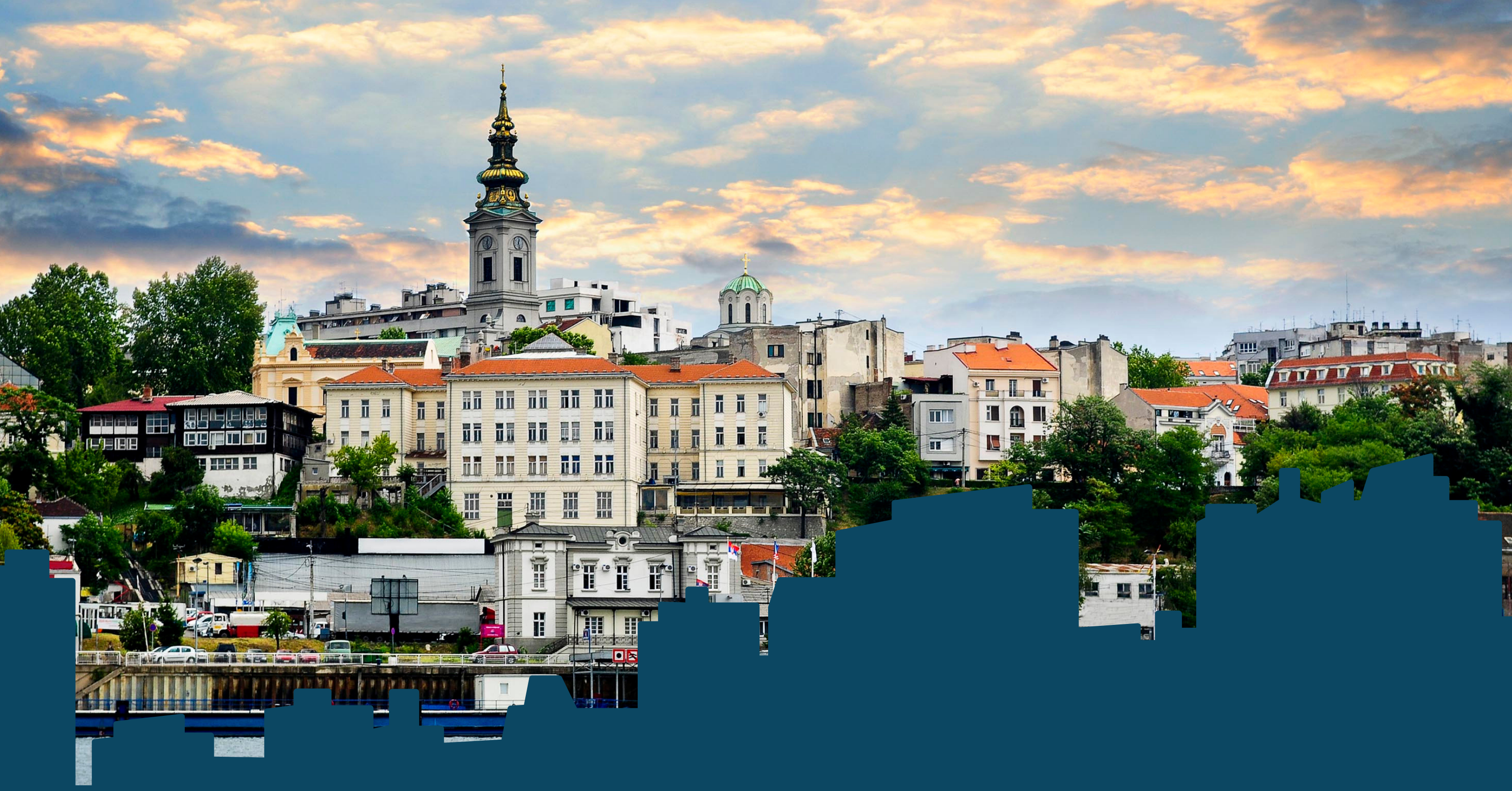

ICACCHE

2nd International Conference on Applications in Chemistry and Chemical Engineering

BOOK OF ABSTRACTS

10 - 14 October 2018 **Belgrade**

www.icacche.com

ICACChE

2nd International Conference on Applications in Chemistry and Chemical Engineering

10 - 14 October 2018 Belgrade

Organized by

Partners

INTERNATIONAL CONFERENCE ON APPLICATION IN CEHMISTRY AND CHEMICAL ENGINEERING (ICACCHE)

ISBN 978-605-67987-1-0

BOOK OF ABSTRACTS OF THE
INTERNATIONAL CONFERENCE ON APPLICATION IN CEHMISTRY AND CHEMICAL ENGINEERING (ICACCHE)
10-14 OCTOBER 2018, BELGRADE

Edited by
Prof. Dr. Ömer Şahin

Published, 2018

info@icacche.com
www.icacche.com

SCIENTIFIC COMMITTEE

1. Prof. Dr. İbrahim DİNÇER-University of Ontario
2. Prof. Dr. Gülhayat NASÜN SAYGILI - İstanbul Technical University
3. Prof Dr. İnci EROĞLU- Middle East Technical University
4. Prof. Dr. Mustafa BÖYÜKATA - Bozok University
5. Prof. Dr. Ferdinand Bego - University of Tirana, Albania
6. Prof. Dr. M. Salih AĞIRTAŞ - Yüzüncü Yıl University
7. Prof. Dr. Spiro Drushku - University of Tirana, Albania
8. Prof. Dr. Mahmut DOĞRU - Fırat University
9. Prof. Dr. Ahmet ÖZER - Fırat University
10. Prof. Dr. Muhtar KOCAKERİM - Çankırı University
11. Prof. Dr. Sinan YAPICI - İnonu University
12. Prof. Dr. Tahir Arbneshi - University of Pristina
13. Prof. Dr. İbrahim DİNÇER - Yıldız Teknik Üniversity
14. Prof. Dr. İsmail ÇAKMAK - Kafkas University
15. Prof. Dr. Ahmet KILIÇ - Harran University
16. Prof. Dr. Ahmet Duran ŞAHİN - İstanbul Technical University
17. Prof. Dr. Mustafa DEĞİRMENCİ - Harran University
18. Prof. Dr. Kozeta Vaso - University of Tirana, Albania
19. Prof. Dr. Zübeyde BAYSAL - Dicle University
20. Prof. Dr. Hasan TOĞRUL - Eskişehir Osmangazi University
21. Prof. Dr. Filiz KARAOSMANOĞLU - İstanbul Technical University
22. Prof. Dr. Fikret AKDENİZ - Kafkas University
23. Prof. Dr. Sermet KABASAKAL - Eskişehir Osmangazi University
24. Prof. Dr. Handan KAMIŞ - Selçuk University
25. Prof. Dr. Ülker BEKER - Yildiz Technical University
26. Prof. Dr. Mahmut KUŞ - Selçuk University
27. Prof. Dr. Hafız ALİSOY - Namık Kemal University
28. Prof. Dr. Ömer YAVUZ - Dicle University
29. Prof. Dr. Mesut AKGÜN - Yildiz Technical University
30. Prof. Dr. Birsen Şengul OKSAL - Giresun University
31. Assoc. Prof. Dr.Koray KÖKSAL - Bitlis Eren University
32. Assoc. Prof. Dr. Naser Troni - University of Pristina
33. Assoc. Prof. Dr. Nasrettin GENLİ - Dicle University
34. Assoc. Prof. Dr. M. Zafer KÖYLÜ - Dicle University
35. Assoc. Prof. Dr. Cafer SAKA - Siirt University
36. Assoc. Prof. Dr. Abdurrahman ASAN - Hitit University
37. Assoc. Prof. Dr. Halil DEMİR - Siirt University
38. Assoc. Prof. Dr. A.Abdullah CEYHAN - Selçuk University
39. Assist. Prof. Dr. Yunus ÖNAL - İnönü University
40. Assist. Prof. Dr. Vedat ADIGÜZEL - Kafkas University
41. Assist. Prof. Dr. Mustafa ÖZDEMİR - Süleyman Demirel University

ORGANIZATION COMMITTEE

Honorary Chairs
Prof. Dr. Murat ERMAN – Rector – Siirt University

Conference Chairman
Prof. Dr. Ömer ŞAHİN – Vice Rector– Siirt University

Members of the Committee

- Assist. Prof. Dr. Orhan BAYTAR - Siirt University
- Assist. Prof. Dr. M. Sait İZGİ - Siirt University
- Assist. Prof. Dr. Sabit HOROZ - Siirt University
- Assist. Prof. Dr. Sinan KUTLUAY - Siirt University
- Assist. Prof. Dr. Arzu EKİNCİ - Siirt University
- Assist. Prof. Dr. Dilek KILINÇ - Siirt University
- Teaching assistant Amra Banda - University of Sarajevo
- Teaching assistant Amina Sivac - University of Sarajevo
- Teaching assistant Boris Avdic - University of Sarajevo
- Teaching assistant Edin Hrelja - University of Sarajevo

Secretariat of the Committee

- Research assistant Yavuz KIRIM-Siirt University
  Tel: +90 541 592 38 60 - yavuzkirim@siirt.edu.tr
- Research assistant Tülin Avcı HANSU - Siirt University
  Tel: +90 539 666 00 69 - tulinn_avci@hotmail.com

WELCOME TO ICACCHE 2018

On behalf of the organizing committee, we are pleased to announce that the International Conference on Application in Chemistryand Chemical Engineering (ICACCHE-2018) is heldfrom October 10 to 14, 2018 in Belgrade - SERBİA. ICACCHE 2018 provides an ideal academic platform to present the latest research finding on design, manufacture and operation of plants and machinery, the development of new materials or substances, developing novel materials and processes, analyzing substances, measuring the physical properties of substances and testing theories. This event gives a chance for all the professionals to gain and share information on Chemistry and Chemical Engineering and other related science branches issues and research.

