ABSTRACTS BOOK

4th International Conference on New Trends in Chemistry
ICNTC 2018

4th INTERNATIONAL CONFERENCE ON NEW TRENDS IN CHEMISTRY

MAY 11-13 2018
Original Sokos Hotel Olympia Garden – St Petersburg/Russia
http://www.icntcconference.com/
ICNTC’2018

4th International Conference on New Trends in Chemistry
St Petersburg/Russia

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Editors:
Assoc. Prof. Dr. Dolunay Sakar Dasdan

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Conference organised in collaboration with Smolny Institute of the
Russian Academy of Education

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Linz Institute for Organic Solar Cells, Linz, Austria

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Dr. Decha Dechechtrirat,
Department of Materials Science, Faculty of Science, Kasetsart University, Thailand

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Escuela Superior Politecnica del Litoral Ecuador
Center of Nanotechnology Research and Development (CIDNA), Guayaquil, Ecuador

Dr. Mauricio Heriberto Cornejo Martinez,
Escuela Superior Politecnica del Litoral Ecuador
Center of Nanotechnology Research and Development (CIDNA), Guayaquil, Ecuador
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Yıldız Technical University – Turkey  
Conference Chair

Assoc. Prof. Dr. Yelda Yalcin Gurkan  
Namik Kemal University – Turkey  
Chemistry Department
Dear Colleagues,

I am honoured to invite and send you this call for papers on behalf of Conference Organisation Board of “4th International Conference on New Trends in Chemistry”, to be held at St. Petersburg dates between 11 – 13th of May 2018.

A 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 in conference will be published in Special Issue Edition of Bulgarian Chemical Communications. (ISSN:0324-1130)

Web site of journal : http://www.bcc.bas.bg/

Bulgarian Chemical Communications is indexed by Science Citation Index Expanded (SCI-E).

We kindly wait for your attendance to our congress to be held on 11–13th of May 2018, 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
4th ICNTC 2018 | 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.
SCIENTIFIC PROGRAM

10 MAY 2018 THURSDAY
18:00 – 21:00 : REGISTRATION

11 MAY 2018 FRIDAY
08:00 - 17:00 : REGISTRATION

MAIN HALL
09:00 – 09:30 : GRAND OPENING CEREMONY

09:30 – 09:40 | B R E A K

HALL 1
09:40 – 09:50
Welcome Speech by Conference Chair
Assoc. Prof. Dr. Dolunay SAKAR DASDAN / Yıldız Technical University , Turkey

HALL 1 / KEYNOTE SPEAKER
09:50 - 10:40
DR. AGATA BARTYZEL,
Department of General and Coordination Chemistry, Faculty of Chemistry,
Maria Curie-Sklodowska University, Poland

Lecture Title: “Multifunctional N,O-donor ligands and their complexation abilities toward d-block metal ions”

10:40 – 11:00 | C O F F E E / T E A B R E A K

HALL 1 / SESSION A

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<td>A. GOMEZ SANCHEZ, Evgen PROKHOROV, G. LUNA BARCENAS, E. M. RIVERA MIÑOZ; M. GRAZIA RAUCCI, G. BUONOCORE.</td>
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<td>Cinvestav, Unidad Querétaro, Querétaro, MÉXICO.</td>
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<td>11:20 – 11:40</td>
<td>INVESTIGATION OF IN-VITRO SALT STRESS ON PEROXIDASE ENZYME OF AMSONIA ORIENTALIS AND PURIFICATION OF PEROXIDASE FROM NON-STRESSED AND SALT-STRESSED PLANTS</td>
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<td>Kocaeli University, Kocaeli, Turkey</td>
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<td>Uskudar University, Istanbul, Turkey</td>
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#### SESSION CHAIR

PROF. DR. F. BEDIA ERİM  
Istanbul Technical University, Turkey

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<td>University of Economics, İzmir, Turkey</td>
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15:40 – 15:50  
COFFEE/TEA BREAK

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Assit.Prof.Dr.Emel AKYOL,  
Yıldız Technical University, İstanbul, Turkey

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<td>Boğaziçi University, İstanbul, Turkey</td>
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13:00 – 14:00  **LUNCH**

## HALL 1 / KEYNOTE SPEAKER

**PROF. DR VURAL BÜTÜN**

*Lecture Title: STIMULI-RESPONSIVE POLYMERS: INTELLIGENT, SURFACE-ACTIVE, SCHIZOPHRENIC, AND SUPERB SOURCE FOR VARIOUS NANOSTRUCTURES “*

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**Presenter:** Pınar TALAY PINAR, Zühre ŞENTURK  
**Affiliation:** Van Yüzüncü Yıl University, Van, Turkey

### Controlled Release of Drug from a New Platform Based Calixarene Nanofiber

**Presenter:** Esra MALTAS CAGIL, Othman HAMEED, Fatih OZCAN  
**Affiliation:** Selcuk University, Konya, Turkey

### Development of Disposable Amperometric Putrescine Biosensor Using Methylene Blue as a Mediator

**Presenter:** Berna DALKIRAN  
**Affiliation:** Ankara University, Ankara, TURKEY

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Bülent Ecevit University, Zonguldak, Turkey |
| 16:50 – 17:10 | Immobilization of Lipase-Producing Bacteria *Acinetobacter Haemolyticus* on Eggshell Membrane | Ceyhun İŞIK, Nurdan SARAÇ, Mustafa TEKE, Aysel UĞUR  
Mugla Sıtkı Koçman University, Muğla, Turkey |
| 17:10 – 17:30 | New Synthetic Methods for Pyrazole Fused Heterocyclic Compounds | Meltem TAN  
Van Yüzüncü Yıl University, Van, Turkey |
| 17:30 - 17:50 | Novel Metal-Based Anticancer Drugs: Synthesis and a New Approach to Drug Delivery | Ayşegül GÖLCÜ  
Istanbul Technical University, Turkey |
| 17:50 – 18:10 | Electrochemical Properties of Lanthanide Series Bis-Pthalocyanines | Efe B. ORMAN, Emre GÜZEL, Baybars KÖKSOY, Ali R.ÖZKAYA  
Marmara University, Istanbul, Turkey |
| 18:10 - 18:30 | Cost and International Network Workshop                                      | Mustafa Ersöz.  
Selçuk University, Konya, Turkey |

**Coffee/Tea Break**

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**Session Chair:** Prof. Dr. İlyas DEHRİ, Çukurova University, Adana, Turkey
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<td>Yıldız Technical University, Istanbul Turkey</td>
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SPECTROSCOPIC AND PHOTOPHYSICAL PROPERTIES OF TWISTED PERYLENE DIIMIDES APPENDED WITH CHELATING N-HETEROCYCLES

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Abstract
Perylene diimides (PDIs) are among the most versatile and functional dyes for supramolecular structures displaying characteristic high absorptions and photo-luminescence properties as the prerequisite for optoelectronic thin film devices. Despite intense investigations on these semiconducting and electro-active materials, details of their electronic structure are still under examination. In particular, non-planar twisted PDIs as an electron acceptor is a promising model system for efficient charge generation and transport processes. Therefore, new dyads and triads based on twisted PDIs carrying different substituents at bay-positions and variety of chelating agents as a new functionality at the imide positions (Fig. 1) have been synthesized. Supramolecular self-assembly of these hybrid materials with metal ions having preference for square-planar geometry, such as Pt(II) and Pd(II) have also been studied. These compounds were fully characterized by FT-IR, 1D-NMR ($^1$H-NMR and $^{13}$C-NMR), 2D-NMR ($^1$H-$^1$H COSY, $^1$H-$^{13}$C HSQC, $^1$H-$^{13}$C HMBC), MALDI TOF mass and UV-Vis spectroscopy. Time-Dependent Density Functional Theory (TDDFT) calculations were carried out for the geometry-optimized electronic ground state and excited state structures in the gas phase. The HOMO-LUMO energy gaps and their photovoltaic properties are discussed.

Fig.1: Twisted perylene dimide molecules.

Key Words: Perylene diimide; N-heterocycles; metal; complex;

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MULTIFUNCTIONAL N,O-DONOR LIGANDS AND THEIR COMPLEXATION ABILITIES TOWARD d-BLOCK METAL IONS

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Abstract

In recent years interest in the design, synthesis, and coordination chemistry of chelating ligands capable of forming stable complexes with metal ions has resulted in the study of a large number of new chelating agents. Schiff bases are ligands which provide such opportunities and for this reason have attracted the attention of researchers for many decades. Nowadays the research field dealing with Schiff bases coordination chemistry has expanded enormously due to their interesting properties and potential applications in various areas such as catalysis, luminescent probes, analytical chemistry, magneto-structural chemistry, agrochemical, biological fields etc [1]. Special attention is paid to the Schiff bases formed during the reaction of diamines with o-hydroxy aldehydes and ketones. These types of imine compounds are stabilized by the intramolecular, strong hydrogen bonds (O-H···N) forming the six membered ring where proton transfer from the phenolic oxygen to the imino nitrogen atom is often observed. As a result, the compounds can exist in the phenol-imine (OH), keto-amine (NH) or zwitterionic (N⁺H···O⁻) forms exhibiting solvato-, thermo- and photochromism. In our study, we have synthesised Schiff base ligands using aliphatic diamines and ketone derivatives of o-phenolic compounds. The obtained ligands rapidly form complexes with transition metals. A special attention was paid to study the impact of various condition factors on the structure of formed complexes. The main factors, which can affect the obtained compounds and were taken into account, were as follows: type of solvent, type of counterion, temperature and stoichiometric ratio M:L. The obtained Schiff bases and their complexes were characterized using FTIR and UV-Vis spectroscopies, X-ray diffraction analysis as well as thermogravimetric methods. The obtained Schiff bases in the solid state exist in the phenol-imine or zwitterionic forms, where strong intramolecular O·-H···N or N⁺·H···O⁻ hydrogen bonds occur. In the polar aprotic solvents the ligands are present predominantly in phenol-imine form while in protic solvent (e.g. MeOH) the stabilization of the more polar, keto-amine form was also observed. In the case of metal complexes formation it was found that the choice of a suitable counterion, type of solvents as well as stoichiometric ratio M:L can significantly influence on the coordination of metallic centres and the crystal packaging of obtained compounds. It was also noted that the solvent molecule played an important role in the stabilization of the structure of studied solvate complexes [2-5].

Key Words: chelating ligands; Schiff base; phenol-ketone tautomerism; metal complexes; crystal structure
References

NOVEL METAL-BASED ANTICANCER DRUGS: SYNTHESIS AND A NEW APPROACH TO DRUG DELIVERY

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Abstract

Cis-platinum ([Pt(NH$_3$)$_2$Cl$_2$]), developed by Rosenberg in 1969 and used for cancer treatment has led many research group to synthesize metal-based drugs (metallodrugs) since those years [1]. Pt(II), Zn(II), Ru(III), Cu(II), Mn(III) and Au(I/IV) are mostly used as the metal ion for the drug development. In all of those studies, the drug molecules act as ligands and form mostly monodentate or bidentate molecular structures by offering pair of electrons to metal atoms [2]. The studies of this topic over the last forty years have been gathered under the roof of “Medicinal Chemistry”. The main objective of Medicinal Chemistry is to identify new anticancer agents and put them into clinical practice procedures. However, as the synthesis of metal-based drugs increases, the problems of water solubility and pharmacological evaluation have come to the fore. Apparently, the solutions to overcome these problems lie not in the synthesis of new anticancer drugs, but in the discovery of appropriate drug delivery strategies. In particular, I will talk about pre-drug, nano-carriers and ligand designs that have been working on for over twenty years and will give examples from anticancer-effective metal-based drugs synthesized in our lab. (This work was supported by a Scientific Research Project Unit (ITU, Project ID: 40917).

References

DEVELOPMENT OF DISPOSABLE AMPEROMETRIC PUTRESCINE BIOSENSOR USING METHYLENE BLUE AS A MEDIATOR

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Abstract

The levels of biogenic amine (BA) are significant for various analytical purposes. Putrescine is a low-molecular-weight nitrogenous base belong to the group of BA. This compound is used for the indication of food quality, because the amount of putrescine in spoiled food increases [1,2]. Therefore, rapid, cost effective, highly sensitive and selective determination of putrescine is of considerable importance. Compared with other analytical methods, such as luminescence, spectroscopy and chromatography, biosensors are one of the best ways of determining species. Recently, the development of nanomaterials modified electrodes have been increased, due to their unique chemical, physical and electronical properties [3]. Artificial mediators are also widely used in biosensor construction, as they can minimize the interference effect of coexisting electroactive species by operating at low potentials [4].

In this study, we report the fabrication of a putrescine biosensor based on Fe3O4 nanoparticles, carboxylated multi-walled carbon nanotubes (c-MWCNTs) and methylene blue (MB). First of all, the putrescine biosensor was constructed by electropolymerization of MB onto the carbon screen printed electrode (SPE) in the potential range of −0.4~1.2 V through cyclic voltammetry. Fe3O4 and c-MWCNT were uniformly dispersed in chitosan matrix, a known amount of homogeneous solution was dropped casted onto the surface of MB/SPE. Diamine oxidase was immobilized onto c-MWCNT-Fe3O4/MB/SPE. The experimental parameters and analytical performances of the biosensor were investigated. Optimum pH and working potential were found to be 8.5 and -0.20 V, respectively. The linear working range of the modified enzyme electrode was 1.9×10^{-5} M−1.5×10^{-4} M with a sensitivity of 1.57 μA mM^{−1}. The biosensor exhibited good long term stability and reproducibility. The proposed biosensor can be used for monitoring various food samples.

Key Words: Putrescine, screen-printed electrode, mediator, biosensor, amperometry

References


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RECOGNITION OF A BROMIDE ION BY THE PROTONATED FORM OF 2-(1H-IMIDAZOL-2-YLTHIO)-3-METHYLNAPHTHALENE-1,4-DIONE)

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Abstract:

Supramolecular chemistry of anions is an important field of research in biological and environmental science. [1] Hosts for different anions are generally formed by protonation of a neutral molecule(s) to offer electrostatic interactions to bind an anion. [2-3] The interactions of various acids, such as hydrochloric, hydrobromic, nitric, perchloric, and tetrafluoroboric acids with 2-(1-Himidazole-2-yltihio)-3-methylnaphthalene-1,4-dione (L) enhance the intensity of the fluorescence emission of L. Exceptionally, the interaction of hydrogen bromide with L not only enhances the emission intensity, but also leads to a sharp characteristic emission at λ = 480 nm (λ_ex=350 nm), which is different from the other acids. Bromide-ion recognition by protonated L is explained on the basis of a tautomeric equilibrium. Various salts of L with the general composition [HL][X] (in which X=Cl (1), Br (2), NO_3 (3), ClO_4 (4), and BF_4 (5)) are structurally characterized. The coordination environment of the corresponding anion in these salts in the solid state is guided by electrostatic N-H···O interactions. [4]

Scheme: Equilibria of L with HBr.

Key Words: (Naphthoquinone, anion sensor, recognition)

References:


This work was supported by The Scientific and Technological Research Council of Turkey (Project No: 116Z159).
AMPEROMETRIC DETECTION OF CADAVERINE WITH c-MWCNTs-CO$_3$O$_4$ MODIFIED SCREEN-PRINTED ELECTRODE

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Abstract

Biogenic amines (BAs) are low-molecular-weight organic bases mainly produced by microbial decarboxylation of amino acids. Cadaverine (Cad) is one of the important BAs related with spoilage in food and can be considered appropriate food freshness indicators with histamine and putrescine [1]. Also, cadaverine has been found to potentiate histamine toxicity [2]. Therefore, the development of sensitive methods for Cad analysis is of great importance [3]. Different techniques have been developed for this purpose [4] and among the various techniques developed for Cad determination electrochemical biosensors represent an interesting alternative.

In this work by combining the advantageous properties of carboxylated multiwalled carbon nanotubes (c-MWCNTs) and Co$_3$O$_4$ nanoparticles, a new Cad biosensor was constructed. In the fabrication process of the biosensor chitosan was used to disperse c-MWCNTs and Co$_3$O$_4$ nanoparticles. Diamine oxidase (DOx) enzyme was immobilized covalently onto c-MWCNTs-Co$_3$O$_4$/SPE using N-ethyl-N'-(3-dimethyaminopropyl) carbodiimide and N-hydroxysuccinimide chemistry (DOx/c-MWCNTs-Co$_3$O$_4$/SPE). The morphology of the c-MWCNTs-Co$_3$O$_4$/SPE has been investigated by scanning electron microscopy, and the electrochemical performance of the biosensor has been researched by amperometric method. Electron transfer properties of the modified electrodes were studied by cyclic voltammetry and electrochemical impedance spectroscopy methods. The optimum amount of c-MWCNTs and Co$_3$O$_4$ nanoparticles were investigated by using central composite design (CCD) approach. CCD was applied to determine the effects of the c-MWCNTs and Co$_3$O$_4$ nanoparticles amounts and to obtain their estimated interactions between each other with minimum numbers of experiments. Optimum experimental conditions such as pH and working potential found to be 8.5 and 0.7 V, respectively. Also, the analytical properties of DOx/c-MWCNTs-Co$_3$O$_4$/SPE like linear working range and detection limit were evaluated and found as: 7.9×10$^{-7}$ M – 1.1×10$^{-4}$ M and 7.7×10$^{-7}$ M, respectively. The developed biosensor is to be used for determination of Cad in food samples.

Key Words: Amperometric biosensor, Biogenic amines, Central composite design, Cadaverine, Diamine oxidase

References


This work was supported by The Scientific and Technological Research Council of Turkey (Project No: 116Z159).
IMMOBILIZATION OF LIPASE-PRODUCING BACTERIA

Acinetobacter Haemolyticus ON EGGSHELL MEMBRANE

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Abstract

Lipases are hydrolases that under aqueous conditions act on the carboxyl ester bonds present in triacylglycerols to liberate fatty acids and glycerol. The long-chain triacylglycerols that form the natural substrates of lipases have very low solubility in water, and the hydrolytic reaction is catalyzed at the lipid–water interface [1]. In addition to hydrolysis, lipases are also involved in a wide range of conversion reactions that include esterification, interesterification, transesterification, alcoholysis, acidolysis and aminolysis in nonaqueous media [2]. This versatility makes lipases the enzyme of choice for potential applications in the food, detergent, pharmaceutical, leather, textile, cosmetic, and paper industries [3].

Immobilization is the process of attaching or entrapping an enzyme to an insoluble material, the matrix, using physical or chemical interactions. The primary objective of immobilization is to reduce the process cost by enhancing enzyme stability and reusability. For further cost minimization, finding a cheap and readily available matrix that can retain maximum enzyme activity is a major challenge in commercial enzyme immobilization applications. Enzymes can be immobilized by several methods, which range from carrier-bound to carrier-free techniques [4].

In this work, lipase (LipAH02–30), first-produced from a soil-olive pomace mixture Acinetobacter Haemolyticus [5] was immobilized onto egg shell membrane (ESM) which is an amorphous natural biomaterial with an intricate lattice of stable and water insoluble fibers. LipAH02–30 was immobilized on to the ESM by adsorption and crosslinking methods. For the optimization of LipAH02–30 immobilization, the amount of ESM, the adsorption time, the unit of LipAH02–30 and the amount of glutaraldehyde were investigated as basic parameters. The optimum temperature, optimum pH, thermal stability, pH stability, kinetic parameters and reusability parameters were investigated in the characterization of LipAH02–30 immobilized ESM prepared under optimum conditions. Also characteristic parameters of immobilized LipAH02–30 compared with free LipAH02–30. Findings from present study will guide development of a low cost biodegradable and biocompatible carrier for LipAH02–30 immobilization.

Key Words: Immobilization, lipase, eggshell membrane, Acinetobacter Haemolyticus

References

BIOSORPTION OF REACTIVE DYES BY KEFIR GRAINS

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Abstract

Dyes are synthetic chemical compounds widely used in dyestuff, textile, leather, paper, plastic, cosmetics, food and pharmaceutical industries. Substantial amounts of colored waste water generated by these industries discharged into the environment is undesirable, not only because of their visual effects, but also because many dyes and their breakdown products are toxic, mutagenic, carcinogenic, or allergenic [1-3].

Several physical or chemical treatment methods including adsorption, precipitation, coagulation, flocculation, oxidation, electrochemical treatment, photo degradation have been used with varying degree of success for removal of dyes from wastewater. Recently, studies focused on microbial biomass for the removal of contaminating dyes from wastewater as treatment by microorganisms is eco-friendly and cost effective[4-5].

The kefir grains are small, gelatinous white/yellow irregularly shaped masses consist of live bacteria (lactic acid bacteria of the genus Lactobacillus, Lactococcus, Leuconostoc and acetic acid bacteria) and yeasts (consist of Kluyveromyces, Candida, Saccharomyces and Pichia) in a slimy polysaccharide matrix [6]. In the literature potential use of many bacteria and yeast for removing the dyes from aqueous solutions have been investigated. Although the kefir grains consist of several live bacteria and yeasts together, their potential use on dye removal has not been reported yet.

