT-IR spectroscopy and dynamic light scattering techniques were used for the characterization.

Key Words: *polythiophene, poly (3,4-ethylene dioxythiophene), thermoelectrics, Seebeck coefficient, magnetic field*

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MODELING PARTICLE SIZE OF POLYACRYLIC ACID-COPPER(II)-BOVINE SERUM ALBUMIN TERNARY COMPLEX IN SALT SOLUTION

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Abstract

Water-soluble polyelectrolytes (PEs)–protein binary conjugates and PE-metal-protein ternary complexes as the functional biopolymer systems represent a specific class of these conjugates and complexes that have been the subject of many studies in the application areas of biotechnology, medicine and pharmacy. The copper complexes interact with DNA, leading to chemically induced cleavage of DNA and, thus, antitumor activity. The mode of action is probably related to the binding of PE-copper(II)-bovine serum albumin (BSA), which is likely to leave some potential donor atoms free and these free donor atoms enhance the biological activity [1].

Particle size and zeta potential of binary conjugates and ternary complexes are among the most important factors affecting biopharmaceutical behavior such as bioavailability, dissolution and immune toxicity of these complexes. For this purpose, in the current study, the interactions between binary and ternary anionic polyelectrolyte, “polyacrylic acid (PAA)”, BSA and copper ions in different salt concentrations were investigated by zetasizer analysis. In this work, the particle size of poly(acrylic acid)-copper (II)-bovine serum albumin (BSA) ternary complex in a salt solution is modeled using extensive regression methods to partial least squares regression from conventional multiple linear regression [2-4]. The effects of particle sizes and zeta potential of binary conjugate as PAA-BSA and ternary complex as PAA-Cu⁺²-BSA are to be investigated systemically increased salt solution into account.

Keywords: particle size, zeta potential, binary conjugate and ternary complex, shrinkage regression

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DEVELOPMENT and OPTIMIZATION of an HPLC METHOD for the SIMULTANEOUS ANALYSIS of a MULTI COMPONENT DRUG PRODUCT by the help of CENTRAL COMPOSITE DESIGN

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Abstract

HPLC analysis of multicomponent pharmaceutical formulations provides some advantages such as rapidity, ease of automation, specificity, precision, accuracy and etc. in quality control laboratories. In order to develop and optimize HPLC techniques, the influences of several variables/factors must be examined by the sophisticated and synchronized practices that need to be studied patiently. HPLC methods were formerly optimizing by time-consuming trial and-error approach (classical approach), which were bringing about limited information related to the separation of analytes and interactions between factors. Thus, chemometric methods such as experimental designs based on response surface methodology are a good option because they are more efficient and practical with a minimum number of experimental run in stead of laborious techniques [1, 2].

In this study, development of a simple and sensitive analytical method based on high-performance liquid chromatography with diode array detection (HPLC-DAD) for the simultaneous determination of doxylamine succinate, dextromethorphan hydrobromide, paracetamol, and pseudoephedrine hydrochloride as active substances, allure red (FD&C Red 40, E129), and brilliant blue FCF (FD&C Blue 1, E133) as colorants and saccharine as an artificial sweetener in a syrup preparation was proposed. Chromatographic separations were performed on an Inertsil C18 column (4.6 mm x 150 mm x 5 µm particle size) along with phosphate buffer and methanol mixture as a mobile phase. Optimum conditions of developed HPLC method were determined through Central Composite Design with a five-level-four factor requiring 30 experiments. The effects of four factors including pH, the composition of mobile phase in first and second steps of gradient elution, and flow rate of the mobile phase were evaluated and then the proposed method was easily and accurately optimized by the help of a chemometric approach.

Key Words: Central composite design, HPLC determination, active substance, colorant, artificial sweetener.

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