Chemistry and Chemical engineering are multidisciplinary branchs of applied engineering and science consisting of the application of physical science (Chemistry & Physics), life sciences including biochemistry with applied mathematics and economics to produce transform and use of chemicals, molecules materials, energy to make the whole production process successful with economic benefits.

Over the last 50 years, the discoveries in the basic sciences and the engineering of these inventions have been targeted at the development of applied technology and the prosperity of mankind and the distant and high quality of life away from environmental destructions for a sustainable future. Mathematics, physics, chemistry, and biology, which are accepted as basic sciences, and their engineering applications are now accepted in the scientific circles that have been intertwined and one of which is not worthless. It is foreseen by sectoral and academic stakeholders that these interdisciplinary relationships will continue to increase over the next several years.

The ability to identify, model, and solve engineering problems, and the ability to apply engineering knowledge develops with the knowledge of basic sciences. So, in terms of engineering education and the application of the engineering profession, the basic sciences have an important place and the necessary importance should be given.

Our goal is to transform this conference into an exchange of views on future vision and scenarios in chemistry, chemical engineering and related sciences, and to make science a tool of peace and justice.

Best regards,

Prof. Dr. Ömer ŞAHİN

ICACChE
2nd International Conference on Applications in Chemistry and Chemical Engineering
10 - 14 October 2018 Belgrade

COMPARATIVE ANALYSIS OF THREE ARTIFICIAL INTELLIGENCE BASED MODELS FOR ATMOSPHERIC TURBIDITY PREDICTION

LAIDI MAAMAR[a], ABDALLAH EL HADJ ABDALLAH[a], CHERIF SI-MOUSSA[a],
HANINI SALAH[a]

[a]MEDEA UNIVERSITY ALGERIA

*maamarw@yahoo.fr

Abstract:

Algeria is one of the countries with the highest solar radiation amount in the world, the knowledge of this solar deposit is mandatory for the use in the design and optimization of solar energy equipments. The measurement of solar energy is always not easy due to high costs, technical complexities and atmospheric turbidity indexes. The atmospheric turbidity represents the attenuation of the solar radiation that reaches the Earth's surface under cloudless sky and describes the optical thickness of the atmosphere. The goal of this work is to model the atmosphere turbidity of some sites in Algeria by means of two parameters, the Linke turbidity factor (TL) and the Angström coefficient (A). This article proposed three machine learning models based on artificial neural networks (ANN), support vector machine (SVM) and Extreme Gradient Boosting (XGBoost) approaches for accurately predicting the non-linear behavior of turbidity indexes in some cities in Algeria using a number of variables involved in physical process. Methods were applied using the free program package MATLAB installed on open source software operating system (Ubunto). Results show the SVM model was more accurate than the XGboost and the ANN models. This SVM model was also interpolated and extrapolated using other cities in Algeria and result show that this latter can be used to predict turbidity indexes with acceptable accuracy.

Keywords: Artificial Neural Networks, Support Vector Machine, Linke Turbidity Factor, Extreme Gradient Boosting, Angström Coefficient.

ICACChE
2nd International Conference on Applications in Chemistry and Chemical Engineering
10 - 14 October 2018 Belgrade

A NOVEL APPROACH BASED ON FRACTIONAL CALCULUS TO PHARMACOKINETIC MODEL

LAIDI MAAMAR[a], ABDALLAH EL HADJ ABDALLAH[a], CHERIF SI-MOUSSA[a], HENTABLI MOHAMED[a]

[a]MEDEA UNIVERSITY ALGERIA

*maamarw@yahoo.fr

Abstract:

Studying the distribution of drugs in the body needs the collection of large numbers of plasma samples to see how the change happens. However, taking large numbers of samples from a patient is difficult. As a consequence, mathematical models based on based on mass balance analysis are used to predict changing drug concentration over time to the body.

The aim of this work is to test the faisability of applying the fractionnal calculus modeling in the field of chemical engineeing. A comprasion between ordinary and fractional differential modeling is conducted to determine the best fractional parameters (n-order kinetic, Caputo fractional derivative of order), the optimization of these parameters has been conducted using hybrid optimization approach based on genetic algorithm and lsqcurvefit algorithm. A database has been collected from literature regarding the distribution of concentration over the time of an intravenous dose in the body.

It has been shown that zero-order differential kinetic with fractional derivative order of 0.5870 describe experimental distribution of the intravenous drug in the body with high accuracy, in comparison with the ordinary differential modeling in terms of a very low average absolute relative deviation AARD of 4.0766% and acceptable correlation coefficient R of 0.9943. The AARD of the ordinary differential modeling is 23.91% and R of 0.9746.

Keywords: Fractional Calculs, Drug Kinetics, Modelling

THE USE OF CARBON NANOTUBE-SUPPORTED CO-CU-B CATALYST İN THE HYDROLYSIS OF SODIUM BOROHYDRIDE

ORHAN BAYTAR[a], ÖMER ŞAHİN[a], MEHMET GÜRSOY[b]

[a]SIIRT UNIVERSITY
[b]KONYA TEKNIK UNIVERSITY

*baytarorhan@gmail.com

Abstract:

The demand for energy increases with increasing population. Existing fossil fuel sources cannot meet this demand. Therefore, researchers are looking for new sources of energy. One of the new energy sources is hydrogen energy.

The carbon nanotube (CNT) synthesized by the chemical vapor deposition method was used as support material for the Co-Cu-B catalyst. Then, the effect of CNT supported Co-Cu-B catalyst on sodium borohydride hydrolysis was investigated. The effects of CNT/catalyst ratio, NaBH4 concentration, catalyst amount and temperature parameters were investigated in sodium borohydride hydrolysis studies. It was determined that sodium borohydride hydrolysis rate increased with increasing catalyst amount and temperature. The initial hydrogen production rates for carbon nanotube-supported Co-Cu-B and unsupported Co-Cu-B catalyst catalysts were 6325 and 1533 ml*min-1*g-1, respectively. Decomposition kinetics and activation energy of sodium borohydride were determined. The order of kinetic and activation energy of sodium borohydride hydrolysis were determined as 0.14 and 53.5 kj*mol-1 respectively. The carbon nanotube synthesized by us was found to increase the active surface area of the Co-Cu-B catalyst used in the hydrolysis of sodium borohydride and to be used in applications.

Keywords: Carbon Nanotubes; Catalyst; Supported

THE SYNTHESIS THE ACTIVE CARBON FROM THE BEECH WOOD AND INVESTIGATION OF ITS EFFECT ON THE CR (VI) ADSORPTION BY SURFACE RESPONSE METHOD

ORHAN BAYTAR[a], ÖMER ŞAHIN[a], AYHAN ABDULLAH CEYHAN[b]

[a]SIIRT UNIVERSITY
[b]KONYA TEKNIK UNIVERSITY

*baytarorhan@gmail.com

Abstract:

In this study, activated carbon was synthesized from beech wood by chemical activation method using ZnCI2 activator. The effect of impregnation rate, impregnation time, activation temperature and activation time parameters were investigated in the synthesis of activated carbon. Iodine numbers of synthesized activated carbons were determined. Characterization of activated carbon-containing high iodine number was determined by BET, SEM and FTIR devices. The surface area of activated carbon was determined as 908 m2/g. Adsorption of Cr (VI) using the synthesized activated carbon was investigated by experiment design. Experimental design was performed with Box-Behnken design model of Surface Response Method in Dizayn Expert package program. The effects of temperature, time and initial concentration parameters were investigated in the experimental design. In the surface response method, the experimental design was carried out by selecting the adsorption capacity (qe) response parameter. It was determined that the best model was quadratic by using Box- Behnken design model. The ANOVA table was created and 3D graphics were plotted to examine the effect of the selected parameters on Cr (VI) adsorption. According to the ANOVA table, the initial concentration of the solution was determined as the most effective parameter for Cr (VI) adsorption. According to ANOVA table, it was determined that single parameters

Keywords: Adsorption; Activated Carbon; Dizayn Expert

COMPARISON OF PROPERTIES OF EU(2+) DOPED ZNS AND EU(3+) DOPED ZNS QUANTUM DOTS

SABIT HOROZ[a]

[a]SIIRT UNIVERSITY

*sabithoroz@siirt.edu.tr

Abstract:

During the past decades, the preparation and characterization of the II-VI semiconductor quantum dots (QDs) have revealed new physics in reduced dimensions and provided possibilities of fabricating novel materials. ZnS is one of the ubiquitous semiconductor materials that has been widely studied as an important phosphor for optoelectronic and photovoltaic energy applications due to its better chemical stability and environment friendliness compared to other chalcogenides [1-2]. Doped semiconductor nanocrystals/QDs are a new class of luminescent materials, which have generated new opportunities for research and also for the applications of nanostructured materials. Doping of ZnS nanoparticles by transition metal ions, e.g. Mn2+, Cu2+ and rare-earth ions of Eu3+/Eu2+, may result in diluted magnetic semiconductors (DMS). Those ions may provide local magnetic moments, which are distributed randomly in the nonmagnetic host lattice and couple with one another by long-range exchange interaction. Depending on the doping, ZnS may show paramagnetic or ferromagnetic behavior [3-5].

Quantum confinement can affect the energy structure of doped nanocrystals and the relative energy positions of the dopants. The excited states of Eu2+ can be moved into the band gap of ZnS by quantum confinement effect. The size dependence of fluorescence of ZnS:Eu2+ QDs was observed by Chen et al [6]. The shift of the Eu2+ intra-ion 4f6d1 (t2g) – 4f7 emission to higher energy for smaller QDs was attributed to the decrease in the electron phonon coupling and crystal field strength.

In the present study, the structural, magnetic and optical properties of Eu doped ZnS QDs have been examined. Both Eu3+ and Eu2+additive materials have been investigated in order to study the effects of the two distinctive Eu ions.