In this study, biosorption potential of living and inactivated kefir grains for reactive dyes Remazol Navy and Remazol Red were investigated with respect to time at different process conditions to determine kinetic and equilibrium models. At all conditions the living kefir grains exhibited higher dye removal efficiencies compared with the inactivated grains. 96.3% and 93% dye removal for Remazol Navy and Remazol Red were obtained with living kefir grains (2.4 g/L) in a relatively short process time of 180 minutes, at pH 2, 25°C and 100 mg/L initial dye concentration. The maximum adsorption capacities by living and inactivated kefir grains were obtained as 134.59 and 56.92 mg/g and 117.94 and 50.47 mg/g for Remazol Navy and Remazol Red respectively. The biosorption rates were found to be consistent with pseudo-first-order model. The biosorption equilibrium data was well described by Temkin and Langmuir models for living and inactivated kefir grains respectively. Overall, the obtained results indicate that the kefir grains was an attractive low-cost biosorbent for the removal of dyes from aqueous solutions.

Key Words: Biosorption, kefir grain, kinetic, equilibrium, reactive dye
References


Poly(ethylene glycol) is a polyether having strongly hydrogen bonds with water and is one of the most studied polymers in current materials science and biotechnology because of not only its unique behaviors in solution but also its wide applications. Polyethylene (PE) based materials are widely used in many fields due to the combination of excellent physical and chemical properties along with low cost. [1-2].

The aim of this study is to investigate the effect of the polyethylene (PE) segments on the charge and particle size of poly(ethylene glycol). For this purpose, to compare the charge and particle size of poly(ethylene glycol) (Scheme 1) and PEG copolymerized with PE segments polyethylene-block-poly(ethylene glycol) (PE-b-PEG) (Scheme 1) with different molecular weights have been examined by Zeta Potential Analyzer. Zeta potential, mobility, and particle size of PEG and PE-b-PEG systems were determined by using the Zeta Potential Analyzer in water as a function of pHs.

Keywords: PEG, PE-block-PEG, particle size, zeta potential, pH effect

Reference

ELECTROCHEMICAL PROPERTIES OF LANTHANIDE SERIES BIS-PHTHALOCYANINES

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Abstract

Phthalocyanines (Pcs) are aromatic macrocyclic compounds with 18-\pi electrons in the phthalocyanine ring. Since their first discovery, these compounds have attracted great attention of scientists due to unique chemical and physical properties. Furthermore, these properties including basic electrochemical ones can be modified by careful selection of central metal ion and substituents, and changing their numbers, positions and types. Thus, double-decker lanthanide phthalocyanines have attracted great attention due to their predominant electrochemical properties for applicability in electrochromic devices \cite{1, 2}.

In this study, voltammetric, spectroelectrochemical and electrochromic properties of a series of 4-(hydroxyethyl)phenoxy-substituted lanthanide bis Pcs including Sm, Eu, Dy and Pr have been performed in solution and in the solid states as Langmuir-Blodgett (LB) films on the ITO electrodes.

Due to the \pi-\pi interaction of Pc rings around the lanthanide metal ion core, the complexes were easily reduced at even positive potentials. Electrochromic characters of the complexes were confirmed by various color changes recorded during the electron transfer reactions, with three distinctive color alternatives, green, orange and red. Electrochromic measurements in the LB thin films of the complexes indicated that the nature of the metal ions in the Pc cavity alter the basic electrochromic parameters of the complexes.

REFERENCES

**ADSORPTION CAPACITIES OF NOVEL ECO-FRIENDLY BIOSORBENTS IN REMOVAL OF CONTAMINANTS IN AQUEOUS SOLUTIONS**

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**Abstract**

Water pollution is one of the most serious problems faced by people today. There is a need to develop efficient, economically feasible and environmentally friendly processes in order to remove pollutants from water [1]. Adsorption, oxidation–ozonation, biological processes, coagulation–floculation, and membrane processes are major technologies that are high operational and maintenance costs, generation of toxic sludge and complicated procedure involved in the treatment [2-6]. The adsorption process is more effective than other methods in removal of contaminants from the water because of convenience, ease of use and ease of design [6-8].

The rising amount of contaminants requires the development of adsorption systems using low cost adsorbents. Low cost biosorbents are found abundantly in the nature or are obtained from an industrial by-products or wastes [9]. They allow successing the removal of contaminants from aqueous solutions and also to contribute to the waste minimization, recovery and reuse [10]. The purpose of this work is to determine both the adsorption capacity and the characterization of low cost biosorbents in the removal of contaminants in aqueous solution. In this context, low-cost bioadsorbents are separated into the following four groups; (i) agricultural waste, (ii) biochar obtained from pyrolysis of agricultural waste, (iii) calcium alginate microbeads and (iv) novel eco-friendly calcium alginate/biochar microbeads.

Zinc and copper are toxic and detrimental for human health and environment. Removal of zinc (II) and copper ions from aqueous solutions is a huge problem for engineers. The various process parameters for removal of zinc(II) using biosorbents are optimized. Adsorption mechanism of Zn(II) and Cu(II) onto biosorbents using a Langmuir, Freundlich, Temkin and D-R isotherms could be well described. The obtained kinetics datas for Zn(II) and Cu(II) adsorption onto biosorbents agreed well with the pseudo-first-order, pseudo-second-order model, intraparticle diffusion and Elovich mass transfer model.

**Key Words:** groundnut husk, biochar, alginate micro beads, biochar-alginate composite micro beads, adsorption, zinc

**References**

CONTROLLED RELEASE OF DONEPEZIL HYDROCHLORIDE FROM PEG-DA HYDROGELS UNDER UV IRRADIATION

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Abstract

Alzheimer’s disease is a neurodegenerative disorder which leads to memory loss, personality changes [1]. Donepezil hydrochloride (DH) is a reversible inhibitor of acetylcholinesterase [2]. Controlled-delivery systems provide the drug at a specific predetermined temporal and/or spatial manner within the body to fulfill the specific therapeutic needs [3]. Photopolymerization carried hydrogels to offer the ability to prepare hydrogels under mild and physiological conditions, on relevant time scales of seconds to several minutes [4]. Polyethylene glycol diacrylate (PEG-DA) hydrogels are attractive materials which used in controlled release [5].

In this study; donepezil hydrochloride (DH) which was encapsulated in to PEG-DA hydrogels which were combined with modified TiO₂ and HAp in via photopolymerization. Fourier transform infrared (FT-IR) spectroscopy and digital microscope were used to characterize the hydrogels. In vitro release studies have been performed for hydrogels in 1.2, 6.8 and 7.4 pH media. Hydrogels were obtained as very useful materials for drug delivery systems.

Key Words: Alzheimer disease, Donepezil hydrochloride, PEG-DA based hydrogels, drug delivery systems, TiO₂

References


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THE RELATIONSHIP BETWEEN SEA SURFACE TEMPERATURES
AND RAINFALL OVER TURKEY

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Abstract

Weather and climate strongly influence coastal water quality. Turkey's 2016-2017 average
monthly temperature, rainfall, and sea temperature were investigated in this study.
The lowest average temperature was in January 2017 and the highest average temperature was
in July and August 2017.
Rainfall between October 1, 2016 and September 30, 2017 in Turkey was below previous
year (October 1, 2015 and September 30, 2016) and norm (October 1, 1981 and September
30, 2010).
Average annual precipitation in Water Year 2016-2017 and 2015-2016 in Marmara region
were respectively 627 mm, and 620 mm. They were below norm (1 October 1981- 30
September 2010). Average annual precipitation in Water Year 2016-2017 was decreased
compared to norm, while it was increased compared to previous Water Year 2015-2016.
While the highest precipitations were in both winter 2015 and 2016, the lowest precipitations
were in both summer 2015 and 2016 in Turkey. 247mm rainfall in winter 2015 was below
208 mm for normal (1981-2010) and 184 mm in winter 2016.
Most monthly rainfall between 2015 and 2016 was in January 2016. Rainfall in January 2016
was increased compared to norm rainfall (1981-2010).
Pearson correlation constant (0.93) showed that rainfall was increased with increase of
precipitation days in Turkey between 2015 and 2016.
The highest sea temperature is in the Mediterranean region. The second highest temperature is
in the Aegean region. Temperatures in the Black sea region and in the Marmara region were
very close to each other. While the highest sea average temperature (1970-2016) was in
August, the lowest sea average temperature (1970-2016) was in February for whole regions.
Average sea temperature was highly negative correlated with rainfall in Aegean, Marmara,
and Mediterranean region. Therefore, precipitation decreases temperature.
Key Words: Coast, Air quality, sea temperature, rainfall

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CONTROLLED RELEASE OF DRUG FROM A NEW PLATFORM BASED CALIXARENE NANOFLYER

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Abstract

Recent years, researchers have fabricated different types of controlled drug delivery vehicles to maintain the drug concentration in the body within its therapeutic range for prolonged time [1-4]. Electrospun nanofiber is one of such systems that have become attractive. The effectiveness of nanofiber as controlled drug delivery system is known to depend on loading efficacy [5-6]. The aim of this study is to develop electrospun calixarene nanofiber based drug delivery system to achieve controlled release of hydrophobic drugs. To accomplish this, we have synthesized a calixarene derivative, 5,17-bis-[Methyl-N-Methyltranylate]-25,26,27,28-tetrahydroxycalix[4]arene of which nanofiber was produced by electrospun method. Drug loading and release kinetics in different physiological pH were studied a fluorescent drug which is thiabendazole (Tbz). Loading and release of the drug were monitored via fluorescence spectroscopy. Data showed that loading amount of Tbz was measured to be as 1.688 µg to the 2.25 cm\textsuperscript{2} of surface in 7.4 of Ph at the end of 120 minutes. The maximum release of Tbz was 0.243 µg at 7.4 of pH. Loading of drug to nanofibers was clarified by SEM, TEM, EDX, AFM and FT-IR analysis.

Key Words: Thiabendazole; Nanofiber; Calixarene; Controlled release, Pharmaceuticals

References

EFFECT OF CHEMICAL TREATMENT ON THE PROPERTIES OF CHITOSAN MULTIWALL CARBON NANOTUBES NANOCOMPOSITE.

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Abstract

Chitosan-multiwall carbon nanotube nanocomposites (CS-MWCNT) are of great interest in different applications including biomedicine, biosensors, drug delivery, among others; this is due in part to their good biocompatibility, high conductivity and mechanical properties. However, poor solubility and the agglomeration of MWCNTs limits their application. One way to prepare well-dispersed MCNTs is its chemical oxidation which allows attaching functional groups onto MCNT’s surface. Despite of the large number of publications in the literature, which are mainly focused on investigations of functional groups in MWCNT and polymer nanocomposite, there are no reports on how different methods of MWCNT oxidation will affect the electrical and mechanical properties of related nanocomposites. The objective of our work is to probe CS-MWCNT nanocomposite’s electrical and mechanical properties by taking advantage of the presence of abundant reactive -NH$_3$ and -OH in the CS molecule; these groups allow one to obtain highly compatible nanocomposites by direct dispersion of MWCNT in CS solution. Nanocomposites have been prepared with functionalized MWCNT (with different wt.%) by chemical treatment in HNO$_3$, carboxyl acids and mixture H$_2$SO$_4$/NHO$_3$. Properties of oxidized MWCNT are evaluated using FTIR to probe functional groups (-CO.OH, -OH, -CO.O) and Raman spectroscopy to quantify the disorder in MWCNTs. Here, we show that MWCNT’s treatment in a mixture of H$_2$SO$_4$/NHO$_3$ is responsible for the appearance of an additional band related to the carboxylate anion and the highest defect concentration. FTIR and SEM analyses show the highest interaction between NH$_3$ groups in CS and functional groups of MWCNT; the best dispersion was observed in nanocomposites with MWCNT treated in H$_2$SO$_4$/NHO$_3$ mixtures. Electrical and mechanical characterization of CS-MWCNT films show the highest conductivity and the best mechanical properties when the concentration of MWCNT is near the electrical and mechanical percolation thresholds; this percolation can be detected by a sharp increase in conductivity and Young’s module. For MWCNT concentrations above percolation threshold, there is a pronounced decrease in conductivity and mechanical properties mainly due to agglomeration of MWCNTs. Both electrical and mechanical percolation thresholds strongly depend upon the method of MWCNT chemical oxidation; this oxidation affects the interaction of CS side groups with MWCNT’s surface groups. Percolation thresholds in CS-MWCNT films obtained by direct dispersion of MWCNT in CS solution increased from 3 wt% MWCNT to 6 wt% with oxidized MWCNTs (presence of carboxyl groups). Similarly, Young’s module increases from 5 GPa in neat CS to 10 GPa in MWCNT nanocomposites. These effects can be related to the enhancement of MWCNT dispersion in CS matrix. It is noteworthy that CS-MWCNT films obtained by treating MWCNTs in mixtures of H$_2$SO$_4$/NHO$_3$ do not exhibit percolation phenomena; conductivity and Young’s module values are practically the same as those of neat CS. These results can be explained in terms of the strong interaction of MWCNT with CS side groups; this suggests the appearance of a “thick” interfacial layer (of a pseudo third component phase). Therefore, good dispersion of MWCNT does not guarantee nanocomposite’s best electrical and mechanical properties.
**Key Words:** chitosan; MWCNT; chemical oxidation; side groups; percolation threshold.

**ALGINATE AND CHITOSAN HYDROGELS AND THEIR COMPOSITES IN DRUG DELIVERY, WASTE WATER TREATMENT, FOOD COATING AGENTS AND WOUND DRESSINGS**

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**Abstract**

Alginate and chitosan based materials has gained importance as promising materials in biomedicine, pharmacology and waste water treatment due to their biocompatible, biodegradable and non-toxic characteristics. In the present study, it will be given examples from our studies on alginate beads in drug delivery and waste water treatment and alginate and chitosan films as food coating and wound dressing materials.

Novel pH sensitive alginate-protein-clay composite beads enhanced protein encapsulation ratio and improved release rate of drug [1]. Similarly, encapsulation of clay in calcium and barium crosslinked alginate-montmorillonite composite beads increased the encapsulation efficiency of vitamin B2 and slows down the release rate significantly [2].

Calcium ions have been using dominantly as crosslinking agent of alginate hydrogel beads. We showed that crosslinking ion highly effect the removal capacity of alginate bead adsorbents against some toxic ions. Barium ion cross-linked alginate beads have shown great affinity to toxic hexavalent chromium ions in aqueous solution in contrast to the traditionally used calcium alginate beads [3]. Our results suggest that aluminum alginate beads can be used as efficient adsorbents for the removal of fluoride from contaminated water [4]. A novel cryogelation-like strategy was developed for alginate montmorillonite composite beads. This process changed the morphology of beads and improved surface area and adsorption capacity of alginate beads against dye pollutants. Turmeric extract incorporated chitosan films can be suggested as potent coating agents with improved film properties and antimicrobial activities against food pathogens [5]. Crosslinking the alginate films with cerium ions and chitosan [6] and incorporation of nano-cerium oxide to chitosan composite films increased the antibacterial capacity of films significantly. These films can be proposed as antibacterial wound dressings.

**Key Words:** Alginate; Chitosan; Drug; Removal;Coating

**References**

CHELATING BENZIMIDAZOLE FUNCTIONALIZED PERYLENE DIIMIDE DERIVATIVES WITH DIFFERENT BAY-SUBSTITUENTS

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Abstract

Perylene diimides (PDIs) are very versatile and promising materials in a variety of technological applications owing to their unique properties such as intense absorption in the visible region, high fluorescence quantum yield, strong electron-accepting character, and excellent photochemical stability [1]. These unique features led to wide applications of perylene diimides in various fields, e.g., in bioimaging, fluorescent sensor, organic solar cells and field-effect transistors (OFETs), and organic light-emitting diodes (OLEDs) [2]. Benzimidazole derivatives are useful intermediates/subunits for the development of molecules of pharmaceutical or biological (such as anticancer, antimicrobial and other medicinal agent) [3]. Hence, PDI incorporating benzimidazole functionality should bring these properties together to enhance the photophysical properties of the new material for application to dye-sensitized solar cells (DSSCs), OLEDs and electrogenerated chemiluminescence systems [4].

In this study, new perylene diimides carrying chelating benzimidazoles at the imide positions and having different perylene core such as non-substituted, tetrachloro-substituted, tetra(4-methoxyphenyl) and tetra(tert-butylphenyl)-substituted were synthesized and fully characterized (Fig.1). The comparative studies based on these molecules should shed light on the substitution effect and intermolecular interactions in their spectroscopic and photophysical properties.

Key Words: Perylene diimide; benzimidazole; synthesis; spectroscopy

References

Acknowledgments:

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SYNTHESIS AND CHARACTERISATION OF NEW 2D OXALAMIDE FUNCTIONALIZED METAL ORGANIC FRAMEWORKS

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Abstract

In the past decade, two-dimensional (2D) materials have attracted attention due to their unique properties [1]. These materials have been investigated for many applications in sensors, photonics, gas separation and catalysis [2]. On the other hand, metal organic frameworks (MOFs) are porous materials with extended skeletons, which exhibit promising capacity for gas adsorption and separation because of their high specific surface areas and tunable porous structures [3]. The MOF design strategy based on integrating polar oxalamide functionalities within the pore surfaces in order to increase the interaction capacity of small gas molecules [4]. In this study we describe the synthesis and properties of KLU-4, KLU-5 and KLU-6 (KLU = Kırklareli University), an oxalamide containing MOF within the bridging ligand 3-OADAH2 (3-OADAH2 = 3,3’-(oxalylbis(azanediyl))dibenzoic acid) whereby oxalamide comprise the bridge between two benzoate groups. This ligands link M2(COO)4 M = Co(II), Zn(II) and Cd(II) paddle-wheels for KLU-4, KLU-5 and KLU-6 to form 2D-MOFs in which the oxalamide is incorporated and placed within the pore surface. The solvothermal reaction of 3-OADAH2 and metal salts in organic solvents under acidic conditions yielded single crystals of \{Co(3-OADA)(DMA)2H2O\}n, \{Zn(3-OADA)(DMA)\}n and \{Cd(3-OADA)(DMA)\}n. The as-synthesized materials are insoluble in common organic solvents and were characterized by elemental analysis, FT-IR, single-crystal X-ray diffraction, powder X-ray diffraction and thermogravimetric analysis. A single crystal structure analysis revealed that non-interpenetrated two-dimensional networks of KLU-4, KLU-5 and KLU-6 crystals hosts DMA as solvent molecule. Moreover, photoluminescence properties of 3-OADAH2 and KLU-5 and KLU-6 were investigated.

Key Words: Metal organic frameworks, Porous coordination polymers, 2D Networks, Ligand design, Coordination chemistry,

References


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THE FT-IR, NMR SPECTROSCOPY AND COMPUTATIONAL STUDY OF THE SUBSTITUTED CARBAZOLE USED IN SYNTHESIZING OF THE STRYCHNOS ALKALOIDS

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Abstract

The substituted carbazole compounds used in the synthesis of the strychnos type alkaloids is an important reagent in pharmaceutical or medicinal chemistry [1]. All quantum chemical calculations have been performed with G09 software [2]. At first, the most stable conformer of studied compound has been obtained from conformational analysis at B3LYP/6-31G(d,p) level of the theory in the gas phase, then, the most stable conformer of the studied compound has been used for further calculations to get the electronic and spectroscopic properties of this molecular system. The free and total energy has been provided by the frequency calculations to estimate the chemical stability behavior of this compound. The solvent effect on the chemical reactivity behavior and quantum chemical parameters have been obtained from conducting the solvent phase calculations in the water phase by PCM (Polarized Continuum Model) [3]. The quantum chemical parameters such as HOMO, LUMO, energy gap, global hardness, electrophilicity index of this compound have been obtained to elucidate the chemical reactivity behavior to nucleophilic and electrophilic attack reactions. Also, HOMO, LUMO and MEP pilots by visualized with GausView 4.1 program [4] have been used to show the electrophilic and nucleophilic site of this compound. The donor-acceptor interactions being important to intramolecular charge transfer have been evaluated by employing the NBO analysis [5]. The FT-IR vibrational modes and NMR shifts of the studied compound have observed and compared with the simulated values.

Keywords: FT-IR, NMR, donor-acceptor, HOMO, LUMO

Acknowledgments

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References

A NOVEL SANDWICHED COMPOSITE ELECTRO-SPUN MEMBRANE FOR FAST OIL-WATER SEPARATION

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Abstract

In recent years, the issue on oil pollution in water has drawn continuous attention of the researchers. The pollution problem are mainly caused by shipping accidents, offshore or marine vessel leakage and illegal discharges of oily wastes. There needs to be more focus on the removal of oil and cleanup methods. Oil absorber sorbents are very commonly used during oil spills for their cost-effectiveness and affordability. An ideal sorbent material should have high hydrophobicity, high oleophilicity, high uptake capacity and rate, adequate buoyancy, and good recoverability of the adsorbed oil. Man-made materials (synthetic sorbents) are designed to remove oil content from water sources due to their oleophilic properties. Among the oil sorbents non-woven fibrous mats are widely used for oil cleanups due to their scalable production.

In the present work, a novel sandwiched composite membrane is generated by electro-spinning technique. The novel sandwiched composite electro-spun membranes were fabricated by sandwiching the Chitosan incorporated Polyvinyl butyral (PVB) nanofiber mat between two layers of Polyacrylonitrile (PAN) electro-spun mats. Firstly, desired amount of PAN polymer was added to 10 mL % N, Ndimethyl formamide (DMF) then the suspension was subjected to electro-spinning process in order to create a first substrate layer. Secondly, 1.0 wt % of chitosan solution was prepared in 2.0 wt% acetic acid solution then added to PVB-ethanol solution with different ratios. Finally, PVB-Ch nanofiber mat was collected on surface of prepared PAN mat by electro-spinning. After reaching desired thickness of PVB-Ch nanofibers, top layer of membrane consisting of PAN nanofiber was composed by electro-spinning procedure under the same circumstances. The generated membrane surface morphology was observed by SEM and other analysis methods. Oil absorption behavior of membranes were investigated and oil absorption capacities were calculated in terms of weight gain. Membrane exhibited excellent absorption capacity up to 100-150 times its own weight for oil.
Abstract

Hemiaminals (N,O-hemiacetals) are tetrahedral intermediates during imine and enamine formation reactions and are usually not isolable. Thus, the synthesis of hemiaminals is a challenging task for organic chemists [1]. The present work describes stereoselective reductions of several heterocyclic compounds to produce hemiaminals and their stereoisomeric assignments. Some of the hemiaminals have been found to be exceptionally stable. Some others have been found to eliminate water with time to produce eneamidines. The elimination products have been exploited to assign configurations to the chiral carbons at C-4 of the heterocyclic ring. The NMR analyses of the hemiaminals showed that the cis and trans hydrogens of the heterocyclic ring have different coupling constants (Figure 1). The C-4 hydrogen of the major isomer had a very small coupling constant (2.0 Hz), whereas the minor one of the same proton coupled with a larger J (6.4 Hz). To assign with certainty the cis and trans isomeric products, the bromination reaction forming the compound 2 has been used. Based on the found NMR results, the smaller coupling constant has been assigned to the cis and the larger to the trans isomer. The M and P isomeric assignments have been done based on the anisotropic effects of the o-aryl substituent.

Figure 1. The $^1$H NMR coupling constants between C-5H and C-4H of 1 and 2.

Key Words: Stable hemiaminals; Chiral hemiaminals; Stereochemical assignments; cis-trans coupling constants; Hemiaminals of heterocyclic compounds

References
Abstract
Drying is simultaneous heat and mass transfer energy intensive operation, widely used as a food preservation technique. In the present study, the applicability of cabinet dryer was investigated at the air temperature of 50, 60, 70 and 80°C for drying of kumquat slices. Freshly harvested kumquat slices were successfully dried from initial moisture content of 440.54 to 42.30% (d.b.) and their drying characteristics and kinetics were evaluated. Results indicated that drying time and slice thickness were more affected by drying air temperature. Drying curves shows that drying occurred in falling rate period and no constant period observed. The effective moisture diffusivity was determined by using Fick’s second law and its mean values ranged between 1.54×10^{-9} and 7.83×10^{-9} m²/s for all investigated conditions. The activation energy was estimated using an Arrhenius-type equation and calculated to be 51.91 kJ/mol. The drying data was fitted to five thin-layer drying models such as Lewis, Henderson & Pabis, Logarithmic, Parabolic and Wang & Singh. The models were compared using statistical criteria based on, the coefficient of determination, root mean square error, and reduced chi-square value. The logarithmic model found to be most suitable to describe the drying kinetics of kumquat slices in the cabinet dryer.

Keywords: Hot-air drying, kumquat, mathematical modelling, Logarithmic model.
INHIBITION EFFECT OF POLYACRYLIC ACID AND ITS MIXTURE WITH POTASSIUM IODIDE ON MILD STEEL CORROSION IN ACID SOLUTION

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Abstract
Organic corrosion inhibitors are one of the most appropriate process for prevention many metals from corrosive environments due to their strong adsorption interactive with metal surface. The molecular structure of inhibitor molecules plays a major role on their adsorption capability. Especially, heteroatoms like sulphur, nitrogen, phosphorus and oxygen, π-electrons and electronegative functional groups offer organic molecules significant adsorption behaviour. The protective adsorption layer become since inhibitor molecules adhere to the metal surface. Synergistic effect offers meaningful way to enhance inhibition efficiency on metal against corrosion. It is well known that inhibition efficiency could be increased with additive of halide ions, especially iodide [1-2].

In this study, the inhibition efficiency of polyacrylic acid (PA) and potassium iodide (KI) mixture has been investigated against mild steel corrosion in 0.5 M HCl acid solution. Potentiodynamic and electrochemical impedance spectroscopy measurements were carried out for better understanding the corrosion process. Surface morphology was studied by scanning electron microscopy. Furthermore, the effect of immersion time was investigated. The results showed that mixture of polyacrylic acid and potassium iodide have good inhibition efficiency for steel corrosion.

Key Words: Synergistic effect, acid solution, corrosion inhibitor

Figure 1. Nyquist plots for mild steel in 0.5 M HCl solution (●) and in presence of 10 % PA with different concentrations of KI: 1.0 mM (□) and 2.0 mM (●).

Acknowledgements
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References
DETERMINATION OF WATER CONTENT IN APROTIC SOLVENT BY ANTRAQUINONE-MODIFIED MULTI-WALLED CARBON NANOTUBES

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Abstract

The Attachment of ethylenediamine bearing BOC (tert-butyloxy carbonyl) by electrochemical oxidation of corresponding diamine linker was achieved onto multi-walled carbon nanotube immobilized at glassy carbon surfaces. Subsequent to removal of BOC protecting group, the coupling of anthraquinone-2-carboxylic acid to amine-terminated surfaces was carried out using solid-phase synthesis methodology. It was demonstrated that anthraquinone exhibits electrochemically two sequential single-electron reductions in aprotic solutions through cyclic voltammetry technique. Peak separation potential between first and second electron transfer step was found to be decreased with the addition of water as a proton source. When the water concentration reaches up to 1 M, only one electrochemical process due to formation of hydrogen bonding between reduced form of anthraquinone and aprotic solvent (acetonitrile) [1-2]. Determination of water content in the aprotic solutions was shown to be quite possible using linear relationship between water concentration and peak separation potential. Limit of detection was also calculated to be around 1.1x10^{-7} M.

Key Words: Carbon nanotubes; Antraquinone; Electrode Modification; Aprotic solvent; Water content.
References


NEW ELECTRODE MATERIALS AND ARRANGEMENTS FOR MONITORING OF TRACE CONCENTRATIONS OF BIOLOGICALLY ACTIVE ORGANIC COMPOUNDS

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Abstract

The presentation will focus on new electrode materials (solid silver amalgams [1], carbon films [2], boron doped diamond, [3] bismuth [4], and antimony[5]) used in our laboratory for voltammetric and/or amperometric monitoring of submicromolar concentrations of various biologically active organic compounds (environmental carcinogens, biomarkers of exposure, treatment or illness, pesticides, nitrophenols and other priority pollutants, dyes, drugs and their metabolites, etc.) in various biological and environmental matrices. Their advantages and disadvantages will be critically compared together with methods of pre-treatment and approaches to prevent their passivation. Attention will be paid to their use both in batch arrangements (voltammetry in single drop of the solution, in membrane separated micro vessels, etc.) and in flowing systems (high performance liquid chromatography or flow injection analysis with amperometric detection using thin-layer, wall-jet, tubular or microcylinder arrangements). At the end the combination of these newly developed methods with advanced methods for preliminary separation and/or preconcentration (solid phase extraction, membrane separation, hollow fibre microextraction, etc.) will be discussed and their applications for the determination of biologically active organic compounds in biological (urine, blood, plasma, etc.) and environmental (drinking, river, and waste water) matrices will be discussed.

Key Words: Solid amalgam electrodes; Carbon film electrodes; Boron doped diamond film electrodes; Bismuth film electrodes, Antimony film electrodes

Acknowledgement

This work was financially supported by the Czech Science Foundation (project P206/12/G151).

References

NEW SYNTHETIC METHODS FOR PYRAZOLE FUSED HETEROCYCLIC COMPOUNDS

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Abstract

Nitrogen-containing heterocycles are key components in a myriad of biologically active compounds. Indeed, recent surveys have reported that greater than 90% of molecules currently under investigation by pharmaceutical companies contain nitrogen heterocycles, especially pyridine derivatives. Pyrazolopyridines constitute an important class of pharmacologically active compounds and are often employed as indole isosteres due to the irreleatively high metabolic stability. Notably, pyrazolo[1,5-a]pyridines, specifically when substituted in the 2-position, are known for their ability to act as dopamine D3 agonists and antagonists and are used in the treatment of psycho-stimulant addictions. Additionally the D3 receptor controls dopamine synthesis, release, and neuronal firing and is linked to the pathophysiology of Parkinson’s disease as well as schizophrenia. Other applications of pyrazolo[1,5-a]pyridines include an adenosine A1 receptor antagonist with potent diuretic activity as well as their use in the treatment of cardiac arrhythmias and for the diagnosis of ischemic heart diseases. Finally, certain pyrazolo[1,5 a]pyridine derivatives have also been found to have superior reactivity than acyclovir and its prodrug valacyclovir as antiherpetic agents [1]. A series of 4-oxo-4,5,6,7 tetrahydropyrazolo[1,5-a]pyrazine-2-carboxamides was synthesized and tested for their inhibition of HIV-1 integrase catalytic activity and HIV-1 replication in cells. [2].

Key Words: Antiherpetic; HIV-1 integrase inhibitor; dopamine D3 antagonist;
References
GENOTOXIC EVALUATION OF ALCOHOLIC AND HEXANE EXTRACTS FROM AN ENDEMIC PLANT THERMOPSIS TURCICA ON LIVER CANCEROUS CELL LINE

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Abstract
Traditional medicines are used for therapeutic purposes all over the world. Many endemic plants all over the world have magical therapeutic potential. These could be explored further for medicinal purposes and hence can be preserved for their proper propagation. Theraposis turcica (\textit{T. Turcica}) is endemic to turkey. It’s general anti-oxidant and anti-cancerous activities are explored, but not study has been observed on liver cancerous cell line in term of its genotoxicity. So, genotoxic evaluation was carried out for the alcoholic and hexane extracts of \textit{T. Turcica}.

Methanol extracts showed the highest DNA damage (20±1) at 250 µg/ml concentration and 11.67±2.52 at 100 µg/ml. Ethanol extracts showed the 2\textsuperscript{nd} highest DNA damage (19±2) at 250 µg/ml concentration and 11 ±1 at 100 µg/ml. While least was observed in the hexane extract (10.33±1.15; 6±2) at both concentrations, respectively. All groups were significantly differ from the control group at both concentrations. A current study concluded that \textit{T. turcica} had the genotoxic effects on the liver cancerous cell line and alcoholic extracts showed the more DNA damage on HepG2 cells.

\textit{Keywords: Endemic plant; Genotoxicity, DNA damage}
NANOSTRUCTURED FUNCTIONAL MATERIALS BASED ON SELF-ASSEMBLY OF BLOCKCOPOLYMERS

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Abstract

Block copolymer (BCP) self-assembly is a promising means to generate nanopatterns, nanopore, nanoarrays on the surfaces with a high density of regularly sized nanoscale pores. Block copolymers consist of macromolecules composed of two or more chemically different blocks which can self-organize into different morphologies with characteristic sizes in the nanometer scale. BCPs with immiscible blocks microphase-separate into domains in which the equilibrium domain size (typically 3–100 nm) and morphology are governed by the Flory-Huggins interaction parameter between the blocks and the degrees of polymerization of each block. Diblock copolymers can self-assemble in their neat state to form spheres, cylinders, gyroids (a complex periodic bicontinuous cubic structure) and lamellae [1-4]. Self-assembled block copolymer is evolving as a powerful yet affordable tool to fabricate nanoporous materials with well defined controlled morphology, form periodic nanopatterns with periods of a few nanometers without any lithographic method. BCP blocks are able to generate structuring a functional materials which can be photonic crystal, or used as a mask to pattern formation for functional nanomaterials, functionalized directly by various chemical approaches, or used as a scaffold to assemble nanostructures. BCPs offer tremendous flexibility in creating nanostructured materials with a range of applications in microelectronics such as circuits, transistors, diods or photovoltaics, nanostructured nanopore membranes, and other devices. The periodicity of the functional structure depends on the molecular weight of blocks and can range from a few nanometers to hundred of nanometers. Many of these applications are based on thin films of BCPs, one of the most widely studied applications is in nanoscale lithography, and the blocks can be removed by etching using chemical, reactive ion etching or plasma process and the remained one is used as a mask to define features in many applications [5].

In this presentation the application of BCPs films for creating of nanostructured functional materials that can be applied in fabrication of nanopattern, nanoarray, integrated circuits, magnetic storage media, sensors, photonic crystals, photovoltaics, or snanostructured nanopore membranes will be presented.

References

APPLICATIONS OF CORE-SHELL COMPOSITE HYDROGELS IN DRUG DELIVERY SYSTEMS

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Abstract

Polysaccharide biopolymers widely used in biomedical field such as for cell encapsulation, drug delivery, wound dressings, contact lenses and tissue engineering because of their unique biocompatibility and biodegradability. However, the hydrophilic nature and porosity of the gels cause easy burst and fast release rate [1-2]. Core-shell hydrogel systems exhibit advantages in drug delivery due to their layered geometry which provide advanced encapsulation. They have a structure that consisting of a core component in the centre and a shell that surrounding the core [3-5].

In this study, core-shell hydrogel beads were synthesized by incorporating metoprolol tartrate in the core component to control the initial burst release. The core of beads was prepared by crosslinking of the mixture of sodium alginate and kappa-carrageenan by using Ca$^{2+}$ and K$^{+}$. Then the core was covered with sodium alginate or kappa-carrageenan. The structure of core-shell hydrogel beads was characterized by Fourier Transform Infrared Spectrophotometer (FT-IR) and Scanning Electron Microscopy (SEM). The results indicated that swelling kinetics, encapsulation efficiency and release behaviour of beads changed with core-shell combination.

Key Words: Hydrogel; core-shell; sodium alginate; kappa-carrageenan; drug delivery.

References

ADSORPTION OF Th(IV) ONTO CHEMICALLY MODIFIED ACTIVATED CARBON

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Abstract

Rapid industrialization has led to the increased disposal of heavy metals into the environment. A wide variety of industries are responsible for the release of heavy metals through their wastewater. Presence of radionuclides and toxic metals in wastes is a major environmental concern [1]. The removal of radionuclides and toxic metals such as uranium and thorium from aqueous waste solutions seems to be a significantly useful subject for environmental control. Thorium is a naturally occurring radioactive element widely distributed over the earth’s crust with nuclear significance. The toxic nature of this radionuclide, even at trace levels, has been a public health problem for many years [2]. Nowadays, various methods have been developed for the separation of Th(IV) from aqueous solutions, including biosorption, liquid–liquid extraction and solid-phase adsorption. Adsorption is considered to be a particularly competitive and effective process for the removal of trace quantities of heavy metals from aqueous solutions [3]. Adsorption based on carbon materials, such as activated carbon, carbon nanotube has been used due to their high adsorption capacity, high thermal and radiation stability. The active carbon surface may exhibit neutral, basic or acidic properties due to the presence of surface functional groups. The aim of the present study is to investigate the influence of various experimental parameters on thorium adsorption and determine the optimum conditions for the maximum adsorption of thorium by chemically modified activated carbon from aqueous solution.

In this work, the granular activated carbon (GAC) was modified with nitric acid and it was called as AC1. The modified material was characterized by X-ray diffraction analysis (XRD), Fourier Transform Infrared (FT-IR) and Brunauer–Emmett–Teller (BET) method. Adsorption of Th(IV) onto AC1 has been evaluated in terms of equilibrium, kinetics and thermodynamics studies. The effects of contact time, pH, initial concentration, and temperature were investigated. The isotherm models, such as Freundlich, Langmuir, Temkin and Dubinin–Radushkevich have been used to describe the equilibrium data. Kinetic data obtained from the batch adsorption studies were fitted to pseudo-first order and pseudo-second order equations. Th(IV) adsorption by AC1 was pH dependent (pH range, 3.0–6.0) and maximum sorption was observed at pH 5.5. Adsorption process is well described by Langmuir isotherm in comparison with Freundlich, Dubinin–Radushkevich (D-R) and Temkin isotherms. Thermodynamic data (ΔH°, ΔS°, ΔG°) were calculated from the temperature dependent sorption isotherms. Results suggested that the adsorption of Th(IV) on AC1 was a spontaneous and endothermic process. According to comparison of kinetic models applied to the adsorption of Th(IV) onto AC1, the experimental data fitted very well the pseudo-second order kinetic model.

Key Words: Thorium, Adsorption, Activated carbon, Modification

References

EXPERIMENTAL AND COMPUTATIONAL CHEMISTRY STUDIES ON THE INHIBITION EFFICIENCY OF PHTHALIC ACID (PHA) FOR THE CORROSION OF ALUMINUM IN HYDROCHLORIC AND TETRAOXOSULPHATE (VI) ACIDS.

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Abstract

In this work, phthalic acid is investigated for its corrosion inhibition properties (for aluminum in solutions of HCl and H₂SO₄) through experimental and computational chemistry methods. The experimental approach was achieved by using gravimetric (weight loss), linear and potentiodynamic polarization techniques as well as two spectroscopic techniques (Fourier transformed infra red and scanning electron microscopy). The theoretical approach incorporated the computation of semi empirical parameters and Fukui functions. Data obtained from weight loss were in strong agreement with those obtained from polarization methods. They generally pointed to the conclusion that phthalic acid inhibited the corrosion of aluminum better in solution of HCl than in solution of H₂SO₄. The inhibition efficiency of the inhibitor increases with increase in concentration but with increasing period of contact and temperature, the inhibition efficiency notably decreased. Confirmation of a physical adsorption mechanism was established by observed low values of activation energy and free energy of adsorption as well as the trend of decrease in inhibition efficiency with temperature. Frumkin and El awardy et al adsorption isotherms best fitted the adsorption characteristics of phthalic acid on aluminium (in both HCl and H₂SO₄ media). The isotherms revealed that the inhibitor occupies more than one adsorption site and exhibited attractive behavior. Calculated quantum chemical parameters were within the range reported for good corrosion inhibitors while Fukui function, Huckel charge, HOMO-LUMO graphs and FTIR analyses indicated that phthalic acid is adsorbed on aluminum surface via the carboxylic oxygen atom.

Key Word: Corrosion, aluminum, inhibition, phthalic acid
SYNTHESIS AND FLUORESCENCE PROPERTIES OF SCHIFF-BASE FLUORINE-BORON COMPLEXES

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Abstract

Schiff base chemistry is a versatile tool in organic synthesis and it has played an important role in the development of coordination chemistry since it is all about the forming complexes with most transitions metals. They have wide applications in analytical chemistry, in medicine and in biological processes including antifungal, antibacterial and anticancer activities [1]. The extensive studies of these compounds have been conducted on the complexation with metals for the construction of new molecular materials due to attractive biological, catalytic and physicochemical properties [2].

Luminescent organic materials have recently received considerable attention due to their potential application, for example, as molecular probes in biomedical labeling and analysis and as organic electronics in material science [3].

Among those, BODIPY (4,4-difluoro-4-bora-3a,4a-diaza-s-indocene) derivatives as the well-known organoboron complexes due to their excellent photophysical properties [4].

Besides the BODIPYs considerable research efforts have been devoted to boron-chelating complexes [5]. Therefore, in this study, the synthesis, the characterizations and the fluorescence property studies of a series of BF₂ complexes of Schiff bases in solution

Key Words: Schiff base; Fluorine-boron complexes; fluorescence; Emission; Quantum yield

References

ELECTROCHEMİCAL BEHAVİOUR OF OFLOXACİN İN PHARMACEUTİCAL AND BİOLOGİCAL SAMPLES USİNG A BORON-DOPED DIAMOND ELECTRODE İN USİNG ANİONİC SURFACTANT

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Abstract

This paper examined use of a boron doped diamond electrode (BDDE) for the electroanalysis of ofloxacin (one of the fluoroquinolone compounds) by cyclic voltammetry (CV) and square wave voltammetry (SWV) in the presence of anionic surfactant (SDS) for the first time. The current signal due to the oxidation process was a function of the amount of ofloxacin, pH of the medium, effect of anionic surfactant (sodium dodecyl sulfate) and scan rate. Cyclic voltammetric studies indicated an irreversible behaviour of ofloxacin in phosphate buffer solution at pH 2.0 with well-defined oxidation peak at +1.24 V (absence SDS) and +1.21 V (presence of SDS) vs. Ag/AgCl, respectively. With optimized experimental parameters, the current response of ofloxacin was proportionally linear in the concentration range from 1.0×10⁻⁷ to 3.5×10⁻⁶ M. A detection limit of 1.76×10⁻⁸ M was observed anodically electrochemical surface pretreatments. The practical applicability of the developed method was demonstrated on the determination of ofloxacin in human urine and pharmaceutical samples. In this way, BDD electrode may represent an efficient alternative to widely used modified electrodes in the determination of fluoroquinolone compounds.