Keywords: Characterization, Doping, Rare-Earth Ions, Synthesis

INVESTIGATION OF THE EFFECT OF SYNTHESIS TEMPERATURE ON THE BAND ENERGY OF CDS NANOPARTICLES

SABIT HOROZ[a], ARZU EKİNCİ[a], ÖMER ŞAHIN[a]

[a]SIIRT UNIVERSITY

*sabithoroz@siirt.edu.tr

Abstract:

In recent time, there has been great drive in the synthesis and characterization of mono dispersed nano particles of II - IV compounds. The reason is that the optical, electronic and thermodynamic properties of the particles in the nanometer range are different from the optical, electronic and thermodynamic properties of the bulk materials, usually due to the quantum confinement. These unique properties can cause interesting linear and nonlinear optical properties such as optoelectronic probes for irregular DNA structures, fluorescence probes in peptides, which have great potential in technological applications [1-3]

Among these II-VI semiconductors, cadmium sulfur (CdS) has a direct band gap of 2.42 eV, corresponding to an optical cut at 515 nm, making it the perfect candidate for promising applications in heroptoelectronic, photonic photovoltaics and photocatalysis. The CdS have unique physical, chemical, optical, and structural properties different from the bulk. These properties are affected by the particle size via the quantum confinement effect. For example, the band gap and thus the band edge absorption is directly controlled by the particle size [4-5].

In our study, we reported the synthesis of un-doped CdS nanoparticles. Samples were prepared by wet-chemical method using 1-thioglycerol as a capping agent at different temperatures. We studied the structural and optical properties of un-doped CdS nanoparticles synthesized at different temperatures. The effect of synthesis temperature on optical properties were discussed.

Keywords: Synthesis, Nanoparticles, Cadmium Sulfide, Optical Properties

COMPARISON OF PROPERTIES OF PBS AND FE DOPED PBS THIN FILMS

ARZU EKINCI[a], SABIT HOROZ[a], ÖMER ŞAHIN[a]

[a]SIIRT UNIVERSITY

*aekinci80@gmail.com

Abstract:

Abstract

One of the most effective methods of improving the quality of semiconductor thin film materials is the alloying of thin films with metal ions. The crystal structure, surface morphology and particle size of the thin film can become controll able by the alloying. Thus, the chemical and physical properties of the synthesized thin films are improved during synthesis. Despite the fact that different studies have produced semiconductor thin films, there is still a shortage to synthesize high quality nanostructured PbS thin films with excellent physical and chemical properties. One of the most important parameters in the alloying process is the lattice matching between the base metal and the alloying metal. For example, the ionic radius of Fe is smaller than the ionic radius of Pb. Thus, it is possible to be easily alloyed Fe metal ions in to the PbS lattice without difficulty. Investigations on the structural, optical and morphological properties of Fe-alloyed PbS thin films have been limited and the photovoltaic properties of Fe-alloyed PbS thin films will be investigated for the first time.

In this study, PbS and Fe-alloyed PbS thin films were synthesized by chemical bath deposition (CBD) technique, which is suitable for cost on glass substrates at room temperature. The structural, elemental and optical properties of the synthesized thin films were characterized by X-ray diffraction (XRD), energy dispersive X-ray (EDX) and optical absorption measurements, respectively. It was observed that Fe dopant alters crystal size and energy band gap of PbS although it does not change the structure of PbS.

Keywords: Keywords: Thin Films, Chemical Bath Deposition, Optical Properties, Particle Size

SYNTHESIS AND CHARACTERIZATION OF CR DODOPED CDZNS NANOPARTICLES

ARZU EKINCI[a], SABIT HOROZ[a], ÖMER ŞAHIN[a]

[a]SIIRT UNIVERSITY

*aekinci80@gmail.com

Abstract:

Hetero-structures based on II-VI group compounds have long been known to be suitable materials for thin-film photovoltaic device applications because of their high optical absorption coefficients. Group II-VI compounds can form ternary and quaternary alloys with a direct fundamental band gap assignment over the entire alloy composition range and high absorption coefficients, which can be used as materials for fabricating hetero-junction photovoltaic devices. Cadmium zinc sulfide (CdZnS) thin films have been widely used as a wide band-gap (2.4 -3.7 eV) window material in heterojunction solar cells and in photoconductive devices. In solar cell systems, where CdS films have been demonstrated to be effective, the replacement of CdS with the higher bandgap ternary CdZnS has led to a decrease in window absorption losses and has resulted in an increase in the short circuit current in the solar cell. However, the resistivity of CdZnS films increases rapidly with the composition of zinc. It is evident that the composition dependence of resistivity is a basic property of the CdZnS solid–solution system and is not appreciably altered by the method of preparation. This high resistivity of CdZnS films limited their utilization as a window material in most heterojunction devices.

In this study, pure CdZnS and chromium (Cr) doped CdZnS nanoparticles at room temperature will be synthesized by chemical precipitation. The structural properties of synthesized nanoparticles using an X-ray diffraction device will be investigated. Furthermore, the size of Cr doped CdZnS nanoparticles will be calculated using the obtained XRD data. The energy band gap of the doped CdZnS nanoparticles will be determined using UV-Vis spectroscopy. Thus, how the Cr dopant affects the structural and optical properties of CdZnS will be examined and the resulting data interpreted.

Keywords: Nanoparticles, II-VI Compounds, Synthesis, Characterization, Doping

EFFECT OF FATTY ESTER-MALEIC ANHYDRIDE COPOLYMER DI-ESTERS ON CRYSTALLIZATION BEHAVIOR OF WAXY CRUDE OIL

REHAB MOHAMED ALI[a], MARWA R. ELKATORY[a], EMAD A. SOLIMAN[a], AHMED I. HASHEM[b]

[a]CITY OF SCIENTIFIC RESEARCHES AND TECHNOLOGICAL APPLICATIONS
[b]FACULTY OF SCIENCE, AIN SHAMS UNIVERSITY

*rehabmohamedali1983@gmail.com

Abstract:

Deposition of large aggregated crystals of wax onto wall of pipelines and tankers at and below the cloud point or wax appearance temperature (WAT) leads to gelation and hence decline the oil flow which is a complex and very costly problem for the petroleum industry. Therefore, the pour point depressants (PPD) are considered as a critical processing aid to improve the flow of waxy crude oil. Therefore, maleinzation of fatty acid esters was investigated in this study to synthesize inexpensive and efficient flow improvers. Where, fatty acid ester and maleic anhydride were copolymerized in the presence of a free radical generating initiator. The resultant copolymers were then esterified with fatty alcohol (C19H36O3). The copolymers and its esterified form were structurally characterized by Fourier transform infrared spectroscopy (FTIR), Nuclear magnetic resonance (NMR) spectral analysis and scanning electron microscopy (SEM). Moreover, the potential interactions between PPD and waxes were investigated by using differential scanning calorimetry (DSC), X-ray diffraction (XRD) and light microscope. The obtained polymeric PPD at dose of 3000 ppm showed good performance by inhibiting the wax crystals from growing to larger sizes and providing a barrier to crystal agglomeration at low temperatures, thus the pour point of the petroleum waxy crude oil was reduced up to 6 °C.

Keywords: Pour Point Depressant; Flow Improvers; Copolymerization; Fatty Acids; Crystallization Of Wax; Waxy Crude Oil

CORRELATION BETWEEN FREE VOLUME HOLES AND MECHANICAL PROPERTIES OF SIDE CHAIN LCP-HDPE GRAFT PRODUCTS

BEHIYE OZTURK SEN[a], UGUR YAHSİ[b], SEDAT CETIN[c], CUMALI TAV[b], MURAT YAVUZ YENER[b], UGUR SOYKAN[d]

[a]SCHOOL OF PHARMACY, ALTINBAS UNIVERSITY
[b]PHYSICS DEPARTMENT, FACULTY OF ARTS AND SCIENCES, MARMARA UNIVERSITY
[c]CHEMISTRY DEPARTMENT, FACULTY OF ARTS AND SCIENCES, ABANT IZZET BAYSAL UNIVERSITY
[d]YENICAGA YASAR CELIK VOCATIONAL HIGH SCHOOL, ABANT IZZET BAYSAL UNIVERSITY

*behiye.sen@altinbas.edu.tr

Abstract:

The aim of this study was to reinforce high density polyethylene (HDPE) with a side chain liquid crystalline polymer (LCP), which is poly(p-benzophenoneoxycarbonylphenyl methacrylate), poly(BPOCPMA) by graft copolymerization of the monomer, BPOCPMA. Graft copolymerization of BPOCPMA (5,10,15,20,30,40% of the reaction mixture) was studied at 140° C for 40 minutes reaction time via bulk-melt polymerization. The content of poly(BPOCPMA) in the products presented as graft units in copolymers, and presented as both the graft units and the homopolymer molecules in the coproducts was determined gravimetrically. The mechanical properties (modulus and tensile strength) of neat HDPE and products (copolymers and coproducts) were determined. Also, products were analyzed by Positron Annihilation Lifetime Spectroscopy (PALS) to determine free volume properties at room temperature and all lifetime spectra were analyzed into three lifetime components. It was also aimed to correlate the free volume properties and mechanical properties of products. It was observed that the free volume size (hole size) and the free volume fraction were anti-correlated with the modulus and the tensile strength. The improvements in the tensile behaviors were accompanied with the reductions in the free volume fraction. Especially, when the content increased from 10.7% to 11.8% poly(BPOCPMA) in the copolymers, the sharp increase in the tensile strength (from 29.40 MPa to 36.3 MPa) and the modulus (from 471 MPa to 514 MPa) were accompanied with the abrupt drop in the free volume fraction (from 4.20% to 3.81%) due to an increase in the resistive frictional force in the molecules and a lower conformational freedom. Moreover, higher mechanical properties of copolymers resulted in lower free volume fraction compared to coproducts owing to the inclusion of the homopolymer molecules in coproducts which was composed of the chains with so large and rigid side groups and this made the material less prone to resist in tensile strength.

Keywords: High Density Polyethyelene, Side Chain Liquid Crystalline Polymer,Positron Annihilation Lifetime Spectroscopy, Free Volume Hole

SOME STUDIES RELATED TO THE DETERMINATION OF FACTORS AFFECTING POSITRONIUM FORMATION OF HIGH DENSITY POLYETHYLENE (HDPE) VIA POSITRON ANNIHILATION LIFETIME SPECTROSCOPY (PALS)

BEHIYE ÖZTÜRK ŞEN[a], UGUR YAHSI[b], CUMALI TAV[b]

[a]ALTINBAŞ UNIVERSITY
[b]PHYSICS DEPARTMENT, FACULTY OF ARTS AND SCIENCES, MARMARA UNIVERSITY

[*]behiye.sen@altinbas.edu.tr

Abstract:

“Positron annihilation lifetime spectroscopy” (PALS) is one of the most important techniques for the determination of local free volume in polymers. In recent years, PALS has been used for the detection of free volume properties of high density polyethylene (HDPE).

Nahid and counterparts studied the effect of trapped electrons on the positronium formation of HDPE below glass transition temperatures. According to experimental results, I3 at 20K was higher compared to I3 at 200K and with increasing temperature, I3 decreased. In addition, the variation in I3 was studied at different irradiation times. By increasing irradiation time, higher I3 was obtained owing to higher inter-track trapped electrons. It can be concluded that at lower temperatures, these trapped electrons are localized and can react with positrons (Nahid et al., 2011).

Suzuki et al. researched the radiation effect on positronium formation of HDPE. The samples were irradiated with γ-ray at room temperature and the variation in positronium formation with the elapsed time was examined for pristine HDPE,1 MGy γ-irradiated PE and annealed of this sample. With regard to results, o-Ps intensity, I3 of 1 MGy γ-irradiated PE was lower than pristine HDPE because of the effect of free radicals on positronium formation in irradiated sample, whereas annealed sample had higher o-Ps intensity, I3 than pristine. Because free radicals were eliminated and the crystallinity of annealed sample was lower than pristine and increased the amount of the amorphous part, which has more trapping sites of electrons. (Suzuki et al., 2001).

Hirade and Kumada investigated the effect of γ-irradiation on the positronium formation of HDPE. The higher irradiation dose led to the lower positronium intensity (Hirade and Kumada, 2001).

We have a project on the radiation effects on molecular weight and thickness dependence of free volume using Slow Positron Beam System at Marmara Positron/Positronium Laboratory Facility.

Keywords: Positronium, Positron Annihilation Lifetime Spectroscopy(PALS), Free Volume, Radiation Effect

HYDROGEN PRODUCTION VIA TIO2 BASED FE (II)–SCHIFF BASE COMPLEX

DILEK KILINÇ[a], ÖMER ŞAHİN[a]

[a]SIIRT UNIVERSITY

*dkilinc@siirt.edu.tr

Abstract:

Hydrogen is a wonderful energy source and a notable clean energy carrier, attracting great interest all over the world [1]. That's why to improve the hydrogen economy, scientists make an effort to find effective hydrogen storage materials with provide safe and green hydrogen production techniques. Recently, H2 is mainly stored in a lot of form like metal hydrides, liquefied hydrogen, organic hydrides, etc. Between them, H2 stored in the form of complex hydrides especially sodium borohydrides has been widely studied because of its specific suitability for all applications [2].

In this study we used Schiff Base complex called 4,4-methylenebis(2,6-diethyl)aniline-3,5-di-tert-butylsalisilaldimin-Fe(II) complex [3] to supported on TiO2 and it was used as a catalyst to hydrogen generation from NaBH4 hydrolysis with based on some parameters. Catalyst was also characterized with some analysis technique. As a result it was seen that TiO2 supported Fe(II) complex is effective catalyst in NaBH4 hydrolysis reaction for H2 production.

References

[1] Mattos LV, Jacobs G, Davis BH, Noronha FB. Chem Rev 2012; 112:4094-123.

[2] Schlapbach L, Zuttel A, Zu¨ttel a. Nature 2001; 414:353-8.

[3] Sahin Omer, Kilinc Dilek, Saka Cafer. Separation Science and Technology 2015; 50:2051-9.

Keywords: Tio2, Hydrogen, Complex, Catalyst

NEW PD-PEPPSI COMPLEXES AND THEIR PROPERTIES

DILEK KILINÇ[a], NEVIN GÜRBÜZ[b]

[a]SIIRT UNIVERSITY
[b]INONU UNIVERSITY

*dkilinc@siirt.edu.tr

Abstract:

Palladium complexes containing NHC ligand, have demonstrate to be useful catalysts in cross-coupling reactions of aryl halides.[1] between the most famous catalysts for this kind of reactions are shown PEPPSI-type palladium–NHC complexes, that have gained practical significance in various catalytic processes,(PEPPSI=pyridine-enhanced precatalyst preparation, stabilization and ınitiation).[2]

Since 2006, various studies has been done with these complexes [3], but only a limited reports available for PEPPSI-Pd catalyzed Mizoroki-Heck Reaction.

In this study, new palladium pyridine (Pd-PEPPSI) complexes which was obtained 3 different NHC ligands were synthesized and the complexes were used as catalysts in Mizoroki-Heck Reaction. Characterization of complexes were done by spectroscopic techniques. It was seen as a result Pd-PEPPSI complexes are very active catalysts in the Mizoroki-Heck cross-coupling reaction.

References:

[1] N. M. Scott, S. P. Nolan in N-Heterocyclic Carbenes in Synthesis (Eds.: S. P. Nolan), Wiley-VCH, Weinheim, 2006, pp. 55–70.

[2] C. Valente, M. Pompeo, M. Sayah, M. G. Organ, Org. Process Res. Dev. 2014, 18, 180–190.

[3] M. G. Organ, S. Çalimsiz, M. Sayah, K. H. Hoi, A. J. Lough, Angew. Chem. Int. Ed. 2009, 48, 2383–2387; A. Chartoire, X. Frogneux, A. Boreux, A. M. Z. Slawin, S. P. Nolan, Organometallics 2012, 31, 6947–6951.

Keywords: Mizoroki-Heck, Peppsi, Cross-Coupling Reaction

INVESTIGATION OF LINER GROWTH RATES OF POTASSIUM PENTABORATE TETRAHYDRATE IN STATIONARY MEDIUM OF SINGLE CRYSTAL SYSTEM

HALIL DEMIR[a], ÖMER ŞAHİN[a], MUSTAFA KAYA[a]

[a]SIIRT UNIVERSITY

*halildemir72@hotmail.com

Abstract:

Although boron minerals are composed of more than 150 compounds containing boron oxide (B2O3) which contain different proportions of boron in natüre. Boron minerals are found naturally in the form of hydrate compounds with Na, K, Mg and Ca elements. Some of the commercial boron compounds produced by crystallization are not investigated as well as sodium compounds. Potassium 1:5 borates (potassium pentaborate tetrahydrate, KB5O8.4H2O) are obtained by maintaining a molar ratio of B2O3 / K2O of the reaction of boric acid and KOH in aqueous medium at 5. The production equation of potassium pentaborate tetrahydrate can be given as follows.

5H3BO3 + KOH → KB5O8.4H2O + 4H2O

In this study, the linear growth rates of potassium pentaborate tetrahydrate in the stagnant medium of single crystal system were investigated due to temperature and supersaturation. It was determined by experimental studies that a single crystal of potassium pentaborate tetrahydrate was scattered at the linear growth rate. In the presence of Ca impurity, linear growth rates due to different supersaturation were investigated and it was determined that scattering continued at growth rates. As the Ca concentration in the solution medium increased, the contraction of metastable zone of Potassium Pentaborat tetrahydrate was also observed.

Keywords: Potassium Pentaborate Tetrahydrate, Growth Rate, Supersaturation, Single Crystal

This work was supported by TÜBIİTAK with the project number 108M043.

ANTICANCER EFFECTS OF POLYFLUORINATED 3-TERT-BUTYL SALICYLALDIMINES ON PANC-1 CELL LINE

FARUK SUZERGOZ[a], HALIL DEMIR[b], VELI KASIM[a]

[a]HARRAN UNIVERSITY
[b]SIIRT UNIVERSITY

*halildemir72@hotmail.com

Abstract:

Schiff bases, condensation products of primary amines with carbonyl compounds, have received much attention due to the biological properties. Schiff bases have been shown to exhibit a wide range of biological activities especially antitumoral effects on cancer cells. In the study, the cytotoxic, antiproliferative and apoptosis induction effects of fluorinated 3-tert-butyl salicylaldimines on Panc-1, a pancreatic epithelial carcinoma cell line, were investigated. The compounds (1-9) were plated 96-well plates 1 nM-1 µM concentrations at triple order. Cytotoxic effects the compounds were determined by luminometric ATP assay. Cytotoxicity power of the compounds was calculated as IC50 values using optical density values obtained from ATP assay. CFSE method was used to calculate proliferative index (PI) values which represents antiproliferative capacity of the compounds. The apoptosis induction on the cells was determined by immunohistochemically using anti-caspase-3 monoclonal antibodies. Apoptosis development on the cells were examined by histopathological methods (giemza, hematoxylin&eosin and Papanicolaou). The most powerful cytotoxic effect on Panc-1 cells was obtained with Compound 5 (F3,5-3TBS) bearing 2 fluorine atoms (IC50:5.1 µM). The strongest antiproliferative effect on Panc-1 cells was obtained with Compound 8 (F3,4,5-3TBS) carrying 3 flourine atoms (PI: 6.4). Compound 5 were induced cleaved caspase-3 expressions on Panc-1 cells indicate that the compound has ability to generate cytotoxic effect Panc-1 cells by induction of apoptosis. Morphological changes observed in the cells confirm that cytotoxic effect of Compound 5 was due to apoptosis induction. We concluded that Compound 5 has potential anticancer activities on Panc-1, pancreatic epithelial carcinoma, cells.