Key Words: Ofloxacin, Sodium Dodecyl Sulfate, Boron-Doped Diamond Electrode, Square-Wave Voltammetry, Biological and Pharmaceutical Samples
EFFECT of PROCESS PARAMETERS on the PRODUCTION of METAL INCORPORATED SILICA AEROGELS

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Abstract
Aerogel is the lightest solid material known in the world used in a wide range of applications due to their unique features such as high porosity (until 99.8%), very large surface area (up to 1200 m$^2$ g$^{-1}$), low density (0.003-0.15 kg m$^{-3}$) and low thermal conductivity (as low as 0.01 W m$^{-1}$ K$^{-1}$). The most charming features of aerogels are the adjustable pore size, pore volume, surface area, and thus aerogels can be conveniently manufactured for several branches of industry. [1, 2].

The aim of this study was to investigate the effect of process parameters (feeding rate and molar ratio of Si:Ca:Mg) on the several properties (density, surface area, pore size, pore volume, elemental compositions and morphology) of metal incorporated silica aerogels. Metal-incorporated silica aerogels are produced via solvent exchange method and dried at ambient pressure. Calcium and magnesium chloride salts are used as the source of metal additive and water glass as sodium silicate source. Characterization tests are evaluated by several techniques such as Fourier transform infrared spectroscopy (FTIR), scanning electron microscope (SEM), inductively coupled plasma optical emission spectroscopy (ICP-OES), tapped density, specific surface area and pore size of aerogels have been analysed by the N$_2$ adsorption and desorption measurements at 77 K via Brunauer–Emmett–Teller (BET) and Barrett–Joiner–Halenda (BJH) methods.

The results showed that calcium incorporated silica aerogel has a lower density (0.16 g cm$^{-3}$), and lowest surface area; magnesium incorporated silica aerogel has the highest surface area (609 m$^2$ g$^{-1}$), and highest density. Further studies should be carried out on the other process parameters and the drying methods to widen the range of silica aerogels with advanced features.

Acknowledgement: The authors are grateful to the TUBITAK (The Scientific and Technological Research Council of Turkey) for the financial support through a 1005 project (Project No: 115M469).

Key Words: Aerogel; Calcium; Magnesium; Silica aerogel; Surface area.

References
MECHANISM OF THE ELECTRON-EXCHANGE REACTIONS BETWEEN MIXED LIGAND Fe(III) COMPLEXES AND CYANO COMPLEX OF Fe(II)

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Abstract

Our interest was to study the reactions of those mixed ligand complexes of Fe(III), where cyanide plays its role as a ligand. We synthesized the mixed ligand complexes of Fe(III) with diimine and cyanide as ligands to form an octahedral geometry with high stability. We adopted previously cited procedures with improvements.\textsuperscript{1,2} The synthesized complexes, $[\text{Fe}^{\text{III}}(\text{diimine})_2(\text{CN})_2]^+$ were reduced by the hexacyano complex of Fe(II) that is well-known for its high stability and octahedral geometry. The reduction was performed in aqueous medium at constant ionic strength 0.06 M. The progress of the reactions was monitored spectrophotometrically by measuring the formation of $[\text{Fe}^{\text{II}}(\text{diimine})_2(\text{CN})_2]$ i.e., increase in absorbance along time. We found that the reduction of the mixed ligand Fe(III) complexes takes place in two phases. The first phase, when the Fe(III) complex is reduced to the neutral Fe(II) complex by following zeroth order kinetics. The second phase was observed to be the rate-determining or slow step in the reduction of each complex, and the electron-exchange took place by an overall second order kinetics. We have also observed a third phase in the reaction pathway, where the rate of electron-transfer and the rate of the insolubility of Fe(II) product competed each other, as we were following the reaction via monitoring the absorbance of $[\text{Fe}^{\text{II}}(\text{diimine})_2(\text{CN})_2]$. As the concentration was increased with the completion of the reaction, the solubility of the neutral product was becoming decreased and though the absorbance decreased. In order to refine our results and to differentiate between the species, which were taking part in the rate-determining step (slow step) and those which were taking part in the fast step, we studied the effect of several parameters on the rate constant. In the view of transition state theory for reactions in solutions, we tried to find out the active species that control the rate of reaction. We studied the effect of protons, ionic strength in various mixed solvent systems, and temperature to calculate thermodynamic parameters of activation. We proposed an outer-sphere mechanism for the electron-exchange between Fe(III) and Fe(II) complexes. The following rate law is proposed for the two electron-exchange reactions.

$$-\frac{d[\text{Fe}(\text{II})]}{dt} = k_1 + k_2[F\text{e}(\text{III})][\text{Fe}(\text{II})] + \frac{k_3[\text{Fe}(\text{III})]}{K_{H^+}[\text{Fe}(\text{II})]}$$

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STRUCTURAL CHARACTERIZATION and IN VITRO BIOACTIVITY of TITANIUM-DOPED 45S5 BIOGLASSES

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Abstract

Bioactive glass has been applied widely in bone tissue engineering applications due to its good bioactivity, biodegradability and osteoconductivity [1]. Recently, modification of conventional bioglass composition by addition of different elements have received much attention in the biomaterials field. The aim of this study was to prepare and characterize novel TiO₂ doped 45S5 bioactive glasses by melt quenching technique using rice husk biosilica as silica source. The properties of bioglasses were evaluated as a function of TiO₂ content (0.5 - 4%) using various techniques (Fourier transform infrared spectroscopy (FTIR), scanning electron microscope (SEM), Vickers hardness measurement). In vitro bioactivity studies of the glasses were investigated by immersion tests in simulated body fluid (SBF) up to 4 weeks while monitoring the composition of the biological medium by ICP-OES analyses. The FTIR, SEM and Vickers hardness studies were executed before and after immersion tests. The hydrolytic degradation behavior of samples was monitored through the pH change and weight loss in the tris-(hydroxymethyl)-aminomethane solution (TRIS). The biocompatibility evaluation of the bioglass samples was carried out through in vitro cell culture (MTT cell viability and cytotoxicity tests of SAOS-2 cells) tests. SEM and FT-IR results indicated that carbonated hydroxyapatite crystals were formed on the bioglasses. Vickers hardness of glasses showed an increase with increasing TiO₂ content. The pH of the TRIS slightly increased with the increment of immersion time. Moreover, it was observed that the biodegradation behavior of bioglasses enhanced with the addition of titanium. The highest weight loss was realized for 1 and 4% TiO₂ doped bioglass samples. In vitro biocompatibility tests revealed that incorporation of TiO₂ to the bioglass promotes differentiation and stimulates bone growth. The high bioactivity and biocompatibility of the TiO₂ doped bioglasses suggest that they can be a potential alternative to the conventional glasses in bone regeneration applications.

Acknowledgement: The authors are grateful to the TUBITAK (The Scientific and Technological Research Council of Turkey) for the financial support through a 3001 project (Project No: 21M647).

Key Words: Biomaterial; Bone repair; Biosilica; Doped bioactive glass; Titanium

References

AXIALLY CHIRAL QUINAZOLINE-4-ONES

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Abstract

The compounds containing the quinazoline scaffold are versatile synthetic building blocks and precursors of many biologically active molecules[1]. Because of their great value, the synthesis of quinazoline derivatives has always received much attention.

The reaction of anthranilic acid and appropriate isothiocyanates in toluene gave the mixture of 1, 2, 3 and 4. When the same reaction was carried out in ethanol only 2-thioxo-3-(o-aryl)-quinazolin-4-ones (1) were obtained. The treatment of the mixture of 1, 2, 3 and 4 with NaOH in methanol gave the compound 1, indicating that compounds 3 and 4 underwent the Dimroth Rearrangement. 2-Thioxo-3-(o-aryl)-quinazolin-4-ones (1) were then converted to 2-(benzylthio)-3-(o-aryl)-quinazolin-4-ones (5) by the reaction of benzylbromide (BnBr) in the presence of NaOH in methanol.

The quinazoline derivatives reported in the present study except compounds bearing phenyl group on N3 are axially chiral due to hindered rotation about N3-Caryl bond and the partial rotation around this bond gives rise to formation of M and P enantiomers. The rotational barriers of these compounds were determined by the thermal racemization of the separated enantiomers [2]. The rotational barriers ranged from 112.7 to 140.8 kJ/mol, depending on size of the ortho substituent. The rotational barriers in 2-(benzylthio)-3-(o-aryl)-quinazolin-4-ones (5) were found to be about 2 kJ/mol higher than the corresponding 2-thioxo-3-(o-aryl)-quinazolin-4-ones (1).

Key Words: Quinazolin-4-ones; Axial chirality; Barriers to rotation; Chiral HPLC; Thermal racemization

References

Abstract

Our main research area is the synthesis and characterizations of different types of stimuli-responsive (co)polymers which have great response to external conditions. They can self-assemble into various nanostructures (micelles, reverse-micelles, flower micelles, gelation, flocculation, etc.) depending on a change of pH, temperature, ionic strength etc. They are getting more and more attention for various applications such as in biomedical technology (as antibacterial agents, drug carriers, controlled releasing systems etc), in sensor technology, in cosmetics... Recently, we have focused on poly(glycidyl methacrylate) based block copolymers and their derivatisations with morpholine, piperazine and tertiary amine type reactants which provide surface activity, water solubility and response to external stimuli. Additionally, derivative polymers can also be converted into different structures with further reactions. They can self-assemble and form core-shell spherical micelles depending on solution conditions due to presence of a block with LCST behaviour. To keep their structure stable, cross-linking chemistry is most commonly preferred pathway which may result with the preparation of core cross-linked (CCL), shell cross-linked (SCL) and/or intermediary layer cross-linked (ILCL) micelles. These cross-linked micelles are good host for the production of nanometal dispersions with a diameter around 5 nm as well. They may also act as suitable drug delivery vehicles for the encapsulation and release of hydrophobic drugs as a function of pH.

Figure 1. Types of spherical cross-linked micelles (SCL, ILCL and CCL, respectively).

Important outcomes of these copolymers are the usages as (i) stabilisers in heterogeneous polymerisations for the production of latex, microgel and nanometal dispersions, (ii) source for novel cross-linked micelles, hydrogels, antibacterial materials, LbL nanofilms, etc. On the other hand, we also succeeded to prepare a novel multi-responsive microgel of a water soluble monomer and “microgel-liposome” system having a potential in drug targeting/releasing applications.

Keywords: Copolymer, self-assembly, cross-linking, micelles, microgels, hydrogels, stimuli-responsive.
SYNTHESIS AND CHARACTERIZATION OF COBALT (II) COMPLEX AND ITS CATALYTIC ACTIVITY ON ALCOHOLS/ALKENES OXIDATION

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Abstract
In catalysis studies, expensive metals such as Pd, Pt, Ru are very active and frequently used, but one of the main objectives in catalytic studies is the use of cheap and active metals in reactions. Conversion of alcohols to carbonyl compounds with oxidation reactions is one of the most important reactions of synthesis of fine chemicals [1].

In this work, we synthesized a new Co(II) complex, [Co(tsabut)(H₂O)(phen)₂]·ClO₄ (where tsabut = 2,2’-(butane-1,4-diylbis(sulfanediyl))dibenzoic acid, phen = 1,10-phenantroline) and characterized through X-ray crystallography. The catalytic activities of Co(II) complex on oxidation of various alcohols (cyclohexanol, cinnamyl alcohol and benzyl alcohol) and alkenes (cyclohexene, styrene and ethylbenzene) were performed in acetonitrile with t-BuOOH as the source of oxygen.

Key Words: Complex, Crystallography, Catalysis, Oxidation.

Figure 1. The molecular structure of Co(II) complex

References
SYNTHESES AND SPECTROSCOPIC CHARACTERIZATIONS OF MONO CYCLO-2,2’-DIHYDROBIPHENYLPHOSPHAZENE BEARING VANILLINATO GROUPS

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Abstract

Cyclotriphosphazenes are an noteworthy class of inorganic cyclic compounds because of active P-Cl bonds enables substitution reactions with different types of inorganic and organic functional groups [1 and 2]. In this study, we synthesised monocyclo-2,2'-dihydrobiphenylphosphazene Then, the gradual Cl replacement reactions of monocyclo-2,2'-dihydrobiphenylphosphazene (2) with the potassium vanillinate resulted in the mono (2a), di (2b, 2c and 2d), tri (2e), tetra (2f) vanillinato substituted phosphazene derivatives (Scheme 1). The synthesized compounds were purified by column chromatography. The FTIR, ¹H, ¹³C and ³¹P NMR techniques were used for the characterizations of new cyclophosphazene derivatves.

Scheme 1 Syntheses route of monocyclo-2,2'-dihydrobiphenylphosphazene bearing vanillinato groups

Key Words: 2,2'-dihydroxybiphenyl, vaniline, hexachlorocyclotriphosphazene, spectral analysis.

References


Acknowledgments

The authors acknowledge the “Karabuk University, Scientific Research Unit” Grant No. KBÜBAP-17-YL-440.
VOLTAMMETRIC SENSING OF TRICLOSAN BASED ON THE ENHANCEMENT EFFECT OF THE CATIONIC SURFACTANT AT CATHODICALLY PRETREATED BORON-DOPED DIAMOND ELECTRODE

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Abstract

Triclosan (TCS) is a non-ionic antibacterial, antimicrobial and antifungal agent, that has been widely used as an antiseptic or preservative for over 50 years in personal care products at concentrations of 0.1-0.3% (w/w), such as deodorants, liquid soaps, shampoos, skin creams, toothpastes as well as in the other consumer products including detergents, food-stuffs, medical devices, clothing, plastic materials, etc. However TCS has been found to be acute toxicity, resistance to biodegradation, environmental persistence and relatively high lipophilicity [1, 2]. Due to its widespread use and toxicity, it is important to develop sufficiently selective, sensitive, simple and rapid analytical methods for the detection and quantification of TCS in commercial formulations and environmental samples at trace levels. In the present study, a simple, cheap, and sensitive electrochemical method based on a cathodically pretreated boron-doped diamond (CPT-BDD) electrode is described for the detection of TCS with the cationic surfactant (cetyltrimethylammonium bromide, CTAB) media. The oxidation of TCS was irreversible and exhibited an adsorption controlled process. The sensitivity of the adsorptive stripping voltammetric measurements was significantly improved with addition of CTAB. Using square-wave stripping mode, a linear response was obtained for triclosan determination in Britton-Robinson buffer solution at pH 9.0 containing 2.5×10⁻⁴ M CTAB at around +0.67 V (vs. Ag/AgCl) (after 30 s accumulation at open-circuit condition). The method could be used in the range of 0.01 to 1.0 μg mL⁻¹ (3.45×10⁻⁸-3.45×10⁻⁶ M), with a detection limit of 0.0021 μg mL⁻¹ (7.25×10⁻⁹ M). The proposed procedure was also applied to determine TCS in spiked tap water samples.

Key Words: Triclosan; Cathodically pretreated boron-doped diamond; Cetyltrimethylammonium bromide; Square-wave adsorptive stripping voltammetry; Tap water.

References

POSSIBLE REACTION PATHWAYS of THE OXYDIBENZENESULFONYL HYDRAZIDE (OBSH) MOLECULE ACCORDING TO THE DFT CALCULATION METHOD

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Abstract

Oxydibenzensulfonyl Hydrazide (OBSH), in some conditions, can react as a foaming agent while also reacting as a crosslinking agent in the curing reaction. It can also be applied in the production of elastomer under room pressure (such as SBR, neoprene, natural rubber), and of thermoplastic products (such as PVC, PE, PS, ABS plastics), or used together with the blends of resin and rubber. It has great ascendancy for manufacturing wire and cable with its good insulatibility [1]. Quantum chemical calculations of Density Functional Theory (DFT) were used to investigate the structural and physical characteristics of OBSH.

The geometric shapes of molecule obtained because of optimization (grey, carbon; red, oxygen; blue, nitrogen; white, hydrogen; yellow, sulphur)

The analysis was made on the probable reaction path of OBSH molecule with OH radicals. The calculation of optimized geometry and the geometric optimization for the determination of the lowest energy status were made via Gauss View 5 and the Gaussian 09 program. Activation energy for the probable reaction paths was calculated and their most stable state from the thermodynamic perspective was determined for the gaseous phase. The aim of this study is to estimate the degradation mechanism of OBSH molecule in gaseous phase. Calculation of the probable reaction path of the activation energy was made, and their most stable state in the thermodynamic frame was determined for this phase.

Key Words: OBSH; DFT; COSMO; Gaussian 09; hydroxyl radical.)

References

INVESTIGATION OF IN-VITRO SALT STRESS ON PEROXIDASE ENZYME OF AMSONIA ORIENTALIS AND PURIFICATION OF PEROXIDASE FROM NON-STRESSED AND SALT-STRESSED PLANTS

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Abstract

In this study, we focused on in vitro salt stress on peroxidase (POD) enzyme activity change of Amsonia orientalis. The plant was subjected to 25, 50, 75, 100, 125 and 150 mM NaCl salinity for 30 days. Change of POD activity was carried out by spectrophotometrically and activity staining assays. Our findings indicated that, POD activity didn’t dramatically change especially when plant exposed to high salinity. The specific activity of POD of non-stressed plant was calculated as 0.74 (U/mg), while the highest specific activity was seen at 50 mM NaCl and the lowest specific activity at 150 mM NaCl as 0.87 (U/mg) and 0.54 (U/mg), respectively. For further analysis of salt stress on POD activity, enzyme was purified from non-stressed and 50 mM salt-stressed A. orientalis. Similar purification profile was observed for non-stressed and 50 mM salt-stressed plant as 4.57 fold purification with 8% yield and 4.10 fold purification with 7% yield, respectively. The molecular weights of purified enzymes from both extract were determined by electrophoretic methods as 81 kDa. These results suggest that POD is a strong defensive enzyme against salinity due to non-change of its activity especially 50 mM NaCl and POD activity monitoring in also crude and purified extract.

Key Words: Peroxidase (POD), Amsonia orientalis, salt stress, purification

References


ADJUSTABLE AC CONDUCTIVITY IN ARDEL/MWCNT COMPOSITES

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Abstract

Ardel is the polyarylate having low specific weight and moisture absorption. This amorphous aromatic copolyester consist of bisphenol-A with terephthalic and isophthalic acid. It has been utilized in wide variety of applications including aircraft, automobile and electrical industries [1]. Additionally, it has excellent mechanical properties with a high glass transition temperature and good electric properties with inherent ultraviolet stability and flame resistance. [2] Carbon Nanotubes (CNTs) and their compounds exhibit extraordinary electrical properties for organic materials, and have a huge potential in electrical and electronic applications such as photovoltaics, sensors, semiconductor devices, displays, conductors, smart textiles and energy conversion devices (e.g., fuel cells, harvesters and batteries). [3]

In the present study, Ardel/Multi-Walled Carbon Nano Tube (Ardel/MWCNT) composites with varying MWCNT concentrations from 1.5 wt. % to 7.5 wt.% were prepared by melt mixing technique [4]. The Fourier Transformed Infrared (FTIR) Spectra, X-ray Diffraction (XRD) and Atomic Force Microscopy images of samples have been analyzed in detail. The micro-structural analyses revealed that a considerable interaction occurs between polymer matrix host and MWCNT guest. The frequency dependences of the real and imaginary components of ac impedance of the samples were determined by impedance analyzer between 10 Hz and 40 MHz in an increasing temperature interval. Additionally, it was observed that the ac conductivity of pure Ardel increases significantly for the higher MWCNT doped samples. The ac conductivity mechanism was also discussed and activation energies of the samples were calculated.

Key Words: Polyarylate; MWCNT; Polymer-MWCNT composites; Electrical properties

References
Abstract

Carbon monoxide is a colorless and odorless gas that, when inhaled, enters the bloodstream and replaces the oxygen on hemoglobin to form carboxyhemoglobin and is therefore a threat to human health. [1, 2] The beneficial effects of CO have been demonstrated in cell culture and animal models of some diseases [3]. CO-releasing complexes are called photoCORMs (photoactivatable CO-releasing molecules). Since the first photoCORM, namely [Mn2(CO)10], was reported by Motterlini et al. [4]

In this study, we investigated the zetasizer measurements of [Mn(phenylimidazole)(2,2-bipyridyl)(CO)3]OTf (Scheme 1) which is a CO-releasing molecule. The Zeta Potential Analyzer was used to measure the Zetasizer Measurements which are zeta potential, mobility and particle size. The stability behavior of complex was determined in different pHs and as function of time in isotonic sodium chloride, dextrose and in PBS.

Scheme 1 Chemical structure of [Mn(phenylimidazole)(2,2-bipyridyl)(CO)3]OTf

Key Words: CO-releasing molecule; phenylimidazole; organometallic manganese complex; zeta potential; particle size; stability; particle charge

References
A TURN OFF FLUORESCENT SENSOR FOR ALUMINIUM IONS

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Abstract

Aluminium is the third most common metallic element and constitutes about 8% of the earth’s crust [1]. Today aluminum is used in wide range in various fields such as cosmetic, kitchen stuff, medicine, cement, cans, foil packing. Although it is very serious threat for the human health, aluminum is used in great amounts thus nowadays many studies about aluminum is done. In studies toxicity of aluminum was determined and it is shown that aluminum causes; neurologic diseases such as Alzheimer and lack of iron based anemia [2]. Serious amount of aluminum, approximately %20, absorbed daily the pots we are cooking our foods which are made of aluminum such as pans, kettles, pots [3].