Keywords: Anticancer, 3-Tert-Butyl Salicyladimines, Pancreatic Cancer, Panc-1.

**This work was supported by TÜBIİTAK with the project number 113Z134*

ICACChE
2nd International Conference on Applications in Chemistry and Chemical Engineering
10 - 14 October 2018 Belgrade

ADSORPTION OF GAS-PHASE BENZENE ONTO FORMALDEHYDE-TREATED WALNUT SHELL: KINETICS, EQUILIBRIUM AND THERMODYNAMICS

SINAN KUTLUAY[a]

[a]SIIRT UNIVERSITY

*kutluays2012@gmail.com

Abstract:

In this paper, the adsorption of gas-phase benzene onto formaldehyde-treated walnut shell was investigated using a laboratory-scale continuous flow fixed-bed reactor system, under atmospheric pressure. According to the knowledge published hitherto, there is no research on adsorption of gas-phase benzene onto formaldehyde-treated walnut shell, in a dynamic system. For this reason, within the context of the main purpose of this research, the effects of process parameters such as nitrogen (N2) flow rate (50-120 mL min-1) as the gas-phase benzene carrier, adsorbent dosage (0.25-1.00 g), concentration of gas-phase benzene at the inlet (10-15 ppm) and the adsorption temperature (293-323 K) on both the adsorption capacity and the adsorption efficiency of gas-phase benzene were studied. For the analysis of adsorption kinetics, pseudo-first-order and pseudo-second-order models were used. Equilibrium isotherm data were analyzed by Langmuir and Freundlich isotherm models. The values of kinetic parameters, equilibrium adsorption capacities, activation energy (Ea), isotherm parameters, correlation coefficient (R2), standard deviation Δq (%) values of adsorption models were calculated and discussed. Thermodynamic parameters such as Gibbs free energy (ΔG°), enthalpy change (ΔH°) and entropy change (ΔS°) were also calculated using van't Hoff equation to characterize the adsorption process of gas-phase benzene. Adsorption capacity of gas-phase benzene onto formaldehyde-treated walnut shell was determined to be 11.69 mg g-1 for 303 K.

Keywords: Benzene Adsorption; Kinetics; Isotherms; Thermodynamics; Walnut Shell

INVESTIGATION OF ADSORPTION KINETICS, EQUILIBRIUM AND THERMODYNAMICS OF TOLUENE VAPOR ONTO FORMALDEHYDE-TREATED WALNUT SHELL

ORHAN BAYTAR[a], ÖMER ŞAHİN[a], SİNAN KUTLUAY[a]

[a]SIIRT UNIVERSITY

*kutluays2012@gmail.com

Abstract:

In this study, the adsorption kinetics, equilibrium and thermodynamics of toluene vapor onto formaldehyde-treated walnut shell was investigated using a laboratory-scale continuous flow fixed-bed reactor system, under atmospheric pressure. According to the knowledge published hitherto, there is no research on adsorption of toluene onto formaldehyde-treated walnut shell, in a dynamic system. For this reason, within the context of the main purpose of this research, the influences of the adsorption conditions such as nitrogen (N2) flow rate (50-120 mL min-1) as the toluene vapor carrier, amount of walnut shell (0.25-1.00 g), concentration of toluene vapor at the inlet (10-15 ppm) and the adsorption temperature (293-323 K) on both the adsorption capacity and the adsorption efficiency of toluene vapor were examined. For the analysis of adsorption kinetics, pseudo-first-order and pseudo-second-order models were used. Adsorption isotherm data were analyzed using the isotherm models of Langmuir and Freundlich. The values of kinetic parameters, equilibrium adsorption capacities, activation energy (Ea), isotherm parameters, correlation coefficient (R2), standard deviation Δq (%) values of adsorption models were calculated and discussed. Thermodynamic parameters such as Gibbs free energy (ΔG°), enthalpy change (ΔH°) and entropy change (ΔS°) were also calculated using van't Hoff equation to characterize the adsorption process of toluene vapor. Adsorption capacity of toluene vapor onto formaldehyde-treated walnut shell was determined to be 16.50 mg g-1 for 303 K.

Keywords: Kinetics; Isotherms; Thermodynamics; Toluene Adsorption; Walnut Shell

AN OPTIMIZATION STUDY FOR PRODUCTION OF PEDOT:PSS BASED CONDUCTIVE POLYMERIC FILMS

DİDEM AYCAN[a], NİHAL DOLAPÇI[a], ÖZGE GÜLÜZAR KARACA[a], NESLİHAN ALEMDAR[a]

[a]MARMARA UNIVERSITY

[*]neslihan.alemdar@marmara.edu.tr

Abstract:

Conductive polymers have the highest possibility to become promising candidates for energy storage, solar cells, supercapacitors and also bio-applications due to provide remarkable difference such as environmental stability, low cost, high capacitance, and high conductivity when compared with metals. In recent years, especially energy storage has been attracting much interest, since conductivity is the key parameter for the materials used in this application area. Poly (3, 4-ethyleendioxythiophene) (PEDOT) is a well-preferred conductive polymer owing to its attractive combination of properties including long-term mechanical and chemical stability coupled with a multiplicity of synthesis options, high transparency and enabling cost-effective mass production.

In this study, the polymeric films were prepared by using different amount of gelatin (Gel), sodium alginate (SA), and hyaluronic acid (HyA) via solvent casting method. Following that, the different amounts of PEDOT:PSS were incorporated into polymeric structure to provide conductivity to polymeric films.

PEDOT:PSS-based conductive polymeric films were characterized by FT-IR analyses. The water uptake capacity of the films was determined via swelling tests gravimetrically. The electrical conductivity of PEDOT:PSS-based conductive films was derived from the sheet resistivity determined by the four-point probe technique.

According to the obtained results, optimum amount of PEDOT:PSS and polymeric content were determined for the best film formulation. Additionally, it was concluded that the obtained polymeric films which were produced based on optimum conditions would be used in energy storage applications for future works.

Keywords: Conductive Polymer, PEDOT:PSS, Energy Storage

THE EFFECT OF PHOTO-INDUCED PHASE TRANSFORMATION ON RGO-CD(1-X)ZNXS PHOTOELECTRODES

DUYGU AKYÜZ[a], ATIF KOCA[a]

[a]MARMARA UNIVERSITY

*duyguakyuz@marun.edu.tr

Abstract:

Increasing global problems such as energy crisis and environmental pollution have accelerated the development and utilization of clean, renewable energy resources. Hydrogen production by solar water splitting via semiconductor photocatalysts is an enhancing technology based on renewable resources[1, 2]. Among the semiconductor, metal chalcogenides (CdS, ZnS) have unique properties such as low band gap, suitable band position for hydrogen production and visible-light response. However, photocorrosion and low solar-to-hydrogen (STH) efficiency limited widely applications of CdS in photocatalytic hydrogen production and photoelectrochemical (PEC) water splitting. Novel nanocomposites (RGO-Cd(1-x)ZnxS) to overcome these limitations were synthesized with loading reduced graphene oxide (RGO) and different co-catalyst (Pt, Ru and Rh) by using solvothermal method. The nanocomposites having cubic phase structure were transformed to hexagonal phase with photo-induced phase transformation (PIPT) with effect of RGO under solar irradiation. This transformation were proved with PEC measurement for the first time. The obtained photoelectrodes were characterized to determine surface structure and morphological properties with various technique such as scanning electron microscope (SEM), transmission electron microscope (TEM) high resolution electron microscope (HRTEM), X-ray diffractometry (XRD), UV-vis diffusion reflectance spectroscopy (DRS), RAMAN spectroscopy and Photoluminescence spectroscopy (PL). Hydrogen production rates, STH efficiency, stability, photocurrent density of photoelectrodes increased with effect of PIPT in PEC system.

Referances

[1] D. Akyüz, A. Koca, Photocatalytic Hydrogen Production with Reduced Graphene Oxide (RGO)-CdZnS Nano-Composites Synthesized by Solvothermal Decomposition of Dimethyl Sulfoxide as the Sulfur Source, Journal of Photochemistry and Photobiology A: Chemistry, (2018).

[2] X. Zong, H. Yan, G. Wu, G. Ma, F. Wen, L. Wang, et al., Enhancement of photocatalytic H2 evolution on CdS by loading MoS2 as cocatalyst under visible light irradiation, Journal of the American Chemical Society, 130(2008) 7176-7.

Keywords: Photo-Induced Phase Transformation, Hydrogen Production, Photoelectrodes, Metal Chalcogenides.

We thank to The Scientific and Technological Research Council of Turkey (TUBITAK, Project Number: 116M567) and Marmara Universit

HYALURONIC ACID BASED SMART HYDROGELS

MÜGE SENNAROĞLU BOSTAN[a], KÜBRA İSEN[a], DUYGU YALÇIN[a], MEHMET SAYİP EROĞLU[a]

[a]MARMARA UNIVERSITY

[*]msennaroglu@marmara.edu.tr

Abstract:

The treatment of inflammatory bowel diseases such as ulcerative colitis, Crohn's disease and colon cancers widely include the admistiration of 5-aminosalicylic acid (5-ASA) although it have some limitations such as gastric irritation, low drug bioavailability and low efficiency. These limitations arises from the fast absorbtion of 5-ASA in stomach and small intestine rather than the colon specific sites. Stimuli responsive hydrogels are smart materials which are sensitive to the changes of environmental conditions. Developing a stimuli responsive and biodegredable smart hydrogel for the controlled release of 5-ASA would overcome these limitations. PNIPA is a widely used temperature responsive synthetic polymer used in controlled drug delivery systems because of having a lower critical solution temperature (LCST) and volume phase transfer temperature (VPTT) close to the body temperature. However PNIPA is not biodegradable and generally crosslinked with bis-acrylamide which is relatively toxic. In this study hyaluronic acid (HA) was methacrylated and used as a biodegradable and bio-compatible crosslinker to prepare HA-PNIPA based temperature sensitive smart hydrogels to overcome these toxicity problems. Methacrylation reaction was characterized using FTIR and 1HNMR spectroscopy. The hydrogels were prepared at four different HA/pNIPA ratios and loaded with 5-ASA. The 5-ASA loading capacity and swelling behavior of the hydrogels in PBS (pH 7.4) were determined at three different temperatures (25, 30, and 40 oC), which are below and over the VPTT of pNIPA. For all the compositions, the maximum drug loading capacity was determined at 25oC and VPTT of hydrogels was sensitively determined using derivative differential scanning calorimetry (DDSC). The 5-ASA release from the hydrogels was monitored using UV-VIS spectrophotometer at 37 °C in PBS (pH 7.4). It is worth nothing that the VPTT of smart hydrogels and thus release rate of loaded drug are tunable by changing the temperature and ratio of HA/ pNIPA.

Keywords: Temperature Responsive Hydrogels, Drug Release, Hyaluronic Acid, Pnipa

A COUNTRY-BASED COMPARISON OF GLOBAL WARMING POTENTIAL OF NATIONAL ELECTRICITY GENERATION

GÜLŞAH YILAN[a], GÖKÇEN ÇİFTÇİOĞLU[a], NEŞET KADIRGAN[a]

[a]MARMARA UNIVERSITY

*gulsah.yilan@marmara.edu.tr

Abstract:

Since the electricity generation activities from fossil fuels are the main contributor to climate change problems, especially for the countries that rely on fossil fuels to supply their electricity demand, impacts associated with the electricity generation activities should be carefully analyzed. As the sustainability concept emerges with the rising environmental awareness, policy-making strategies have changed in a way to consider all related issues like technical, environmental, and socio-economic factors. Among these factors, environmental issues are one of the least studied ones compared to financial and technical aspects. In order to investigate the environmental impacts related with electricity sector in Turkey, a life cycle assessment methodology is applied for the 2014 electricity generation mix. The IPCC 2013 impact assessment method is used for calculating the global warming potential of electricity generation activities. As the computation results indicate, fossil fuel technologies are the main responsible for environmental burdens generated. In a global warming potential basis, country-based comparisons are also conducted with electricity mix of various countries. In this study, environmental impacts for 2014 electricity mix is compared with other studies concerning Turkey and also with different countries as follows: the Czech Republic, China, Portugal, India, US, Thailand, and New Zealand. Selected studies apply the same methodology with this paper in terms of functional unit and impact assessment method. The comparison is conducted with environmental impacts of national electricity mix expressed in kg CO2 equivalents per kWh. The GWP scores for fossil fuel technologies are consistent with Turkey-specific studies available in the literature with respect to their order of magnitude affirming the reliability of the inventory data.

Keywords: Country-Based Comparison, Electricity Generation, Global Warming Potential, Sustainability, Turkey

**This study is financially supported by BAPKO,*

ELECTRICITY SECTOR INVESTMENTS IN TURKEY WITH THE COMPARISON OF ENVIRONMENTAL BURDENS GENERATED

GÜLŞAH YILAN[a], GÖKÇEN ÇİFTÇİOĞLU[a], NEŞET KADIRGAN[a]

[a]MARMARA UNIVERSITY

[*]gulsah.yilan@marmara.edu.tr

Abstract:

Energy generation activities are the main contributor to environmental burdens generated country-wide. In order to suggest environmental-friendly policies for future energy planning studies, a comprehensive analysis is required to depict the actual generation profile. With this aim, an impact assessment analysis of electricity generation activities in Turkey for the year 2014 is conducted via life cycle assessment methodology. The midpoint CML 2001 impact assessment method is used for calculating the environmental burdens of electricity generation. As the computation results indicate, fossil fuel technologies are the main responsible for each category of environmental impacts generated. The results also state that increasing the share of renewable technologies are essential in response to meet the increasing energy demand. However, electricity sector investments do not reflect the best case in terms of environmental issues. According to the investments made in the energy sector since 2014, new investments of the Turkish electricity market still depend on fossil fuel technologies despite its being a country of considerable potential regarding renewable energy sources. The trend of investments does not show a linear change throughout the years not only for the total installed power but also for any type of technologies. The fluctuation in the new investments may result from the socio-eco-political situation of the country, the increase in energy efficiency scores of available technologies, and also the public opinion of related power generation technique. Even the investment trend cannot be received from the short-term statistics, renewable energy shares can be supposed to increase from a broad perspective in order to meet sustainable policy-making goals.

Keywords: Electricity Generation, Energy Investment, Environmental Burdens, Turkey

[*]*This study is financially supported by BAPKO, MARMARA UNIVERSITY.*

METAL CHALCOGENIDES-BASED NOVEL PHOTOCATALYSTS: SYNTHESIS, CHARACTERIZATIONS AND PHOTOCATALYTIC HYDROGEN PRODUCTION APPLICATIONS

ATIF KOCA[a], DUYGU AKYÜZ[a]

[a]MARMARA UNIVERSITY

[*]akoca@marmara.edu.tr

Abstract:

Photocatalytic solar hydrogen production for water splitting has attracted a great deal of attention since the need for renewable energy has increased (1,2). Metal chalcogenides-based photocatalysts as semiconductor has potential to solve both energy and environmental problems. In addition, carbon materials also have shown great efficient to enhance the photocatalytic hydrogen-production performance of semiconductor photocatalysts (2,3). This review presents, to overcome the limitations such as photocorrosion, light absorption, charge carrier generation, charge transport, separation and recombination were studied with carbon materials and metal chalcogenides. Reduced graphene oxide (RGO) included transition metal chalcogenides (TMC), RGO-Cd(1-x)ZnxS nanocomposites, synthesized by using the different synthesis strategies such as sulphurization and solvothermal method. The synthesized photocatalysts were characterized to determine surface structure and morphological properties with various technique such as scanning electron microscope (SEM), transmission electron microscope (TEM) high resolution electron microscope (HRTEM), X-ray diffractometry (XRD), UV-vis diffusion reflectance spectroscopy (DRS), RAMAN spectroscopy and photoluminescence spectroscopy (PL). RGO-Cd(1-x)ZnxS nanocomposites were tested as active photocatalysts in photocatalytic hydrogen production system under solar irradiation. Moreover, the effect on the photocatalytic hydrogen-production efficiency of RGO based TMC photocatalysts are discussed and determined photocatalytic system parameters.

Referances

1. Koca, A., & Şahin, M. (2002) International Journal of Hydrogen Energy, 27(4), 363-367.

2. Akyüz, D., & Koca, A. (2018) Journal of Photochemistry and Photobiology A: Chemistry.

3. W Li, (2017) Rengui. Chinese Journal of Catalysis, 38.1: 5-12.

Keywords: Transition Metal Chalcogenides, Hydrogen Production, Photocatalysts.

[*] *We thank to The Scientific and Technological Research Council of Turkey (TUBITAK, Project Number: 116M567) and Marmara Universit*

THE SYNTHESIS OF SOME NOVEL FLAVONE COMPOUNDS AS ANTICANCER AGENTS

OYA BOZDAĞ DÜNDAR[a], IŞILAY YÜCEİLYAS[a], TUĞBA SUBAŞ[a], FILIZ BAKAR ATEŞ[a]

[a]ANKARA UNIVERSITY

*Oya.Bozdag@pharmacy.ankara.edu.tr

Abstract:

Cancer is a fatal disease characterized by out-of-control cell growth. While many chemotherapeutic strategies for cancer treatment have been proposed, tested and in some cases implemented in the past few decades, these diseases remain tenacious and deadly. Today, there is a need for new drugs that can be effectively used for treatment. Thus, further research in this area is being continued.

Flavonoids consist of a large group of polyphenolic compounds having a benzo-y-pyrone structure and are ubiquitously present in plants (1). They are useful as chemopreventive/chemotherapeutic agents. It is well known how high intake of fresh fruits and vegetables, rich in vitamins A, C, E, B-carotene, flavonoids and other constituents, confers cancer protection against several common human cancer such as: lung, breast, prostate, and colon cancers (2).

Flavones can express anticancer activity through different modes of action: inhibition of cancer promotion (apoptosis, autophagy and cell cycle arrest) (3), blocking of cancer progression (inhibition of angiogenesis and metastasis) as well as prevention of DNA damage (4). Thus, they are considered as important dietary substances with a high capacity of tumor chemoprevention (5).

Within the scope of this study, it was synthesized some new flavone compounds for evaluating their anticancer activities. The chemical structure of synthesized derivatives will be elucidated by Elementary Analysis, IR, NMR and mass spectral data after the pureness control of them done by ITK and melting point analyses. The synthesized compounds have also been investigated for their anticancer activities through inhibition of cell growth.

References

1) M. F. Mahomoodally, A. Gurib-Fakim, A. H. Subratty. Pharm Biol. (2005), 43, 237.
2) N. Pathak, S. Khan, A. Bhargava et al., Nut Cancer (2014), 66, 857.
3) X. Cao, B. Liu, W. Cao, W. Zhang, F. Zhang, H. Zhao, R. Meng, L. Zhang, R. Niu, X. Hao, B. Zhang, Chin. J. Cancer Res. 25 (2013), 212-222.
4) P. Batra, A.K. Sharma, Biotech. 3 (2013), 439-459.
5) P. Kittakoop, Studies in Natural Products Chemistry (2015), 44,251-307.