So far Photochemical Electron Transfer (PET), Flame Atomic Absorption Spectrophotometer (FAAS), inductively coupled plasma atomic emission spectroscopy (ICP-AES) Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES), Electrothermal atomic absorption spectrophotometer (ET-AAS), High Pressure Liquid Chromatography (HPLC) methods are used to determine the aluminum. These methods have some disadvantages like time consuming, need for some pretreatment, have high cost.

In our work, polymeric fluorescent sensor was prepared towards Aluminium ions in aqueous solutions. In this way a new reusable turn off fluorescent sensor was developed for the rapid and high sensitivity determination of aluminium. The influences of experimental parameters such as pH, time and foreign ion concentrations, which may have an effect on the fluorescence intensity, were investigated. The proposed method was successfully applied for determination of aluminium content in water.

This work was supported by Marmara University, Commission of Scientific Research Project (M.Ü. BAPKO).

Key Words: Aluminium, Optical Sensor, Fluorescence, UV-curing.

References

A NOVEL APPROACH FOR QUANTITATIVE ANALYSIS OF UNCONJUGATED BISPHENOL A LEVELS IN MATERNAL AND UMBILICAL CORD BLOOD

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Abstract

Bisphenol A (BPA) is a chemical widely used in manufacturing polycarbonate and epoxy resin, materials that are commonly used in the production of various types of food and beverage containers, including the lining of metal cans [1]. BPA is an endocrine disrupter that can mimic human hormones, recent studies have found that human exposure to BPA results in adverse health effects, such as altered hormone levels, reproductive effects, or increased incidence of diseases, including cancer. The European Food Safety Authority (EFSA) reduced the tolerable daily intake for BPA from 50 to 4 µg/kg /day [2]. Prenatal exposure to BPA can lead to substantial adverse effects on fetal growth and development [3]. This study was conducted to assess BPA concentration in pregnant women and umbilical cord blood to investigate whether maternal BPA exposure affected fetal outcomes. This application presents a simple, fast, and effective method for the determination of the BPA levels in maternal and umbilical cord blood with 1 µg/kg limit of quantitation. We measured the BPA levels of maternal blood (n = 25) and umbilical cord blood (n = 25) with a triple quadrupole tandem LC-ESI-MS/MS system. BPA in blood serum was extracted into acetonitrile, centrifugated and upper phase injected after dilution with water. LC-MS/MS analysis was performed using a pentafluoro phenyl-phase (PFP) column (3 µm, 2.1 × 100 mm) with Varian 325-MS system linked to an electrospray (ES) ionization interface. The injection volume was 50 µl and the column oven was maintained at 40°C. The separation was performed using a gradient with mobile phase from 0.5 mM ammonium acetate in distilled water (Mobile phase A) and acetonitrile (Mobile phase B). The flow-rate was 0.4 ml/min. We observed the range of BPA was from non-detection to 55.03 ng/ml. The mean BPA concentrations in the groups of maternal blood sera were 20.15 ± 0.775 ng/ml and highest level of maternal BPA exposure was 55.03 ng/mL and for umbilical cord blood 25.22 ng/mL was the highest BPA exposure indicator. Elevated prenatal BPA exposure increased the risk of low birth weight, small for gestational age and adverse actions of adipokines in neonates, especially in male infants. These results provide further evidence that maternal exposure is correlated with adverse birth outcomes.

Key Words: Bisphenol A, LC-MS/MS, Umbilical Cord Blood, Endocrine disruptors.

References

PARTICLE CHARGE and STABILITY BEHAVIOUR OF [Mn(2-mercaptobenzimidazole)(2,2-bipyridyl)(CO)$_3$]OTf IN DIFFERENT pHs and SIMULATED BODY FLUIDS

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Abstract

Zeta potential is the charge that develops at the interface between a solid surface and its liquid medium. The net charge at the particle surface affects the ion distribution in the nearby region, increasing concentration of counterions close to the surface. The zeta potential has proven to be extremely relevant to the practical study and control of colloidal stability and flocculation processes. [1] Pharmacological chemists are interested in the development of so-called carbon monoxide releasing molecules (CORMs). These molecules act as inert molecular vehicles that capable of carrying bound CO through the blood stream and only releasing their load when subjected to do so by a specific trigger at defined tissues. [2]

In the present work, the particle charge and stability behaviour of [Mn(2-mercaptobenzimidazole)(2,2-bipyridyl)(CO)$_3$]OTf (Scheme 1) which is a CORM were determined via Zeta Potential Analyzer in different pHs and as function of time in dextrose and in PBS. The Zeta Potential Analyzer was used to measure the Zetasizer Measurements, which are zeta potential, mobility and particle size.

Scheme 1 Chemical structure of [Mn(2-mercaptobenzimidazole)(2,2-bipyridyl)(CO)$_3$]OTf

Key Words: CO-releasing molecule; 2-mercaptobenzimidazol; manganese complex; zeta potential; particle size; stability; particle charge

References

ELECTROCHEMICAL, SPECTROELECTROCHEMICAL AND ELECTROCOLORIMETRIC CHARACTERIZATION OF NOVEL PT(II) AND PD(II) COMPLEXES OF PYRIDINE APPENDED PERYLENE DIIMIDE FOR ELECTROCHROMIC APPLICATIONS

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Abstract

Functionalized perylene diimids (PDIs) and their derivatives display interesting electronic and electron transfer properties such as high quantum yield, photoluminescence, thermal, chemical and photochemical stability, as well as desired optical and electronic properties [1]. All of these properties are important for applications in electrochromic and optoelectronic systems, and can be modulated as a function of the substitution pattern. Therefore, the identification of the electrochemical, spectroelectrochemical and electrocolorimetric properties of new examples of PDI compounds is of vital importance for the evaluation of their usability in various technological areas, especially in electrochromic devices.

In this study, redox and electrochromic properties of pyridine appended PDI ligand and its Pt(II) and Pd(II) complexes have been identified by electrochemical, in situ spectroelectrochemical and in situ electrocolorimetric measurements in DMSO and DCM. The measurements showed that the novel chromophores display fast electron reduction and oxidation processes with considerably narrow electrochemical HOMO-LUMO band gaps, due to high π-electron conjugation in the PDI core. The reduction of the novel compounds at modest potentials suggested that these novel chromophores are good electron acceptors. Pyridine appended PDI and its complexes with Pt(II) and Pd(II) displayed very similar redox behaviour. Accordingly, a remarkable difference between the redox behaviours of palladium and platinum complexes was not observed, since these metals are in the same group with similar chemical and electronic properties. Therefore, it appeared that platinum and palladium metal sides are redox-inactive and all redox processes are PDI ligand-based. The HOMO–LUMO band gaps of the compounds were also calculated from both electrochemical redox data and the spectral data reflecting the relevant electronic transitions. These values within the range of 1.92–1.98 eV were lower than the band gaps of various N,N'-disubstituted-PDI compounds [2] and suitable for their usability in photovoltaic and optoelectronic applications as organic semiconducting materials. Spectroelectrochemical and electrocolorimetric measurements showed the ability of the compounds to give net colour changes between the blue, pink and green colours and thus, their suitability for electrochromic applications.

Key Words: Perylene diimide, Pt(II) and Pd(II), Electrochemistry, Spectroelectrochemistry, Electrochromism

Acknowledgment: This study was supported by The Turkish Scientific Research Council of Turkey, TUBITAK (Project no: 214Z090).
References

DEGRADATION RATE OF PAPER DYED WITH RHEUM RIBES L.

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Abstract

History of dyeing and painting are older than written records and as many fields, were applied on paper too [1]. Generally natural color of the paper is not admired so paper is colored via chromatic methods. There is no evidence on addition of colorants to pulp during initial stages of paper production and cross sections of colored papers show that inner fibers are whiter in tone than those on the surface. This indicates the application of colorant after formation of paper [2]. Palette of organic dyes and pigments used widely at traditional dyeing was limited with natural dyes until development of modern chemistry in 19th century [3]. As dye and pigment source minerals, insects and plants were widely used [4]. Manuscripts as paper based materials go through physicomechanical, chemical and optical changes and running accelerated ageing experiments is beneficial to realize degradation mechanisms [5]. During accelerated ageing of cellulose paper acid catalysed hydrolysis, oxidation, cross-linking and degradation work together. In kinetic studies Arrhenius equation is used with DP (degree of polymerisation) [6]. In this study model papers were dyed with a natural dye obtained from plant Rheum ribes L. and subjected to accelerated ageing tests. In order to estimate the degradation constant, viscosity measurements were performed and data collected were processed in terms of DP. Kinetic constants were evaluated via Arrhenius equation. Spectrophotometer was used to monitor color changes that occur after ageing and results were obtained in CIEL* a*b* color space. In addition, pH values were measured via flat electrode on surfaces of model papers.

Key Words: accelerated ageing; degree of polymerisation, cellulose, degradation, natural dye

References


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ELECTROCHEMICAL INVESTIGATION OF INTERACTION BETWEEN NIMESULIDE AND Cd(II) IONS IN THE ABSENCE AND PRESENCE OF HYDROGEN PEROXIDE

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Abstract

Hydrogen peroxide (H\textsubscript{2}O\textsubscript{2}) is an indispensable substance in chemical industry, food industry, pharmaceutical industry, clinical medicine and environmental monitoring. Catalase, a typical peroxidase, is a natural enzyme to detect and decompose H\textsubscript{2}O\textsubscript{2} into oxygen and water. Such natural enzymes act as an efficient biocatalyst to increase the rate of reaction by reducing the activation energy of the chemical reaction \cite{1}.

Nimesulide (NIM), is a weakly acidic non-steroidal anti-inflammatory drug. It differs from other non-steroidal anti-inflammatory drugs (NSAIDs) in that its chemical structure contains a sulfonanilide moiety instead of carboxylic group. NIM presents high antiinflammatory, antipyretic, and analgesic activities in addition to low toxicity, a moderate incidence of gastric side effects, and a high therapeutic index \cite{2}. The use of metal ions and their compounds in the treatment of human illness is known for centuries \cite{3}. Thus, it is important to research the interaction of drugs with metal ions.

The aim of this study was to investigate the interaction of Cd(II) ions with NIM at phosphate buffer (pH=7.40) in the absence and presence of H\textsubscript{2}O\textsubscript{2} by using square-wave voltammetry technique. Cd(II) gave a reduction peak at -0.94 V in the absence of NIM or H\textsubscript{2}O\textsubscript{2}. At physiological pH (7.40) NIM and H\textsubscript{2}O\textsubscript{2} gave a reduction peak at -0.78 V and -1.30 V, respectively. Additionally, a new peak (Cd(II)-NIM) was observed at -0.48 V and the current of this peak increased as NIM was added. The reduction of Cd(II)-NIM complex may be shown as follows:

\[ \text{Cd(II)NIM}_\text{complex} + 2e^- \rightarrow \text{NIM} + \text{Cd(Hg)} \]

When the H\textsubscript{2}O\textsubscript{2} is added to Cd(II)-NIM solution, the peak currents of NIM and Cd(II) ions increased. Consequently, it was found that H\textsubscript{2}O\textsubscript{2} exhibited a catalytic effect at the reduction of NO\textsubscript{2} group on the NIM molecule, in the presence and absence of Cd(II) ions. Also, H\textsubscript{2}O\textsubscript{2} prevented the complexation of NIM with Cd(II) ions.

\textbf{Key Words:} Nimesulide, Complex, Voltammetry
References

EXTRACTION OF PHENOLICS IN CARROT WITH METHANOL SOLVENTS HAVING DIFFERENT pH VALUES

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Abstract

Carrot (*Daucus carota* L.) is a widely consumed vegetable, and it is an important source of Vitamin A, carotenoids and phenolics [1,2]. Carotenoids, phenolics and vitamin A have been proved to possess antioxidant activity [1,3].

Synthetic antioxidants are largely employed as preservatives by pharmaceutical, cosmetic and food industries, even if they are suspected of being responsible for liver damage and carcinogenesis in laboratory animals [4]. There is need to replace synthetic antioxidants with natural and probably safe ones. Some factors effect the extraction of natural antioxidants like extracting solvent type and concentration, extraction pH, extraction time [5]. The aim of this study was to investigate the effect of solvent pH on the extraction of the phenolics of carrots, and to determine antioxidant activity values of those extracts.

For the extraction of phenolics, 70% (v/v) methanol solvents of which pH were adjusted to pH=2.0, pH=4.0 and pH=6.0 were used. At the end of the study, it was found that the extracts prepared with methanol having pH value of 2.0 had the highest content of phenolic compounds and antioxidant activity. This result shows that pH=2.0 is the most proper methanol solvent pH for the extraction of phenolics in carrot.

**Key Words:** carrot; phenolic; antioxidant; extraction; pH

References

ANTHOCYANINS and DIFFERENT METHODS OF EXTRACTION from SOME FRUITS and VEGETABLES

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Abstract

Phenolic compounds are secondary metabolites and they are divided into two groups as phenolic acids and flavonoids. Anthocyanins are a member of flavonoids group. They are natural colorant and are responsible to form colors pink, red, blue and purple for vegetables, fruits, fruit juices and wines. Raspberry, blackberry, pomegranate, strawberry, cherry, sour cherry, grape, plum, eggplant, beet and cabbage are known as rich in terms of anthocyanins [1,2]. Most commonly found anthocyanins in nature are cyanidin, delphinidin, pelargonidin, peonidin, petunidin and malvinidin. Pelargonidin gives orange, cyanidin gives orange-red, delphinidin gives blue, peonidin gives red, petunidin gives blue-red and malvinidin gives red-blue color [3]. So they are commonly used as colorant to make food (snacks etc.) more attractive. Besides they known as natural antioxidants. These bioactive components have lots of benefits when they are consumed regularly. Reducing the atherosclerosis and total cholesterol, inhibitory effect on cancer cells proliferation, preventive effect on cardio-vascular diseases are just some of these benefits for human health. [1,3,4]. Different methods are used for the extraction of anthocyanins from fruits and vegetables. Supercritical fluid extraction, accelerated solvent extraction, solid phase extraction, ultrasound assisted extraction, pH differencies methods are some of procedures to obtain anthocyanins from fruits and vegetables [4,5,6].

In this study we aimed to compile information about the anthocyanins and their extraction methods from some fruits and vegetables.

Key Words: Anthocyanin, phenolic compounds, extraction, fruits

References

PARTICLE SIZE PREDICTION OF COPOLYMER-DRUG CONJUGATE USING PARTIAL LEAST SQUARES REGRESSION

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Abstract

Particle size of the copolymers and the associated polydispersity are among the most important factors affecting biopharmaceutical behaviour in a wide variety of therapeutic applications. Particle size provides valuable properties of particles or molecules in liquid medium. This characteristic directly affects bioavailability, dissolution and immunotoxicity. Predicting the particle size would skip many preliminary studies usually required to optimize formulations [1-6].

In this work, the particle size of copolymer-drug conjugates was tried to be estimated using partial least squares regression (PLS). The aim was to build a mathematical model capable of predicting the particle size of copolymer-drug conjugate produced by a pharmaceutical polymer of choice. Partial least squares regression can be seen as a hybrid of multiple regression and principal component analysis and PLS is a method for constructing predictive models when the factors are many and highly collinear. In the present study, to calculate the particle size of the copolymer-drug conjugate, we used the zeta potential and the particle size of the copolymer and drug, and different pH’s values as inputs.

Key Words: partial least squares regression, copolymer-drug conjugate, particle size

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References


Abstract

*Lycium barbarum* L. (goji berry or wolfberry) belongs to Solanaceae family, widely grows in arid and semi-arid regions of Southeastern Europe, Mediterranean countries and Northwestern China [1,2]. Recently, it has been extensively used as functional food for its beneficial effects such as antipyretic, anti-inflammation and anti-senile properties. Goji berry is also known for its bioactive properties which prevent or treat various chronic diseases such as diabetes, hyperlipidemia, thrombosis, immunodeficiency, cancer, hepatitis and male infertility [1]. These bioactive properties have been provided by synergistic interactions of its chemical constituents including carotenoids, flavonoids, betaine, cerebroside, β-sitosterol, trace minerals, vitamins and aminoacids [1,3]. Important bioactives are related to phenolic compounds sand antioxidant activity [3]. Goji berry can be consumed as fresh fruit, fruit juice or dried fruit in order to prevent microbial and chemical spoilage during shipping and storage. But in various studies it has determined that drying method and storage time affects the antioxidant activity and phenolic compounds of goji berry samples. The goji berry extracts were prepared with using 70% methanolic solvents. The content of total phenolics was determined spectrometrically according to Folin-Ciocalteu procedure and calculated as gallic acid equivalents [5]. Antioxidant activities af goji berry samples were determined according to DPPH method and calculated as Trolox equivalents [6].

It was found that the phenolic compounds of the goji berry samples have varied between 910.88 and 1848.96 mg GAE/100g dry weight. Also the antioxidant activities of goji berries have determined between 613.21 and 1160.24 µmol Trolox/100g dry weight. The reason of these results is considered that the drying method and storage conditions have affected the antioxidant activity and phenolic compounds of goji berry samples.

**Key Words:** *Lycium barbarum*, *goji berry*, *antioxidant*, *phenolics*
REFERENCES
DETERMINATION THE COLOR VALUES OF RED CABBAGE EXTRACTS HAVING DIFFERENT pH VALUES

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Abstract

Red cabbage (Brassica oleracea L. var. capitata L. f. rubra) is grown as a vegetable and is rich in anthocyanin pigment [1]. Anthocyanins are responsible for most of the red, blue and purple colours of flowers and fruits. These pigments are also widely used in the food industry to colour soft drinks, jams and dairy products [2]. Anthocyanins are relatively unstable compounds. Depending on the pH of a solution, they undergo reversible and irreversible transformations, which lead to visible changes in the color of the solution [1]. Color is one of the quality characteristics used in sensory evaluation and it plays a key role in food choice [3].

The aim of this study was to determine color values of red cabbage at different pH values. In the study, color pigments present in red cabbage were extracted by ethanol, and pH values of extracts were adjusted between 2.0 and 12.0. Then, the color values of extracts were determined by a Hunter LabMini Scan XE model colorimeter [4]. The Hunter color values were expressed as L* (whiteness or brightness/darkness), a* (redness/greenness) and b* (yellowness/blueness). In color analysis, significant increases in redness of extracts were determined by decreasing pH value from pH=8.0 to pH=4.0, and significant increases in greenness were determined by increasing pH value from pH=9.0 to pH=12.0. All b* values were positive in the study. When the extract of pH=6.0 had the highest b* value, the extracts of pH=9.0 and pH=11.0 had the lowest b* values. These results show that the colors of foods or other materials having red cabbage would change by the differences in pH values.

These results may be important for the food industry as well as for other industries, which may allow the use of natural coloring materials in the dyeing of certain materials such as; textile fibers, baby toys and other products, etc.. Thus, Haddar et al. [4] studied the effect of dye bath pH on the dyeability of wool and silk fabrics by the aqueous extract of red cabbage in the range of pH=2.0–pH=8.0, and at the end of the study they underlined that red cabbage extract could prove an alternative to toxic synthetic colourants. It is thought that it will be beneficial to increase such studies.

Key Words: Red cabbage; anthocyanins; color value; pH; natural coloring.

References

Abstract
Carbon monoxide-releasing molecules (CO-RMs) are a class of organometallo carbonyl complexes capable of delivering controlled quantities of carbon monoxide (CO) gas to cells and tissues thus exerting a broad spectrum of pharmacological effects. [1] Metal containing CO-releasing molecules have been designed as an effective cancer treatment strategy. CORMs are responsible for releasing controlled amounts of CO to cells and tissues. CO is an important signaling molecule, which plays significant roles in the pathogenesis of cancer. Delivering precise and controlled amounts of CO to tissues and organs is an essential biochemical process due to toxic effect of CO at high concentrations. [2]

In this work, [Mn(2-isopropylbenzimidazole)(2,2-bipyridyl)(CO)₃]OTf (Scheme 1) which is the CO-releasing molecule was characterized by Zeta Potential Analyzer. The Zeta Potential Analyzer was used to measure the Zetasizer Measurements, which are zeta potential, mobility and particle size. The stability behavior of complex was determined in different pHs and as function of time in dextrose and in PBS.

Scheme 1 Chemical structure of [Mn(2-isopropylbenzimidazole)(2,2-bipyridyl)(CO)₃]OTf

Key Words: CO-releasing molecule; 2-isopropylbenzimidazole; manganese complex; zeta potential; particle size; stability; particle charge

References
DETERMINATION OF PARTICLE SIZES OF NANOPARTICLES BY NMR SPECTROSCOPY

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Abstract

The sizes of nanoparticles can be measured by NMR besides TEM (Transmission Electron Microscopy), SEM (Scanning Electron Microscopy) and DLS (Dynamic Light Scattering). In this study, particles sizes of nanoparticles were measured with diffusion-ordered nuclear magnetic resonance spectroscopy (DOSY). In order to determine diffusion coefficient, a pulsed-field gradient experiments were done. According to these results, hydrodynamic radius of nanoparticles was calculated by using Stokes–Einstein equation. In order to check the conformity of the diameters calculated by NMR experiments and equation, particle size of the nanoparticles was measured by SEM and DLS. And then, in order to check agreements between NMR results and SEM, DLS results, correlation graphs were drawn. So, DOSY NMR experiments have proved to be accurate and reliable in order to calculate sizes of nanoparticle.

Keywords: NMR, Particle Size, DOSY
INVESTIGATION OF INTERACTION BETWEEN 2-THIOURACIL AND TiO$_2$ THROUGH NMR, FT-IR, RAMAN SPECTROSCOPIC METHODS AND DFT

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Abstract

In this study, the adsorption of 2-thiouracil on TiO$_2$ has been investigated by FT-IR, Raman, NMR spectroscopic methods and DFT. Result show that there is a interaction between TiO$_2$ and title molecule. NMR experiments were carried out in 500MHz NMR. NMR results show that chemical shift of peak of proton of OH group was observed in the NMR spectrum. Moreover, T$_1$ relaxation time of them decreased. FT-IR and Raman spectra show that new peaks were observed and especially changes of bands of OH and SH groups were observed. It has been observed that the interaction between TiO$_2$ and title molecule is over the OH and SH groups. All theoretical computations have been calculated using the (DFT) method at B3LYP/LanL2DZ level of theory to study the vibrational spectra and to assign the vibrational modes of the investigated molecule. It was observed that there was a good agreement between experimental and theoretically obtained results.

Keywords: 2-Thiouracil, TiO$_2$, NMR, Vibrational Spectroscopy, DFT
A COMPUTATIONAL APPROACHES ON THE STRUCTURAL, ELECTRONIC AND SPECTROSCOPIC PROPERTIES OF THE PHENYLHYDRAZINE

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Abstract

Phenyl hydrazine is well known a starting material to produce heterocyclic indoles via Fischer indole synthesis as well as it is included in many kinds of the reactions that are Bartoli reaction, Bischler-Möhlaub reaction, and etc [1]. Furthermore, Phenyl hydrazine is used as a chemical agent in pharmaceutical, analytical and especially medicinal chemistry. Potential surface scan analysis has been employed to obtain the stable conformers of the phenyl hydrazine compound in the gas phase by using the B3LYP/6-31G(d,p) level of the theory. The stable conformers have been re-optimized at 6-31G(d,p), 6-311++G(3d,p) basis sets in both the gas and water phases. The polarized Continuum Model (PCM) [2] has been used to obtain the thermochemical properties of all stable conformers as well as the quantum chemical descriptors. Gaussian 09W [3] software package has been used to perform all calculations and GausView 4.1 program [4] has been used to perform the HOMO, LUMO and MEP diagrams as well as to verify the vibrational modes of the phenyl hydrazine molecule.

Keywords: FT-IR, NMR, MEP, HOMO, LUMO

Figure 1. The stable conformers on the Potential Energy Surface (PES) scan of the Phenylhydrazine at the B3LYP/6-31G(d,p) level of the theory in the gas phase.

Acknowledgments

The author thanks to Scientific Research Projects Department of Cumhuriyet University (Project No: CUBAP: EİT-072). All calculations have been conducted at TUBITAK ULAKBIM, High Performance and Grid Computing Center.

References

Abstract

The accumulation of synthetic plastics, mainly from food packaging, is causing a serious environmental problem. It is driving research efforts to the development of biodegradable films and coatings. Edible films and coatings play an important role for conservation, distribution, and marketing of food products and they are very important alternatives to non-biodegradable materials. The biopolymers used as raw material to prepare biodegradable films should be renewable, abundant and low-cost. Chitosan is a promising biopolymer for developing of edible films and coatings on an industrial level because of its film-forming, biodegradable, non-toxic, and antimicrobial characteristics. Edible films based on chitosan have with good mechanical properties and a selective permeability to CO$_2$ and O$_2$. However, chitosan films are highly permeable to water vapor limiting their use in food products.

In this work, edible films were prepared by using solution casting method using chitosan and glycerol in various ratio. To determine the best conditions required to achieve the adequate response in terms of the shape stability of edible films, the effect of chitosan concentration, plasticizer ratio, and crosslinking degree were evaluated. The biofilms were characterized by physical, mechanical and optical properties such as moisture content, swelling degree, water vapor permeability (WVP), tensile strength and transparency as their structures were confirmed by FTIR. Experimental results show that chitosan concentration and plasticizer ratio affected the film properties.

Keywords: Biopolymer, edible film, chitosan, glycerol, crosslinking
EXCELLENT CORROSION INHIBITION PERFORMANCE
PYRAZINECARBOXAMIDE ON MILD STEEL IN 0.5 M HCl

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Abstract

Inhibition performance of Pyrazinecarboxamide (PA) against corrosion on mild steel (MS) in 0.5 M HCl solution investigated by potentiodynamic polarization, electrochemical impedance spectroscopy (EIS) and linear polarization resistance (LPR) methods. The inhibition efficiency increased with increasing inhibitor’s concentration. The potentiodynamic polarization results indicated that all the studied inhibitors act as mixed type. Pyrazinecarboxamide adsorption on the MS surface obeyed the isotherm of Langmuir and the thermodynamic parameters; $K_{ads}$, $\Delta G^{\circ}_{ads}$ were also calculated and discussed.

Key Words: Mild steel, Corrosion, Inhibitor, Pyrazinecarboxamide.

Figure 1. Nyquist plots for the mild steel in 0.5 M HCl acid solution (○) and containing 10 mM PA (●).

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References

THE INVESTIGATION OF STRUCTURAL ALTERATION OF RAW MATERIALS USED TO ATTAIN GRAPHENE QUANTUM DOT IN DIFFERENT PROLYSIS CONDITIONS

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Abstract

Graphene which is one of the carbon allotrope become widespread an industrial usage due to the unique optical and electrical properties [1]. Grafen Quantum Dots (GQDs) is obtained from the materials such as graphite, glycine, alginate, glucose whose structure contains carbon atoms. In addition, to that GQDs has a spectacular characteristic and unique optical and electrical features in the energy application.[2] It promises a great potential on the research areas with several properties such as low toxicity, high solubility in various solvers, chemical regression and high electrical and heat conductivity [3].

In this study, molasses that are used to attain GQDs are carbonized at the temperature of 200, 250, 300, 350 and 400 °C for 2, 3, 4, 5 and 10 hours. The DTA method was used to determine the melting temperature of the molasses. In order to determine the elemental and optical properties of the obtained graphene quantum particles, XRD, SEM-EDAX, Elemental Analysis, Fluorescence Spectrometry techniques and UV–visible spectroscopy are used. BET techniques have been used for the detection of the pore structure of carbonized materials. Mass loss values was also determined and studied its effects were the outcome. The results obtained from these techniques show that the material obtained from the molasses is GQDs.

Key Words: Graphene Quantum Dots (GQDs), Molasses, Carbonization

References


Acknowledgments
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Abstract

The N-Acylhydrazone (NAH) moiety is considered a privileged structure in Medicinal Chemistry, since it can be recognised by many distinct receptors, leading to a broad range of pharmacological activities. In fact, several reports have demonstrated the importance of N-acylhydrazone derivatives as antitubercular, antiviral, analgesic and anti-inflammatory, anticonvulsant, antitrypanosomal, antipsychotic and vasodilatory agents, amongst others [1]. It was observed that phenylcarbamoylbenzoic acid derivatives, carrying the acid hydrazide moiety, showed moderate antioxidant activity (55.21% inhibition), in comparison to L-ascorbic acid [2]. The synthesized molecules (3a-c) are also the starting materials of these substances which can show biological activity. Previous studies have demonstrated that benzoicain-containing local anaesthetics and novel derivatives exhibited antimicrobial activity against different species, either Gram-positive, or Gram-negative, or fungal strains [3].

Key Words: Antioxidant activity; antitubercular; antiviral

References

PREPARATION OF AMINO MODIFIED RECYCLED POLYETHYLENE TEREPTHALATE NANOFIBERS AND INVESTIGATION OF USAGE IN WASTE WATER FILTRATION

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Abstract

Waste water treatment is an area of research with an increasing popularity worldwide. Main cause of this popularity is the fact of water shortage closer than ever. Keeping drinkable water accessible and affordable relies on filtration technology. Contaminants in waste water causes illness and harmful to environmental populations.

In filtration technology, nanofibers become more and more important due to their incredible surface area, high porosity and ability to modified as needed. There are many advantages compare to common filtration techniques such as disuse of additional chemical agents or high-pressure necessity.

In this study, we aimed to preparation of recycled PET nanofibers using electrospinning method, surface modified with branched polyethylene imine and gaining functional material. The polyethylene imine covalently bonded nanofiber matrix will use in waste water filtration process.

The source of polyethylene terephthalate polymer is waste water bottles. Thus, this source allows us to solve an environmental problem with waste material.

Modified nanofiber membrane characterized by Fourier-Transform Infrared Spectroscopy (FTIR). Nanofiber diameter and morphology were analysed by Scanning Electron Microscopy (SEM). Thermal properties of membranes were examined by Thermogravimetric Analysis (TGA). The amount of heavy metal ions in waste water were investigated by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) before and after the filtration process. The filtration of wastewater indicates that the nanofiber matrix can be suitable for the wastewater applications.

This work was supported by Marmara University, Commission of Scientific Research Project (M.Ü. BAPKO) under grant FEN-C-YLP-081117-0628

Key Words: PET, Recycled Material, Nanofibers, Waste Water, Filtration.

References

THE MODIFICATION OF THE SURFACE OF POLYACRYLONITRILE FIBER BY GRAFTING OF GLYCIDYL METHACRYLATE MONOMER

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Abstract

Polyacrylonitrile (PAN) Fiber is a remarkable material due to its good thermal stability, low gas permeability, compatibility with polar materials, hardness and high abrasion resistance [1]. However, due to containing the high polar nitrile groups, it also has some undesirable properties that limit its application, such as high static charge, low humidity charm, low paint affinity [2]. In order to improve these properties, functional monomers can be incorporated into PAN fiber structure by graft copolymerization method [3-5]. Since the superior properties of the components can be combined with the graft copolymer structure to be formed, fiber material having wide using potential can be prepared.

For this purpose, glycidyl methacrylate (GMA) with a reactive functional group was selected as the monomer to be grafted. The grafting was carried out at suitable concentrations by the addition of solution of the benzoyl peroxide initiator in the acetone to the mixture containing PAN fibers and GMA solution. Preparation of PAN fibers grafted GMA at different percentages was investigated by varying the polymerization conditions such as initiator and monomer concentration, polymerization temperature and duration. The grafting percentages were gravimetrically determined and the highest grafting efficiency as 95% was achieved under the conditions investigated. The structure and morphology of the PAN fiber-g-GMA copolymer prepared were characterized by ATR-FTIR, XRD and SEM techniques, respectively.

Key words: Polyacrylonitrile; Fiber; glycidyl methacrylate; grafting, functional polymer

References

NOVEL TETRAKIS 4-(1-PYRIDIN-4-YL)ETHOXYL) SUBSTITUTED METALLOPHTHALOCYANINES: SYNTHESIS AND ELECTROCHEMISTRY

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Abstract

One of the most important drawbacks for fuel cell applications is the catalysts with high cost. Therefore, it is substantial to develop alternative, cost-effective and easy-to-be prepared catalysts to remove the need for the precious ones such as Pt or IrO2. Since cobalt (II) phthalocyanines was reported as electrocatalyst in oxygen reduction, cobalt an iron macrocyclic complexes have been studied extensively in oxygen reductions (1, 2)

Nowadays, the most useful electrocatalysts for polymer electrolyte membrane fuel cells (PEMFCs) are Pt-based materials which are not only rare but also very expensive. Many strategies have been used to tackle with the catalyst cost. One of them is to reduce the Pt loading, and the other is to replace Pt-based catalysts with non-precious metal catalysts. Among the non-precious metal catalysts explored, transition metal macrocyclic complexes and their pyrolyzed materials have attracted the most attention worldwide for PEMFC applications (2, 3).

Motivated by the advantage of pyridine nitrogen in the N-doped carbon materials, a novel tetrakis 4-(1-(pyridin-4-yl)ethoxyl) substituted metallophthalocyanines with redox active metal center have been synthesized and characterized with elemental analysis, FTIR, 1H-NMR and MALDI TOF mass spectroscopy methods. Their electrochemical properties and catalytic activity have also been investigated.

Key Words: Phthalocyanine, Synthesis, UV-vis, Electrochemistry

References

SYNTHESIS AND ELECTROCHEMISTRY OF NOVEL TETRAKIS 2-
DIBENZYLAMINOETOXYL SUBSTITUTED
METALLOPHTHALOCYANINES

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Abstract

Electrocatalysis can be used to produce eco-friendly electricity. However, to become widespread of fuel cell technology remains restricted by high costs and limited resistance. It is well known that Pt and IrO2 are the most popular electrocatalysts on oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). Due to the high cost and shortage of catalysis materials, works are concentrated on non-precious metal-based compounds in recent years. Since a transition metal N4-chelate had been used on oxygen electrocatalysis by Jasinski first in 1964, various N4-macrocycles such as transition metal phthalocyanines (MPcs) and porphyrins were used on oxygen electrocatalysis (1-3).

Inspired by the advantage of N4-macrocyclic structure, a novel tetrakis 4-(2-(dibenzylamino)ethoxy) substituted metallophthalocyanines with redox active metal center have been synthesized and characterized with elemental analysis, FTIR, ¹H-NMR and MALDI TOF mass spectroscopy methods. Their electrochemical properties and catalytic activity have also been investigated.

Key Words: Phthalocyanine, Synthesis, UV-vis, Electrochemistry

References

ELECTROSPUN POLYVINYL ALCOHOL/ZNO NANOFIBER AS A NEW CARRIER FOR LIPASE IMMOBILIZATION: AN OPTIMIZATION STUDY

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Abstract

Due to wide band gap of Zn⁺², ZnO-Polymer composites offer many advantages as inexpensive, semiconductor, eco-friendly and have many applications as gas sensors, piezoelectric materials, optoelectronic devices, varistors, transparent conductors, short-wave light emitting diodes, organic photovoltaic cells.

In this submitted work, electrospun Polyvinyl alcohol/ZnO nanofibers were used for lipase immobilization. The nanofibers were prepared by electrospinning technique with the most appropriate operational parameters as electric voltage, distance between tip and collector, concentration of PVA and ZnO, injection speed were found as 13 kV, 17 cm, 9% PVA, 1% ZnO and 0.5 ml/h respectively. The morphology and structure of the nanofibers was characterized by scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and thermal gravimetric analysis (TGA). According to the results, ZnO were successfully embedded in the hybrid fibers due to chemical interactions between PVA and ZnO. The effect of operational parameters was investigated for optimizing the PVA/ZnO nanofiber morphology by using SEM technique. Obtained nanofibers were randomly-organized, smooth and round-shaped. SEM results showed that resulting nanofibers had the narrow diameter distribution. Lipase immobilization was carried out in which the most suitable nanofiber formation was observed. The enzyme was immobilized onto the nanofibers by adsorption and then cross-linking methods. For the optimization of lipase immobilization, the amount of nanofibers, the adsorption time, the amount of lipase and the amount of glutaraldehyde were investigated as basic parameters. The optimum values for amount of nanofibers, amount of lipase, adsorption time and glutaraldehyde concentration were found as 5 mg, 0.75 mg/ml, 15 min and 4%, respectively.

Key Words: Nanofiber, Electrospinning, Immobilization, Lipase, PVA/ZnO
References

Funding
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LIPASE IMMOBILIZED ELECTROSPUN POLYVINYL ALCOHOL/ALGINATE NANOFIBERS FOR EFFECTIVE AND ENHANCED STABILITY

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Abstract
Nanofibrous materials could be produced with the methods such as self-assembly, template synthesis, phase separation, and electrospinning [1]. It was reported that among these methods, the electrospinning is the most efficient and most versatile method for producing the nanofibers having uniform diameter and the appropriate functional group depending on used polymers [2]. At the point of flexibility, cost efficiency and being easy to handle, electrospinning method is also advantageous among the others [3]. As reported in literatures, some nature carbohydrate polymers like alginate and chitosan could not be prepared electrospun nanofiber form alone [4]. Because, especially alginate has rigid and long worm-like molecular chains which inhibits fiber formation during electrospinning. Alginate could be electrospinned by blending it with polyvinyl alcohol or polyethylene oxide etc.

In this submitted study, lipase was successfully immobilized by adsorption and cross-linking on polyvinyl alcohol/alginate nanofibers that were prepared by electrospinning. Results showed that nanofibers enhanced the stability properties of porcine pancreas lipase. When the free lipase lost its all activity after 40-60 min at high temperatures, lipase immobilized nanofibers kept almost 70% activity at the same time. The lipase immobilized polyvinyl alcohol/alginate nanofibers protected approximately all of their activities until pH 9. Lipase immobilized polyvinyl alcohol/alginate nanofibers maintained 60% of their activities after 14 reuses. The morphology of nanofibers was characterized by Scanning Electron Microscope, Fourier Transform Infrared Spectroscopy and Thermal Gravimetric Analyzer. The nanofibers provided the huge specific surface area. As a result, the nanofiber production method, electrospinning, is simple, versatile and economical for preparing appropriate carrier to immobilize the enzymes. The lipase immobilized alginate based electrospun nanofibers have high enzyme loading capacity, high catalytic activity and improved stability properties. So, they may have great potential for industrial applications like biodiesel production, transesterification, aminolysis and alcoholysis.

Key Words: Nanofiber, Lipase, Immobilization, Polyvinyl alcohol, Alginate
References

Funding
This work was supported by a grant from the Muğla Sıtkı Koçman University Scientific Research Project (No: 13/182).
NEW IMPROVEMENTS ON SUPERCRITICAL DYEING MACHINES

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Abstract

Application of supercritical fluid dyeing principle on the textile material dyeing processes is an interesting alternative to the conventional aqueous processes with its promising environmental benefits. Supercritical fluid dyeing is a waterless dyeing process that exploits the unique properties of supercritical fluids. Carbon dioxide (CO2) is particularly attractive for such applications because of its reasonable price, non-flammable and nontoxic properties, and its critical temperature point (Tc = 31.1 °C, Pc = 73.7 bar) is lower than that of many other fluids.

During this dyeing process water is completely eliminated, where textile waste water and chemical auxiliary consume and related environmental problems are also eliminated. Required carbon dioxide can be recycled; excessive amount of used dyestuff which is not adsorbed on the textile substrate can be collected and reused subsequently. Although the purchase cost of a supercritical dyeing machine is higher than that of an aqueous one, the operating cost is lower and this results in a 50% savings on the overall cost of supercritical process. The necessary energy consumption in this process is relatively lower than is needed to heat water in conventional methods of dyeing. Due to the elimination of drying process, saving on energy and time becomes possible. Required dyeing time cycle is shorter compared to the traditional methods.

The typical configuration of a supercritical fluid dyeing plant consists of a CO2 tank, a compression pump, a heated dyeing vessel, a dye container and a circulation pump. First, the autoclave is loaded with the textile material (yarn bobbins or fabrics wound on a dyeing beam), then the system is pressurized and heated at the requested working conditions. The dyeing step is performed by circulating the supercritical bath from the dye container and the dyeing vessel through the circulation pump; an option to reverse flow in the dyeing bath from inside-to-outside (I/O); to outside-to-inside (O/I) of the textile beam (yarn or fabric) is generally available. At the end of the dyeing step, the system is typically partially depressurized and washed with clean supercritical CO2 to remove the excessive unfixed dye. Finally, the autoclave is unloaded and both the CO2 and the residual dye are recovered for a subsequent dyeing run.

Key Words: Supercritical fluid; Supercritical dyeing; Supercritical dyeing machines; Waterless dyeing; Textile dyeing
References

APPLICATION OF SUPERCRITICAL FLUID DYEING PRINCIPLE FOR THE SYNTHETIC TEXTILE FIBERS

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Abstract

Traditional aqueous dyeing procedure requires a large amount of water, changing between 70–120 litres of fresh water per 1 kg of fiber. The advantages of supercritical carbon dioxide dyeing method are found promising especially on synthetic fabric dyeing process. The main technological solutions of the super critical fluid dyeing (SFD) process, related to the operative conditions and equipment design, were developed and optimized for the dyeing of polyester (PET) fiber, even though reports of experiments conducted on other synthetic and natural fibers can also be found. Natural fiber types of cotton, than wool and silk fibers have been dyed in supercritical carbon dioxide beside the synthetic fiber groups.

Synthetic textile fibers, such as PET fibers, are semi-crystalline polymers with a glass transition temperature generally in the range of 80–125 °C, depending on orientation and crystallinity. When the polymer is in contact with the supercritical dyeing bath, the small CO2 molecules can easily penetrate into the free volume of the amorphous parts of the polymer and increase the segmental chain mobility (plasticization effect). The CO2 sorption and the plasticization action result in the reduction of the glass transition temperature, which is shifted down by at least 20–30 °C, and in the increase in the free volume of the polymer (swelling). This phenomenon promotes the diffusion of the dye molecules to the fiber structure resulting permanent dyeing effect. At the end of the SFD process of textile material, the system is depressurized and the CO2 is released by the polymer.