Keywords: Flavone, Sulfonamide, Anticancer, Cytotoxicity, Synthesis

**This work was supported by the scientific and technological council of Turkey (TUBITAK), Turkey (project no: 217S489).*

STUDIES ON THE SYNTHESIS OF SOME NEW QUINAZOLINYLFLAVONYLSULFONAMIDE COMPOUNDS AS ANTICANCER AGENTS

TUĞBA SUBAŞ[a], IŞILAY YÜCEILYAS[a], FILIZ BAKAR ATEŞ[a], OYA BOZDAĞ DÜNDAR[a]

[a]ANKARA UNIVERSITY

*Tugba.Subas@ankara.edu.tr

Abstract:

Cancer is defined as uncontrolled cell growth and may affect any part of the body. The growing cells often invade surrounding tissue and can metastasize to distant sites [1].

Flavonoids are secondary polyphenolic metabolites which are occured commonly in many fungi and plants [2]. The studies have reported that they can inhibit cell proliferation, induce apoptosis and suppress angiogenesis by interfering with growth factor signalling [3].

Nitrogen-rich heterocycles, particularly quinazolines and quinazolinones, represent a unique class of diversified frameworks displaying a broad spectrum of biological functions [4].

In this study, in view of the anticancer property of quinazoline ring and flavone, a new series of flavonyl quinazolinyl sulfonamide compounds has been synthesized. The structural evaluation of the synthesized compounds is based on the 1H NMR, Mass and elementary analysis data. The synthesized compounds have also been investigated for their anticancer activities through inhibition of cell growth.

References:

[1]. W.A. Denny, G.W. Rewcastle, A.J. Bridges, D.W. Fry, A.J. Kraker, “Structure-activity relationships for 4-anilinoquinazolines as potent inhibitors at the ATP bindings site of the epidermal growth factor receptor in vitro”, Clin. Exp. Pharmacol. Physiol., vol 23, pp. 424-427, 1996.
[2]. D. Raffa, B. Maggio, M.V. Raimondi, F. Plescia, G. Aidone, “Recent discoveries of anticancer flavonoids”, Eur. J. Med. Chem., vol. 142, pp.1-16, 2017.
[3]. G.V. Sherbet. “The Anti-Cancer Potential of Flavonoids”. Molecular Approach to Cancer Management, Chapter 17, pp. 151, 2017.
[4]. I. Khan, S. Zaib, S. Batool, N. Abbas, Z. Ashraf, J. Iqbal, A. Saeed, “Quinazolines and quinazolinones as ubiquitous structural fragments in medicinal chemistry: An update on the development of synthetic methods and pharmacological diversification” Bioorg. Med. Chem., vol,24 pp.2361-2381, 2016.

Keywords: Flavone, Sulfonamide, Quinazoline, Cytotoxicity

**This work was supported by the Scientific and Technological research Council of Turkey (TUBITAK), (project no: 217S489).*

IT STUDIES ON THE SYNTHESIS OF SOME NOVEL QUINOXALINYL FLAVONE COMPOUNDS AS ANTICANCER AGENTS

IŞILAY YÜCEILYAS[a], TUĞBA SUBAŞ[a], FILIZ BAKAR ATEŞ[a], OYA BOZDAĞ DÜNDAR[a]

[a]ANKARA UNIVERSITY

[*]yuceilyas@ankara.edu.tr

Abstract:

The role of dietary flavonoids in cancer prevention is well established and widely discussed. Many mechanisms of action have been identified including cell cycle arrest, induction of apoptosis, inhibition of angiogenesis, antioxidant effect and inhibition of some functional enzymes like cyclin-dependent kinases, tyrosine kinases, aromatases, topoisomerases and glycogen phosphorylases [1,2].

Quinoxaline derivatives are an important class of heterocyclic compounds, in which N replaces one or more carbon atoms of the naphthalene ring [3]. Quinoxaline nucleuses exhibit potential anticancer activity, which makes them an important basis for the anticancer drugs [4].

In this study, a new series of quinoxalinyl flavone compounds has been synthesized for their evaluation of anticancer property through inhibition of cell growth. The structural evaluation of the synthesized compounds was based on the 1H NMR, Mass and elementary analysis data.

References

[1] W.J. Craig, "Health-promoting properties of common herb "Am. J. Clin. Nutr. Vol 70 pp.491-499 (1999).

[2] A.R. Tan, S.M. Swain, "Review of flavopiridol, a cyclin-dependent kinase inhibitor, as breast cancer therapy"Semin. Oncol. Vol 29 pp. 77-85 (2002).

[3] Y. Deepika, P. N., K. Sachin, S. Shewta, "Biological activity of quinoxaline derivatives" Curr. Pharm. Rev. Res. Vol 1(3) pp. 33-46 (2011).

[4] A. Husain, D.Madhesia ,"Recent advances in pharmacological activities of quinoxaline derivatives."

J. Pharm. Res. Vol 4 (3)pp. 924-929 (2011).

Keywords: Flavone, Sulfonamide,Quinoxaline,Cytotoxicity

[*] *This work was supported by the scientific and technological council of Turkey (TUBITAK), Turkey (project no: 217S489).*

INCREASING THE CATALYTIC ACTIVITY FOR THE HIGH YIELDING SYNTHESIS OF ARYL AMINES USING ORGANOZINC REAGENTS

TAHIR DAŞKAPAN[a]

[a]ANKARA UNIVERSITY SCIENCE FACULTY DEPARTMENT OF CHEMISTRY

*daskapan@science.ankara.edu.tr

Abstract:

Organozinc reagents are not reactive toward ketoximes at room temperature; there is need to an efficient catalyst. The use of CuCN as a catalyst allowed obtaining aryl amines in low to moderate yields [1].

In this work, the synthesis of aryl amines in high yields by an easily applicable electrophilic amination method using organozinc reagents was provided by increasing the catalytic activity of copper catalyst by means of a dipolar aprotic solvent (DAS). For this purpose, we used 10 different dipolar aprotic solvents (1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU), hexamethylphosphoramide (HMPA), dimethyl sulfoxide (DMSO), N-methyl-pyrrolidin-2-one (NMP), propylene carbonate (PC), 1,3-dimethyl-2-imidazolidinone (DMEU), N,N-dimethylacetamide (DMAC), tetrahydrothiophene 1,1-dioxide (sulfolane), N,N,N',N'-tetramethylurea (TMU) and N,Ndimethylformamide (DMF)), as dipolar aprotic solvents, in the CuCN catalyzed electrophilic amination reaction of organozinc reagents and determined their effect on increasing the catalyst activity.

All reactions involving organometallic reagents were performed in flame-dried glassware with standard syringe / cannula techniques under an atmosphere of dry, oxygen-free argon. Arylamines as the final products were isolated as their N-benzoyl derivatives and these known compounds were identified from their melting points and 1H NMR spectrums.

Acknowledgements: We would like to thank the Ankara University Research Fund for their financial support (grant no. 06B4240002).

References

1. T. Daşkapan; Arkivoc. 2011, v, 230.

Keywords: Organozincs, Amines, Copper Catalysis, Amination, Ketoximes

This study is supported by Ankara University Research Fund (grant no. 06B4240002).

ELECTROPHILIC AMINATION OF ORGANOZINC REAGENTS WITH SP3-NITROGEN CONTAINING AMINATING REAGENT

TAHIR DAŞKAPAN[a]

[a]ANKARA UNIVERSITY SCIENCE FACULTY DEPARTMENT OF CHEMISTRY

*daskapan@science.ankara.edu.tr

Abstract:

Organozinc compounds are an important class of main-group organometallic reagents. They are suitable reagents for the synthesis of functionalized important organic compounds and for their reactions, since the high covalent character of C-Zn bond [1,2].

For this reason, we decided to focus on the preparation of primary arylamines which are key intermediates in the synthesis of various practically important organic compounds [3] by electrophilic amination of ordinary organozinc reagents with sp3-N containing aminating reagent. The reactivity of organozinc reagents can be increased by using transition metal catalysts. Copper catalysis has been known to promote the reactions of organozinc reagents.

We observed that, CuCN catalyzed the reaction of organozinc reagents with methoxyamine (MeONH2) as sp3-N containing aminating reagent to form primary aryl amines in low to good yields. The use of a suitable co solvent promoted the electrophilic reactions of organozinc species and supplied increase in the yield of amine or lessened the amount of catalyst and reaction time.

This method is an alternative to the methods developed for the synthesis of primary amines [4] because it can be carried out under mild reaction conditions and is easily applicable.

All reactions involving organometallic reagents were performed in flame-dried glassware with standard syringe / cannula techniques under an atmosphere of dry, oxygen-free argon. Arylamines as the final products were isolated as their N-benzoyl derivatives and these known compounds were identified from their melting points and 1H NMR spectrums.

Acknowledgements: We would like to thank the Ankara University Research Fund for their financial support (grant no. 06B4240002).

References

[1] P. Knochel, P. Jones (Eds), Organozinc Reagents: A Practical Approach. Oxford University Press: Oxford, 1999.
[2] Z. Rappoport, I. Marek (Eds), Patai's The Chemistry of Organozinc Compounds,Wiley-VCH: Chichester, 2008.
[3] S. A. Lawrence, Amines: Synthesis, Properties and Applications, Cambridge University Press: Cambridge, 2004.
[4]. T. Daşkapan; Arkivoc. 2011, v, 230.

Keywords: Organozincs, Amines, Copper Catalysis, Amination, Hydroxlamines

---

**This study is supported by Ankara University Research Fund (grant no. 06B4240002).*

SYNTHESIS OF N-SUBSTITUTED PYRROLE COMPOUNDS FROM HYDRAZIDE DERIVATIVES

HAKAN CAN SÖYLEYICI[a]

[a]ADNAN MENDERES UNIVERSITY, BUHARKENT VOCATIONAL SCHOOL,
DEPARTMENT OF ELECTRICITY AND ENERGY

*hcsoyleyici@adu.edu.tr

Abstract:

Pyrrole is a compound which is widely used in organic synthesis and electroactive material applications owing to aromaticity that is possessed within heterocyclic compounds and delocalization which is provided in the attended structure. Synthesis of pyrrole with Paal-Knorr method is an old method however this method is usually applied with aromatic and aliphatic amines.