Key Words: Supercritical fluid; Supercritical dyeing; Polyester yarn ; Waterless dyeing; Textile dyeing

References

EFFECT TO LYOTROPIC LIQUID CRYSTAL MEDIA AND ELECTROCHEMICAL PROPERTIES OF SCHIFF BASE METAL COMPLEX

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Abstract

Liquid crystals (LC) are known as an intermediate phase which has symmetry and order between solid and liquid state. As a kind of liquid crystal, lyotropic liquid crystal (LLC), contains mixture of amphiphilic molecules [1]. Amphiphilic molecules are arranged according to solvent type, amphiphilic molecule concentration and temperature such as cell model, disc, hexagonal texture etc. and also structure order determine phase type of LLC [2]. In the recent times LLCs are used to synthesize organic or inorganic nano materials [3], in drug delivery systems [4], as solvent for NMR [5]. A great deal of Schiff base with thermotropic liquid crystal properties, have been researched but in LLC media very few. A new Schiff base was synthesized with stoichiometric amounts of 2-hydroxy-4-octyloxybenzophenone and 1,2-etilenediamine by condensation reaction and then nickel complex was obtained. In this study, properties of the synthesized Schiff base metal complex was investigated in LLC medium. The LLC medium was comprised of decylammonium chloride (CH₃(CH₂)₉NH₃⁺Cl⁻)/(DACl) /KCl/Limonene/water. At the beginning cholesteric phase occured due to limonene, which is a chiral molecule and then adding Schiff base metal complex induced to form hexagonal phase. And also metal complex of Schiff base researched by cyclic voltammetry. Cyclic voltammetry is a common used method for application of electrochemical methods to the study of coordination of transitional metal complex. It provides a rapid location of redox potentials of the electroactive species and effect of media on the redox process [6].The cyclic voltammogram of nickel complex shows two cathodic and two anodic peaks. The anodic peaks are at +0.68 and +1.179 and the cathodic peaks of complex are at -0.91 and -0.274 V, respectively. It is revealed that metal center of the complex is effective on the electrochemical behaviour.

Key Words: Schiff base, Metal complex, Lyotropic liquid crystal, Cyclic voltammetry, Polarized light microscope

References
POLY(METHACRYLOYLOXY ETHYL PHOSPHATE) GRAFTED PVDF POLYMER ELECTROLYTE MEMBRANES VIA SURFACE INITIATED ATRP

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Abstract

Rechargeable lithium polymer batteries have been considered to be one of the most important next-generation power sources. The energy density and battery safety factors are important criteria guiding the advancement of novel battery systems [1,2]. Polymer electrolyte membranes are promising advanced materials for fuel cells and Li-polymer battery applications as well as for super capacitors [3]. Poly(vinylidene fluoride) (PVDF) and its copolymer have been widely studied for applications in rechargeable batteries. PVDF homopolymer help to enhance the ionic conductivity and thus improve cell rate capability [4].

In this study, electrospun poly(vinylidene fluoride)/poly(methacryloyloxy ethyl phosphate) polymer electrolytes have been prepared for application in lithium polymer batteries. PVDF nanofiber was first prepared by electrospinning. Then, poly(methacryloyloxy ethyl phosphate) brushes were grafted onto PVDF nanofiber via atom transfer radical polymerization. The chemical structure of the prepared poly(vinylidene fluoride)/poly(methacryloyloxy ethyl phosphate) is confirmed by FTIR analysis. The morphology of the PVDF based nanofibers was investigated by SEM. Ionic conductivity and electrochemical stability studies of the nanofiber electrolytes were measured. The conductivities of Li-salt containing nanofibers are between the range of $3.41 \times 10^{-3}$ S cm$^{-1}$ and $8.26 \times 10^{-4}$ S cm$^{-1}$. In addition to these results, lithium-doped nanofiber polymer electrolyte shows a good electrochemical stability between in the range of 3.0 and 6.0 V vs Li at room temperature.

References


THE PREPARATION OF FLUORINE AND GRAPHENE OXIDE CONTAINING HYDROPHOBIC NANOCOMPOSITE COATINGS

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Abstract

The development of polymer nanocomposites with hydrophobic properties have become a prominent area of current research and development. Flourine containing nanocomposites have been attracted great attention by owing to the characteristics of fluorine atoms such as excellent surface properties, water resistance, corrosion resistance, low refractivity and low dielectric constant [1]. In addition excellent physical and mechanical properties of graphene and its derivatives as nano fillers make it more preferable for designing the corrosion resistant coatings than the other nano-materials. Graphene oxide has high surface area and nanometric thickness, which shows the barrier property preventing oxygen and water permeability of the coating [2].

In this study, a new fluorine and graphene oxide based hydrophobic polyurethane-silicone nanocomposite coatings were developed. The nanocomposite coatings were prepared by using a sol-gel process from the alkoxysilane modified polyurethane prepolymer and perfluoroctylalkoxysilane. In addition, graphene oxide was added into the prepared sol-gel mixture. Hydrophobic and anti-corrosive coatings were fabricated with incorporation of the mixture of the graphene oxide and sol-gel into nanocomposite formulations. Structure analysis of alkoxysilane modified polyurethane was confirmed by FTIR. The surface morphology of the nanocomposite coatings was investigated by Scanning Electron Microscopy analysis. The contact angle results show that the obtained coatings have good hydrophobic properties.

References


INTERMOLECULAR INTERACTIONS BETWEEN SULFADIAZINE AND SACCHARIN

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Abstract

Sulfadiazine (4-Amino-N-(2-pyrimidinyl)benzesulfonamide) (SD) has been widely used as an antibiotic. Saccharin (benzoic sulfimide) (SAC) is known as an artificial sweetener. In current study, intermolecular photoinduced electron transfer in the SD-SAC complex has been investigated to determine its structure and photophysical properties by using quantum chemical methods. The conformational analyses of investigated molecules were performed to determine initial structures. Full optimizations were performed with Gaussian 09 [1] at the B3LYP/6-311++G(d,p) level. In order to explore the solvent effect, solvation calculations were performed by Tomasi’s Polarizable Continuum Model (PCM) [2,3] using Dimethylformamide (DMF) as the solvent. Molecular orbitals and energy differences of frontier orbitals and electrostatic potentials (Figure 1) for studied molecules were calculated at B3LYP/6-311++G(d,p) level in gas phase and in DMF. SDSAC complex is stable in the gas phase and DMF and shows intermolecular charge transfer (Figure 1) between HOMO-LUMO orbitals by S₁ excitation.

Figure 1. Calculated UV-Vis absorption spectra of SDSAC complex in DMF

Key Words: Density functional theory; UV-Vis absorption spectra, Sulfadiazine, Saccharin

References

We acknowledge computer time on FenCluster provided by Ege University Faculty of Science.
INTERMOLECULAR INTERACTIONS BETWEEN SEROTONIN AND PROMAZINE USING COMPUTATIONAL METHODS

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Abstract

Serotonin (5-Hydroxytryptamine) (SE) has been implicated in a broad range of behavioral disorders involving the sleep cycle, eating, the sex drive and mood [1]. Promazine (PZ) is a psychotropic drug which is used extensively in mental disorders and anticancer activities. Its interactions in metabolism with the serotonin are important in terms of its biological activity. In this study, intermolecular interactions between photophysically excited promazine and naturally occurring hormone (serotonin) in the human body at ground-state will be investigated using computational tools. Conformational analyses have been performed to determine the initial structures for promazine and hormone (serotonin) using Spartan 08 [2]. Ground state geometry optimizations are first performed with Gaussian 09 [3] at the ω-B97XD/6-31G(d,p) level of DFT theory without symmetry constraint in gas phase and water phase, solvation calculations were performed by Tomasi’s Polarizable Continuum Model (PCM) [4,5]. The electronic transitions were calculated by the time-dependent density functional theory (TD-DFT) with CAM-B3LYP, B3LYP and ω-B97XD methods using 6-311G++(d,p) basis set in gas phase and in water. Molecular orbitals, energy differences of frontier orbitals and electrostatic potentials for studied molecules were investigated. Intermolecular charge transfer between HOMO-LUMO orbitals of SE-PZ complex was observed in both media.

Key Words: Density functional theory; UV-Vis absorption spectra, Promazine, Serotonin

References


We acknowledge BAP (2013FEN063) for financial support of this research work and computer time on FenCluster provided by Ege University Faculty of Science.
Abstract

In recent years, adsorption of protein molecules has been playing an important role in many areas such as biology, biotechnology, biochemical and environmental science. Hydroxyapatite (HAP) is one of the important biocompatible materials that can be used in protein adsorption. HAP widely used in separation of biological molecules is preferred due to its chemical and structural similarities with the bone [1-4].

In this study, the adsorption of bovine serum albumin (BSA) onto HAP crystals produced under different conditions was investigated. The experiments were carried out at 37°C at pH 6.0 and 7.4. The adsorption capacity of HAP crystal increased with increasing pH and decreased with increasing adsorbent production temperature. Adsorption kinetics data were tested using pseudo-first-order and pseudo-second-order model. The evaluation of the results showed that the pseudo-second-order kinetic model is more convenient to represent the adsorption kinetics.

Key Words: Protein adsorption; hydroxyapatite; bovine serum albumin; isotherms; kinetics.

References

COMPARISON OF U(VI) ADSORPTION ONTO DIFFERENT ADSORBENTS

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Abstract

Activated carbon (AC) has been recognized as one of the most popular and widely used adsorbent in water and wastewater treatment throughout the world [1,2]. Their large sorption capacity is linked to their well developed internal pore structure, surface area and the presence of a wide spectrum of surface functional groups. Oxygen, hydrogen, sulphur and nitrogen are generally present in AC in the form of functional groups and/or atoms chemically bonded to the structure. In the carbon structure, the main functional groups which, in general, are considered to be responsible for uptake of pollutants include carboxyl, carbonyl, phenols, lactones, quinones besides others. The unique adsorption properties of AC can be significantly influenced by these functional groups. The nature and concentration of surface functional groups may be modified by suitable thermal or chemical treatments to improve the performance of AC for specific contaminants removal [3]. The modifications of the surface chemistry of carbons are acidic treatment, base treatment, impregnation, micro-wave treatment, ozone treatment and biological modifications.

In this work, granular activated carbon was modified with acidic treatment (with HNO₃), base treatment (with NaOH) and surface oxidation (with KMnO₄). The modified materials were called as AC1, AC2 and AC3, respectively. The influence of various experimental parameters on U(VI) adsorption by different adsorbents is investigated and conditions for the adsorption of uranium from aqueous solution were compared for modified adsorbents.

The results showed that the adsorption kinetic behaviour of U(VI) on AC1, AC2 and AC3 followed the pseudo-second order kinetic. U(VI) adsorption by three adsorbents were pH dependent and average sorption pH for adsorbents was observed between pH 4.5 and pH 5. Maximum uranium uptake capacities of AC1, AC2 and AC3 obtained from batch studies were 98.89%, 99.0% and 94.38%, respectively. The equilibrium data in aqueous solutions were represented by the isotherm models. The adsorption equilibrium data fitted very well to Langmuir model for three adsorbents. The thermodynamic parameters, ΔH°, ΔS° and ΔG°, were evaluated as well. The negative value of ΔG° indicates the spontaneity and the positive value of ΔH° shows the endothermic nature of the adsorption process for three adsorbents.

Key Words: Uranium, Adsorption, Activated carbon, Modification

References

ELECTROCHEMICAL DETERMINATION OF LUTEOLIN İN BIOLOGICAL SAMPLE AT A CATHODICALLY PRETREATMENT BORON-DOPED DIAMOND ELECTRODE IN THE PRESENCE CATIONIC SURFACTANT USING SQUARE-WAVE ADSORPTİVE STRIPPING VOLTAMMETRY

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Abstract

Luteolin (3’,4’,5’,7’-tetrahydroxyflavone) is a type of flavonoid that is abundant in many plants such as celery, green pepper, parsley and perilla leaf. Luteolin has many biochemical and pharmacological effects, including anti-oxidative, anti-bacterial, anti-viral, anti-inflammatory and anti-carcinogenic effects. Recent reports indicate that luteolin exhibits anti-proliferative activity against cancer cells and suppresses oxidative damage of DNA, lipid, proteins and carbohydrates [1]. The electrochemical behavior of luteolin was studied in 0.1 M HClO₄ at a boron-doped diamond electrode (BDDE) by cyclic voltammetry (CV) and square-wave voltammetric method (SWV). The oxidation process was produced in different supporting electrolyte media. The oxidation process was irreversible and exhibited adsorptive-stripping controlled. For analytical purposes, very resolved voltammetric peaks were obtained using square-wave mode. The linear response was obtained in the range of 0.174 - 1.74 µM for the first and second oxidation steps in 0.1 M HClO₄ using SWV. These method was used for the determination of luteolin in human urine. The first oxidation step was chosen as indicative of the analysis of luteolin in biological media. The methods were successfully applied to spiked human urine sample.

Key Words: Luteolin, Surfactant, Boron-Doped Diamond Electrode, Square-Wave Voltammetry, Biological Sample

REFERENCES

EFFECT OF BENZOPHENONE DERIVATIVE SCHIFF BASE TO CONTAINING METAL SALTS LYOTROPIC LIQUID CRYSTAL

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Abstract

Lyotropic Liquid Crystal (LLC) is a mesophase, which is sensitive many exciting such as electric, magnetic field. In nature LLC emerge commonly in from cell membrane to biological secretions and this material also are used to commerically from polymer synthesize to drug delivery systems. An amphiphilic molecule, which has polar and apolar sections self-assembly spontanenously and this unique organization ensure stable different phases thermodynamicly [1].

Benzophenone is a ketone and has been used in food industry as a flavour, in plastic industry as a additive, in cosmetic industry as UV-absorber and agricultural industry as a precursor. Benzophenone and derivatives have been used in myriad research and many type of Schiff base synthesized until now. due to antibacterial properties [2-3]

In this study, unique structural symmetry, thermodynamic stability and simple control over the structural parameters with polar and apolar region is reason of why is prefer of LLC. A chiral amphiphilic molecule [(L-alanine hydrochloride decylester (L-ADE)] was used for preparing cholesteric phase, which micelles arrange a helical structure. Cholesteric phase was occurred from L-ADE/ NH₄Cl/ H₂O and this system also prepared with metal salts (CuCl₂, NiCl₂, ZnCl₂, CoCl₂) and effect of metal salts investigated with polarize optical microscope (POM). Then a Schiff base synthesized from 2-hydroxy-4-octyloxybenzophenone and 1,6-hexane diamine was added prepared metal and free metal LLC systems and effect of this compound was researched with polarized light microscope.

Key Words: Schiff base, Benzophenone, Lyotropic liquid crystal, Metal salts, Polarized light microscope

References

ENZYMATIC TREATMENT ALTERNATIVES IN TEXTILE

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Abstract

Global enzyme market is growing continuously and reached over 4.4 billion US$ at the end of 2015. Share of technical purposed utilization of the enzymes is estimated about 38% in the total consumption. Share of textile, fur and leather in this amount is about 17% (289 million US$). Utilization of enzymes in textile industry, allow the development of environmentally friendly technologies in fiber processing and strategies to improve the final product quality [1]. Applications of enzymes in textile starts with starch removal process of Amylase enzyme. Currently it is reported that the main classes of enzymes involved in cotton pre-treatment and finishing processes are hydrolase and oxidoreductase [2]. Commonly used enzymes in textile applications are Amylase for desizing of starch from the woven fabric; Cellulose for cotton fabric softening purpose (especially for the denim finishing); Catalase for bleaching; Laccase for non-chlorine bleaching and fabric dyeing; Pectatlyase for bioscouring; Protease for removal of wool fiber scales and degumming of silk; Lipase for removal of size lubricants and denim finishing, Ligninase and Collagenase for wool finishing; and Cutinase for cotton scouring and synthetic fiber modification. Processing recipe of the enzymes are also influential factor on the environment. Enzymatic treatments on cotton fiber based textile products can be applied in acidic, neutral and alkali environment which are also influential on environment. Increasing utilization of enzymes in the textile industry is an encouraging step for the application of white/industrial biotechnology, which allows the development of environmentally friendly technologies in fiber, yarn, fabric and garment processing steps [3]. Traditional wet processing techniques in textile industry causes high amount of waste water and resulting environmental side effects to the rest of the nature. Increasing global demands on textile products show increasing potential use for the enzymes in various sub applications on the textile production path. Current enzymatic treatments on textile and their increasing potential brings new possibilities to the textile sector such as higher quality, decreased environmental pollution and cost effectiveness [4-6].

Key Words: Enzymes, Textile Finishing, Environment

References

APPLICATION OF SUPER ABSORBENT POLYMERS IN TEXTILE PRODUCTS

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Abstract

The super-absorbents polymers SAPs can be classified as a special case of hydrogels. Principle idea were implemented about 80 years ago (in 1938) and first application in textile products had been introduced in the 1980’s in the components of body hygiene products and disposable baby diapers. Eventually Super Absorbent Fiber (SAF) form of the SAPs are developed and more of the textile application potentials were improved. Fiber form of the SAPs are generally utilized in the manufacturing process of nonwoven textile surfaces. Such products are advised to be used as absorbent vests, tops, and single sweat-absorbing elements, as well as for inlays for layered technical textile based clothing and items. Kitchen paper towels, sponges, disposable mats for outside doorways and bathrooms, household pet litter, bandages and wound dressings are some other textile products that SAPs and SAF can be utilized in the manufacturing stages of the items. Application of SAPs on to the nonwoven based textile items can be completed in the form of powder or pulverization onto the nonwoven textile substrate. Fixation of the powder or pulverized SAPs onto the surface is one major issue that is still open to development for each individual product design and construction phases. Utilization of SAF in yarn and eventually in fabric form show promising product development possibilities for SAP in textile products, especially in medical and personal hygiene products. SAF containing yarn types can be used to manufacture complying special requirements in unique textile based product applications and development.

Key Words: Super Absorbent Polymers, SAP, Functional Textile Products

References

REDUCTION OF PYRIDINE COMPOUNDS TO THEIR HEMIAMINAL DERIVATIVES

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Abstract

Hemiaminals (N,O-hemiacetals) are unstable species and cannot be isolated after their formations [1]. However, theoretical studies revealed that hydrogen bonding plays a vital role in stabilization of the tetrahedral hemiaminals [2]. In this study we have synthesized a series of 3-(pyridin-2-yl)-2-(pyridin-2-ylimino)thiazolidin-4-ol derivatives regioselectively from 2-iminothiazolidin-4-one derivatives using LiAlH$_4$ in THF (Scheme 1). For these compounds because of the intramolecular restricted rotation around the N$_3$-aryl single bond, formation of $M/P$ isomerization is possible. The solid state structures of the synthesized hemiaminals have been shown to be stable due to the formation of an intramolecular hydrogen bond between the N$_3$ pyridine nitrogen and the hemiaminal OH (Figure 2). In this way the $RM$ and $SP$ enantiomeric pair has been isolated. The enantiomeric ratio has been determined by $^1$H NMR in the presence of chiral auxiliary $(R)$-TFAE as 1:1.

\[
\text{Compound 1: } R_1=\text{H} \\
\text{Compound 2: } R_1=\text{CH}_3 \\
\text{Compound 3: } R_1=\text{H} \\
\text{Compound 4: } R_1=\text{CH}_3
\]

Scheme 3. Synthesis of stable hemiaminals from pyridine compounds.

\[
\text{Figure 1. The expected six membered ring structure stemming from the intramolecular hydrogen bonding.}
\]

**Key Words:** Stable hemiaminal; Chiral auxiliary; Axially chiral hemiaminals; Pyridine compounds; Intramolecular hydrogen bonding

References

Graphene is the name given to one of the honeycomb structures of the carbon atom. The strong carbon bonds in the landscape make it one of the strongest materials on the earth. Due to these properties, graphene has attracted increasing attention in recent years some fields such as physics, chemistry and material science. In addition, it is of great importance in terms of increasing application areas of composites prepared with various inorganic materials, metals and polymers. Polyphenols have attracted great attention of research due to their perceived health-beneficial effects. They occur in a variety of fruits, vegetables, nuts, seeds, flowers, bark, beverages, and even some manufactured food, as a component of the natural ingredients used.

In this work, graphene oxide (GO) was prepared by Hummer’s method from graphite (G). Reduced graphene oxide (RGO) with various nanosize has been prepared by Green Method using white cabbage. “Folin-Ciocalteu” Method was applied to get polyphenol of white cabbage. Then, white cabbage extracts were used to reduce GO. Nanocomposites were obtained utilizing various nanosize of prepared RGO and clay minerals. The results showed that RGO/clay nanocomposites were successfully synthesized. SEM, TEM, XRD, FTIR, TGA / DTA techniques were used for the characterization of the nanocomposites.

**Key Words:** Nanocomposite; reduced graphene oxide; green synthesis; white cabbage; clay.

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**References**


PREPARATION AND CHARACTERIZATION OF POLY(SODIUM 4-STYRENESULFONATE)-DECORATED SnO₂ NANOPARTICLES BY HYDROTHERMAL METHOD

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Abstract

In this study, PSS-Tin Oxide (PSS-SnO₂) nanocomposites were properly synthesized using PSS and Pre-synthesized SnO₂ nanoparticles size of 16.4 nm with PEG as the surfactant via hydrothermal process in the presence of dimethyl formamide (DMF) for 2 hours at 0°C reaction temperature. The structure, morphology and elemental analysis of PSS-SnO₂ nanostructure were analyzed by field emission scanning electron microscopy (FESEM), energy dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy. The results showed that the SnO₂ surface successfully was covered with PSS under strong π-π interactions and with an encapsulation ratio of 39.53 wt%.

Key Words: Nanoparticle, tin oxide, PSS, PEG.

References

Abstract

Recently, the preparation of POSS-polymer composites has attracted the attention of materials scientists due to the unique properties of POSS (1-2). In this study, novel polyimide (PI) / POSS was prepared. Precursor of polyimide, which is the poly(amic acid) (PAA), was successfully synthesized with 3,3′,4,4′-Biphenyltetracarboxylic dianhydride (BPDA), 2,6-Diaminopyridine (DAP) in the solution of N-methylpyrrolidone. The amount of POSS in the composites was varied from 0 wt% and 1 wt%. The structure, thermal, surface properties and dielectric constant of polyimide composites were characterized by scanning electron microscopy (SEM), ATR-FTIR, thermogravimetric analysis (TGA), impedance analyzer. SEM and FTIR results showed that POSS / polyimide composites were successfully prepared. PI matrix decreased the dielectric value of pure PI from 7.1 to 8.6.

This work was supported by Marmara University, Commission of Scientific Research Project (M.Ü. BAPKO).

Key Words: POSS, Polyimide, Dielectric

References

FLUORIMETRIC SENSOR FOR CYANIDE IONS

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Abstract

Cyanide, known as a very dangerous and toxic substance, can be released into the environment in industrial sources, besides the organic and inorganic varieties found in nature due to its industrial use. Cyanide and its derivatives are used frequently in the production of many chemical substances, textile, leather, acrylic and plastic production, photography, painting etc. For these reasons, people are inevitably exposed to cyanide. Known for many years as a deadly poison, cyanide can pose a danger that could lead to death if it enters the body in any way (1-2). Therefore, it is a very important issue to be able to determine cyanide precisely and reliably.

The studies in the literature for the determination of cyanide ions generally include chemical reactions, potentiometric, spectrophotometric and spectrofluorometric methods (3-5). These methods have some disadvantages, such as loss of cyanide from the sample matrix during steps such as distillation or extraction of the complex formed with an organic reagent, and also requiring careful control of the analysis conditions, which causes the results to be erroneous.

In our work, a polymeric fluorescence sensor was prepared by UV-curing technique for used in the determination of cyanide ions in the aqueous medium, and a new spectrofluorometric method was developed for the rapid and high sensitivity determination of cyanide using this sensor. Variables such as pH, time, foreign ion effect, etc., which may have an effect on the fluorescence intensity, have been examined in detail and the method has been successfully applied to different water samples.

This work was supported by Marmara University, Commission of Scientific Research Project (M.Ü. BAPKO).

Key Words: Cyanide ions, Fluorescence, Sensor, UV-curing.

References

COMPREHENSIVE SCREENING OF BEE PRODUCTS FLAVONOIDS CONTENTS WITH TIME EFFECTIVE AND SENSITIVE HPLC-UV METHODOLOGY

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Abstract

Bee products are natural food product well known for theirs nutritional and medicinal values. They are strong antioxidant sources and the health benefits offered by these products are attributed mainly to the presence of phenolic compounds [1]. Flavonoids and phenolic acids constitute the most important polyphenolic classes. Flavonoids exhibit a wide range of biological effects including anti-bacterial, anti-inflammatory, anti-carcinogenic, anti-atherogenic, anti-trombotic, anti-allergic and antioxidant activities [2]. The antioxidant activity of flavonoids and phenolic acids depends on the number and positions of the hydroxyl groups and the nature of substitutions on the aromatic rings. Analysis of the flavonoids in honey, propolis and pollen is a very promising subject for the authentication and the nutraceutical research [3]. This work describes a novel, time effective, feasible and sensitive methodology for the rapid analysis of flavonoids at bee products. The objective of this study is to develop HPLC and sample preparation methods for identifying different types of flavonoids quantitatively. The sample preparation includes salting out liquid-liquid extraction using ethyl acetate and sodium chloride for honey samples. Pollen and propolis samples prepared via ultrasound assisted methanol extraction. Separation and quantification of 31 flavonoid compounds were accomplished with HPLC-PDA system. The chromatographic gradient separation was performed on a C18-Pentafluorphenyl (PFP) 250x4 mm column with a mobile phase consisting of 0.5% (v/v) formic acid and methanol. The chromatograms were monitored at 280nm. Honey samples (100), pollens (50) and propolis (50) samples from different regions and origins were analyzed and the results indicated that, relatively high amounts of taxifolin, epi-catechin, rutin hydrate, 4-OH benzoic acid, protocatechunic acid, caffeine acid and gallic acid were identified in all honey extracts. Protocatechuic acid (avg. 12.12 mg/kg), 4-OH benzoic acid (avg. 3.85 mg/kg) and rutin hydrate (avg. 2.25 mg/kg) are major flavonoids in Turkish pine honey where quercetin (avg. 1.45 mg/kg), gallic acid (avg. 7.17 mg/kg) and chlorgenic acid (avg. 2.01 mg/kg) were main flavonoid components in polifloral honeys. Pinocembrin, CAPE, chrysin and galangin are the most common flavonoids in propolis extracts with above the average value of 23.02 mg/L. Unlike honey and propolis, kaempferol, naringenin and resveratrol flavonoids were detected in pollen sample extracts.

Key Words: Flavonoids, HPLC, Honey, Propolis, Pollen.
References
FUNCTIONALIZED CELLULOSE ACETATE MEMBRANES.
SYNTHESIS, CHARACTERIZATION AND APPLICATIONS

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Abstract

The use of polymeric membranes is very well known, especially for water purification, separations or concentrations [1]. There are several methods for improving the separation properties of polymeric membranes, the most facile being the synthesis of composite membranes, the filler adding more value to membrane properties in terms of mechanical and thermal resistance and also separation efficiency [2, 3].

By functionalization, highly performance polymeric membranes can be obtained, also for other processes than separations. This work describe a new method for obtaining cellulose acetate membranes covalent functionalized with resveratrol [4], respectively sericin [5] for improving osseointegration at the interface between bone and metallic implants. For this purpose, cellulose acetate membrane is hydrolyzed in the presence of potassium hydroxide, followed by covalent immobilization of aminopropyl triethoxy silane (APTS). Sericin, respectively resveratrol were immobilized onto membranes using glutaraldehyde as linker.

Scanning electron microscopy revealed morphological changes (due to the crosslinking effect of APTS and glutaraldehyde reactions), correlated with water flows through synthesized membranes and proteins retention. Covalent immobilization of resveratrol, respectively sericin was proved by FT-IR, Raman, XPS and thermal analysis. The obtained membrane materials were also evaluated for osseointegration potential and cytotoxicity using MC3T3-E1 cells, proving their biomedical potential. Author potential applications for functionalization method, like analytical separations will be discussed for obtained materials.

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Key Words: membranes; covalent functionalization; cellulose acetate; biomedical applications

References

INVESTIGATION OF SUPEROXIDE DISMUTASE ACTIVITY, GLUTATHIONE AMOUNT AND PROTEIN CARBONYL LEVEL AT Cyprinidae Family EXPOSED TO VARIOUS STRESSORS

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Abstract

“Kangal Hot Spring with fish” is famous for the treatment of skin diseases. The thermal spring is situated 13 km outside the town of Kangal in Sivas. Mean temperature of the slightly alkaline water is 35°C with 2.9 ppm oxygen concentration. Trace elements of the water were determined previously and interestingly the water contains relatively higher selenium concentration (1.3 mg/L). Two different Cyprinidae family fish species so called "doctor fish" inhabit in the pools of the spring. The two species, Cyprinion macrostomus macrostomus (striker) and Garra rufa obtusa (licker), feed on phytoplankton and zooplankton [1,2]. However, higher temperature in the pools limits the amount of plankton, making them predatory and aggressive in seeking food. The scaly skin of psoriatic patients partially prevents food deficiency and make patients target for nutrients. These two fish species are under stress for life because of high temperature, high altitude, and insufficient nutrition and oxygen supplies in the pools.

Oxidative stress represents a shift on equilibrium between reactive oxygen species and detoxifying reagents on behalf of reactive oxygen species. Production of peroxides and free radicals damages macromolecules of a cell in adverse conditions. Living organisms form first line of defence against oxidative stress through an increase in superoxide dismutase (SOD), catalase, and glutathione peroxidase enzyme levels [3].

In this study changes of Superoxide dismutase (SOD) activity and amount of glutathione and level of protein carbonyl were investigated in two fish species living in Sivas Kangal Hot Spring. Fishes was exposed to various stressors such as heavy metal, pH, selenium, oxygen deficiency, temperature and nutritional deficiency. Fish muscle was used in all experiments.

Although glutathione levels were increased by the stress effects, there was no significant change in the amount of glutathione under nutritional deficiency in Garra rufa obtusa fish muscle. It was observed that the amount of glutathione decreased by the temperature effect, there was no change in nutritional deficiency, and the other stress effects increased the amount of glutathione in Cyprinion macrostomus macrostomus fish muscle.

In both fish species, stress effects caused changes in protein carbonyl levels and the highest increase was observed in temperature and nutritional deficiency effects.

SOD activity was decreased by the effect of nutritional deficiency and temperature effects and SOD activity was increased by the other stress effects in Garra rufa obtusa fish muscle. Nutritional deficiency, temperature and pH effects caused a decrease in SOD activity, while other stress effects caused an increase in SOD activity in Cyprinion macrostomus macrostomus fish muscle.

Key Words: Oxidative stress; SOD; Glutathione; Protein carbonyl

References

Abstract

The application of enzymes in their native form biochemical, biomedical, biotechnological, and food industrial fields is not always suitable and optimal. Binding of enzymes on a solid support is an advantageous modification of their application. Enzymes are immobilized onto or into a solid matrix to increase their thermostability, operational stability and recovery. Other benefits obtained as well, include better operational control, flexibility of reactor design, and ease of product recovery without catalyst contamination [1].

A great number of synthetic or natural carriers with different shapes/sizes, porous/non-porous structures, different hydrophilicities and binding functionalities, have been specially designed for various bioimmobilization and biosensor procedures [2].

Free and immobilized catalase can be of great value in food industries. Immobilized catalase has useful application in the food industry in the removal of hydrogen peroxide from food products after cold pasteurization and in the analytical fields as a component of hydrogen peroxide and glucose biosensor systems [3].

In this study we used paraffin wax as a support material for immobilization [4]. Paraffin wax (petroleum by product) is mostly found as a white, odorless, tasteless, waxy solid, with a typical melting point between about 47°C and 64°C. Paraffin wax is formed of straight chain hydrocarbons (18 to 40 carbon atoms) having an average molecular weight between 360 and 420. It is insoluble in water, but soluble in ether, benzene, and certain esters. Paraffin is unaffected by most common chemical reagents, but burns readily. Moreover, it is highly thermoplastic with a macro-crystalline structure. It exhibits excellent water repellency.

The first aim of this study to prepare catalase immobilized in paraffin wax and second, to investigate the kinetic parameters, operational, thermal and storage stability of immobilized catalase and free catalase in batch systems [3].

Catalase has been successfully immobilized into paraffin wax. Catalase activity decreased with immobilization. Optimum pH and optimum temperature for activity of free and immobilized catalase did not change. This study shows catalase can be immobilized in to paraffin wax and it can be used for practical applications.

Key Words: Catalase; Immobilization; Paraffin wax

References

PRECONCENTRATION OF COPPER, LEAD, GOLD AND PALLADIUM BY MICROEXTRACTION TECHNIQUE BASED ON IONIC LIQUID

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Abstract

Separation and preconcentration procedures are considered of great importance in elemental analysis as they eliminate or minimize matrix effects and concomitants, lowering the detection limit and enhancing sensitivity of detection techniques towards metals and their species [1]. Microextraction techniques are very useful and popular for the preconcentration and separation for organic and inorganic contaminants in environmental samples at trace levels since the last ten years due to their advantages like simple procedure, high extraction efficiency and low consumption of toxic organic solvents [2,3]. Ionic liquids (ILs) have been considered as green solvent. Its low vapor pressure, viscosity and the miscibility with water and other organic solvents made it have great applications in many fields [1]. Due to this properties, ionic liquids are very important and green alternative to organic solvents in classical extraction techniques. Various works have been presented by the usage of ionic liquids on the preconcentration and separation of trace heavy metal ions in the environmental samples [4].

In this work, ionic liquid based dispersive liquid-liquid microextraction method has been developed for enrichment copper, lead, gold and palladium in the various natural waters, waste water and tap water samples. 1-hexylpyridinium hexafluorophosphate solution was used as the ionic liquid in this method. Acetonitrile was used dispersive solution. Analytical concentrations after extraction were determined by flame atomic absorption spectrometry (FAAS) with microsample injection system. After the optimization of the variables was established, the method was applied to various water samples. The accuracy of the method was controlled with industrial waste water standard reference material (SPS-WW2 BATCH 114). The detection limits for Cu(II), Pb(II), Au(II) and Pd (II) in the determination by DLLME-AAS (3s, N=16) were found to be 2,22 µg/L, 2,48 µg/L, 3,21 µg/L and Pd (II) 2,65 µg/L, respectively.

Key Words: Ionic Liquid; Microextraction, Preconcentration

References

SELECTIVE EXTRACTION OF IRON, GOLD AND PALLADIUM WITH DISPERSIVE LIQUID LIQUID MICROEXTRACTION METHOD

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Abstract

The liquid phase microextraction techniques has received a growing amount of attention due to its simplicity, low consumption of organic solvent, low cost, ease of operation and possibility of obtaining high enrichment factor [1]. Dispersive liquid-liquid microextraction (DLLME) is the new microextraction techniques introduced in 2006 [2]. In this technique, an appropriate mixture of an extraction solvent and a disperser solvent is rapidly injected into an aqueous sample so that a cloudy solution is formed. The analyte in the sample is then transferred to the fine droplets of the extraction solvent and phase separation is performed by centrifugation. The advantages of this method are: simplicity, rapidity, low cost, low organic solvent volume, high recovery and enrichment factor [3].

In this study, dispersive liquid-liquid microextraction method was developed for the sensitive and selective determination of Fe (III), Au (II) and Pd (II) ions in various water samples. The main factors affecting the DLLME, such as pH of sample solution, amount of carmine as a ligand, extraction and disperser solvent types and their volume, were optimized for the best extract efficiency. Under the optimum conditions, i.e., sample volume: 5 mL, amount of carmine: 0.2 mg, extraction solvent: 250 μL CHCl₃, disperser solvent: 1 mL acetone, a quantitative recovery value was obtained. The preconcentration factor was calculated to be 10 for 5 mL sample volume and 0.5 mL last volume. The relative standard deviation was better than 5%. The method was validated by analysing the certified reference materials and the water sample spiked with analyte ions and then applied to various samples.

Key Words: Gold, Palladium, Iron, Microextraction, Preconcentration

References

ANODICALLY PRETREATED BORON-DOPED DIAMOND ELECTRODE FOR ANTITHYROID DRUG METHIMAZOLE DETERMINATION IN THE PHARMACEUTICAL FORMULATIONS

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Abstract

Methimazole (MMZ, 1-Methyl-2-mercaptoimidazole) prevents the thyroid gland from producing too much thyroid hormone. Therefore, MMZ is widely used in medicine for treatment an overactive thyroid gland (hyperthyroidism) [1]. MMZ is an orally taken drug to manage hyperthyroidism associated with Grave’s disease, however it causes side effects such as liver cirrosis, irritation of the skin, nephritis, allergies and pharyngitis with fever as well as impaired taste, auditory disorder and olfactory [2, 3]. Hence, developing a rapid, cheap and simple method for MMZ quantification is important for medical and/or pharmaceutical research.

In this study, a rapid, cheap, simple and modification-free electroanalytical methodology based on anodically pretreated boron-doped diamond (APT-BDD) electrode is described for the detection of MMZ. The oxidation of MMZ was well-defined irreversible and presented a diffusion controlled process. Using square-wave voltammetric (SWV) technique, a linear response was obtained for MMZ determination in 0.1 mol L⁻¹ Britton-Robinson (BR, pH 5.0) buffer solution at +0.89 V (vs. Ag/AgCl). Linearity was found between the oxidation peak currents and the concentration of MMZ within 0.5 to 25.0 μg mL⁻¹ (4.38×10⁻⁶-2.19×10⁻⁴ mol L⁻¹), with a detection limit of 0.085 μg mL⁻¹ (7.45×10⁻⁷ mol L⁻¹). The proposed method can be used for the determination of MMZ in the pharmaceutical formulations with acceptable recoveries.

Key Words: Methimazole; square-wave voltammetry; anodically pretreated boron-doped diamond electrode; pharmaceutical formulations.

References

Abstract

Capsaicin is also known as trans- 8-methyl- N- vanillin -6- nonamid and quite strong and stable, an alkaloid occurs only in hot pepper crystal in nature. The Solance falier Capsicum annum or obtained from Capsicum frutescens' and ' olorein capsicum ' (OC) as an oil derived from paprika known. Medicine in addition to its use in many areas; alcohol, ether and pepper spray hood from 1-10% capsaicin solution dissolved in organic solvents such as chloroform is done. In order to eliminate the harmful effects of capsaicin fragmentation reactions with OH radical was investigated. Quantum chemical calculations of Density Functional Theory (DFT) were used to investigate the structural and physical characteristics of capsaicin.

The geometric shapes of molecule obtained because of optimization
(grey, carbon; red, oxygen; blue, nitrogen; white, hydrogen)

The calculation of optimized geometry and the geometric optimization for the determination of the lowest energy status were made via Gauss View 5 and the Gaussian 09 program. Activation energy for the probable reaction paths was calculated and their most stable state from the thermodynamic perspective was determined for the gaseous phase. The aim of this study is to estimate the degradation mechanism of capsaicin molecule in gaseous phase and solvation phase. Calculation of the probable reaction path of the activation energy was made, and their most stable state in the thermodynamic frame was determined for these phases.

Key Words: Capsaicin; Pepper Gas; Gaussian 09; DFT

References

ELECTROCHEMICAL, SPECTROELECTROCHEMICAL AND ELECTROCATALYTIC CHARACTERIZATION OF NOVEL PHTHALOCYANINE COMPOUNDS INCLUDING 1,1'-THIOBIS(2-NAPHTOL) MOIETIES

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Abstract

Phthalocyanine (Pc) complexes with the conjugated 18 double bonding electrons system display Pc and/or metal based redox properties [1-2]. These properties can be modified in a broad scale by changing the nature and number of peripheral or nonperipheral substituents and the metal ion in the centre. The modifiable rich redox properties make these compounds applicable in various electrochemical technology areas such as electrochromic display devices [1] and electrochemical energy conversion and storage systems such as polymer electrolyte membrane fuel cells (PEMFCs), direct methanol fuel cells and metal-air cells [2]. Accordingly, these compounds have attracted considerable attention of many scientists and researchers.

The detailed identification of their redox properties has vital importance for the determination of the possibility of the usage of Pc compounds in the technological applications. In this study, electrochemical redox properties of novel Pc complexes including 1,1'-Thiobis(2-naphtol) moieties were identified by electrochemical techniques such as cyclic voltammetry, square wave voltammetry, and chronocoulometry. Moreover, in situ spectroelectrochemical measurements were also carried out in order to provide additional support for the assignment of the redox processes since it is not possible to completely distinguish such processes by voltammetry alone. The compounds usually showed one-electron metal- and/or ligand-based reversible or quasi-reversible reduction and oxidation processes. The ratio of anodic to cathodic peak currents for the redox couples were usually near unity and anodic to cathodic peak separation ranged 60 to 100 mV, suggesting reversible to quasi-reversible behaviour. The color changes associated with the redox processes were also identified by in situ spectroelectrochemistry and in situ electrocolorimetry, with the aim of identifying the possibility of the usage of the compounds as electrochromic materials. The catalytic performances of the metal Pcs for oxygen reduction were also tested by dynamic voltammetry using the combined system of a rotating ring-disk electrode and a bipotentiostat, in the media similar to PEMFC and metal-air cell working conditions since one of the main tasks of the current research associated with these battery applications is the availability of efficient, stable and cost-effective electrocatalysts promoting the overall four-electron reduction of the oxygen molecule.

Key Words: Phthalocyanine, Thiobis(2-naphtol), Electrochemistry, Spectroelectrochemistry, Electrocatalysis

Acknowledgments: This study was supported by Marmara University The Commission of Scientific Research Projects.
References


Abstract

Antibiotics are a group of emerging substances used in both human and veterinary medicine for the treatment and prevention of bacterial infections. Currently, there is growing interest in the presence and persistence of antibiotics in the environment because, even at low concentrations, they can lead to the proliferation of antibiotic-resistant bacteria leading to untreated human disease [1]. 50% of these compounds can be removed from the water by conventional methods, and the removal performance can reach a certain level. The present work aims to solve current problems regarding the reactive separation of antibiotics by obtaining new cellulose acetate (AC) and hydrotalcite (LDH) composite membranes and subsequent modification of the optimal composite membranes in order to remove antibiotic traces left. LDH (see scheme 1) are anionic clays which have exceptional properties such as high specific surface area, increased porosity, high anion exchange capacity and good thermostability, making it ideal for sewage treatment [2]. The hydrotalcite will be introduced into the polymer matrix in order to increase porosity and pore diameters, e hydrophilicity and mechanical strength, and membrane permeability to water.

Key Words: Antibiotic retention, membranes, hydrotalcite, surface modification

References

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