2,5-di(2-thienyl) substituted pyrrole derivatives are particularly used to obtain of electro-conductive materials. The major advantage of such compounds is that thiophene is relatively much more readily polymerized than pyrrole and the conductivity of the thiophene-pyrrole-thiophene (SNS) chain without interruption in electron delocalization.

The monomer 2,5- di(2-thienyl) pyrroles (SNS) compose of thiophene and pyrrole rings interconnected by their a-positions which allow further improvement of the properties. In literature, 2,5-di-(2-thienyl)-1H-pyrrole (SNS) derivatives have very useful properties for optoelectronic applications and there are lots of SNS derivatives, having substituted alkyl derivatives, phenyl derivatives and, ferrocene, pyrene, bipyrrole. However, except our group's studies, there is no study related to hydrazide substituted SNS derivatives in the literature. The recent studies have shown that using hydrazide instead of amine is not only increase product yield but also improve optical and electrical properties of the corresponding polymer

In the present study, N-amide substituted pyrrole compounds (SNS) were synthesized with aromatic hydrazides instead of amines. The structures of these new derivatives were characterized using nuclear magnetic resonance (NMR) spectroscopy.

Keywords: Paal-Knorr, Pyrrole, Nmr

**TUBITAK P.N. 115Z665, ADU BAP-17001*

DEVELOPMENT OF CATHODE SURFACES FOR FUEL CELL APPLICATIONS USING CARBON BASED COMPOSITES; ELECTROCHEMICAL REDUCTION OF OXYGEN

ÇAĞRI CEYLAN KOÇAK[a]

[a]DOKUZ EYLÜL UNIVERSITY

[*]ceylan.kocak@deu.edu.tr

Abstract:

The cathodic oxygen reduction reaction (ORR) is the greatest performance restrictor of fuel-cell applications. Improving catalysts would thus significantly important effect on the efficiency of the fuel cell, and in this regard the preparation of cathode catalysts has been the focus of substantial research over the past few decades. Nano-sized materials with various carbon based supports were promising alternatives for this purpose [1-3]. Metal nanoparticles modified electrodes have been extensively used in electrochemical studies due to their higher catalytic activity, electron transfer rate, and increased electrode surface area compared to the common regular electrodes. Combination of metallic nanoparticles with carbon based materials has attracted great interest in many applications especially in ORR due to their synergistic catalytic effect[4].

In this study, various carbon based materials investigated as cathode material for oxygen reduction reaction in alkaline medium. Carbon based composite materials modified on glassy carbon surfaces with simple technique and followed by deposition of various metal nanoparticles (Au, Pt, Cu etc. or their bimetallic forms) on this modified GCE. In order to improve the activity of catalytic surface some parameters were optimized such as; concentration of supporting electrolyte, carbon based composite material ratio, metal nanoparticles type, concentration, and cycle number. The electrocatalytic activity of the composite electrodes are studied with respect to oxygen reduction using both static and rotating-disk electrodes in an alkaline solution The obtaining results were compared with other modified electrodes. All composite electrodes are characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray photoelectron spectroscopy (XPS), X-Ray Diffraction (XRD) and electrochemical impedance spectroscopy (EIS).

References

[1] Koçak C.Ç., Dursun Z., Turkish Journal of Chemistry., 2018, 42, 623 – 638.
[2] Yavuz E., Özdokur K.V., Çakar I., Koçak S., Ertaş F.N., 2015, Electrochimica Acta 151, 72–80.
[3] Aoun S.B. Dursun Z., Sotomura T, Taniguchi I, Electrochemistry Communications, 2004, 6-8, 747-752.
[4] Koçak C.Ç., Şahin N., Polat R., Dursun Z., Journal of Electroanalytical Chemistry, 2011, 662, 275–280.

Keywords: Fuel Cell, Oxygen Reduction, Carbon Based Materials, Metal Nanoparticles

ELECTROCHEMICAL OXIDATION OF HYDRAZINE AT THE METAL NANOPARTICLES AND POLYMER FILM MODIFIED ELECTRODES

SÜLEYMAN KOÇAK[a], MÜGE HATİP[a]

[a]MANISA CELAL BAYAR UNIVERSITY

*dr.suleymankocak@gmail.com

Abstract:

Electrocatalysis, which is a special area of electrochemistry, has made an important contribution to the development of analysis techniques. Electrocatalysts are used in fuel cells. A fuel cell (FC) is an electrochemical device that enables the conversion of the chemical energy of fuels directly into electrical energy as long as fuel is supplied. A fuel cell exploits the oxidation of fuel in the anode and oxygen reduction in the cathode. The fuel cell system provides high conversion efficiency and extremely low emissions [1-3].

Hydrazine is also an ideal fuel for a direct fuel cell system with high hydrogen content (12.5 wt%). Hydrazine decomposition products (nitrogen and water) are environmentally friendly. There are several reported techniques for the determination of hydrazine. Among these methods, electrochemical techniques offer an opportunity for a portable, rapid, sensitive and economical methodologies. However, the oxidation of hydrazine in carbon electrodes has slow kinetic and high voltage. By modifying the electrodes, the electron transfer rate of hydrazine can be increased and the excess potential can be reduced. Metal nanoparticle modified electrodes on polymer surfaces are densely the subject of the researches. Both physical and chemical characteristics of the substance is changed in nanometer sized dimensions and resulted in an increase in active surface area of material [1-4].

In this study, different conductive polymers were studied on the CNT/GC electrode surfaces and the electrochemical behavior of hydrazine were investigated. These surfaces were modified with metal (Au, Pt, etc.) nanoparticles. The concentration and cycle number of of monomer and metals, pH of solution was optimized. Modified electrodes were characterized by SEM-EDX, XPS, XRD techniques.

Reference

[1] Koçak S., Aslışen B., Koçak Ç.C., Analytical Letters, 2016, 49, 990-1003.
[2] Koçak, S., Aslışen B., Sensors and Actuators B: Chemical, 2014, 196 , 610-618.
[3] Koçak C.Ç., Altın A., Aslışen B., Koçak S., Int. J. Electrochem. Sci., 2016,11, 233 – 249.
[4] Koçak S., Altın A., Koçak C.Ç., Analytical Letters, 2016, 49, 1015-1031.

Keywords: Fuel Cell, Hydrazine, Conductive Polymers, Cnt

OPTIMIZATION OF ELECTROCHEMICAL PROCESSES FOR THE TREATMENT OF RAW WOOLEN YARN DYE WASTEWATER

KUBRA ULUCAN-ALTUNTAS[a], FATIH ILHAN[a], CAN DOGAN[a], UGUR KURT[a]

[a]YILDIZ TECHNICAL UNIVERSITY

*kulucan@yildiz.edu.tr

Abstract:

The textile industry is an important source of pollution due to its intensive water consumption and the toxic content of dye, and this wastewater deteriore the quality of water when they received to surface waters. In this study, electrochemical treatment methods, which are less costly than many treatment methods, has been investigated for raw woolen yarn dye wastewater. Four iron electrodes connected parallely for electrocoagulation process. As opmitization method, response surface methodology was applied by having current density (20 -100 A/m2), reaction time (5-25 minutes) and initial pH (pH 4-pH 8) as independed conditions. The highest Colour and COD removal were obtained as 95% and 40.5%, respectively. High colour removal rate can be achieved in as little as 15 minutes. Electrocoagulation can reduce the time required for colour treatment. In order to obtain these results, it is necessary to apply a current density of 65A/m2 to the wastewater which has been set to an initial pH of 5 and 15 minutes. Although the color removal is high, COD removal does not meet discharge standards. In order to enchance COD removal rate, electrofenton process was also applied. Electrofenton process increased COD removal rate to 77%, where the colour removal rate stayed the same as 96,5%.

Keywords: Electrocoagulation, Electrofenton, Paralel Electrodes, Iron Electrodes, COD, Colour

RECENT ADVANCES IN METAL DOPED GRAPHENE NANOPARTICLES

KUBRA ULUCAN-ALTUNTAS[a]

[a]YILDIZ TECHNICAL UNIVERSITY

*kulucan@yildiz.edu.tr

Abstract:

Graphene has unique properties due to its two-dimensional nanostructure properties. It is an important material that draws attention recently because it has an excellent mobility of charge carriers, superior chemical stability, and high specific surface area. Graphene oxide, a derivative of graphene, has many oxygen functional groups on the surface and has similar advantages of graphene. Graphene and graphene oxide are nanomaterials used in many different industries and in particular for the adsorption of pollutants due to its many advantages such as high pore volume and surface area. Over the past decade, researchers have been developing a variety of materials such as graphene oxide based composites, graphene oxide carbon nanotubes, and metallic nanoparticle production. Metal doped graphene nanoparticles as photocatalysts have begun to attract attention as novel materials for water treatment and environmental remediation applications. These graphene based composites are doped with various metals, making them more effective in many areas. These nanoparticles synthesized by doping of various metals can be produced with low cost, and researchers gain great attention in applying as photocatalysts in the removal of pollutants. This review summarizes the recent advances in pollutant removal of graphene based nanoparticles, which have recently been investigated as an innovative nanomaterial.

Keywords: Graphene, Graphene Oxide, Photocatalyst, Nanoparticles

DETERMINATION OF VEMURAFENIB IN URINE SAMPLES BY UPLC METHOD

AYŞE ÖZDEMIR[a], SENEM ŞANLI[a], SÜLEYMAN GÖKÇE[a]

[a]UŞAK UNIVERSITY

*ayse.ozdemir@usak.edu.tr

Abstract:

Vemurafenib is the first selective, potent and orally bioavailable inhibitor of the serine/threonine-protein kinase B-Raf protein encoded by the V600E mutated BRAF(T1796A; amino acid change in the BRAF protein = Val599→Glu599) gene [1]. Vemurafenib is chemically propane- 1-sulfonic acid {3-[5-(4-chlorophenyl)-1H-pyrrolo [2,3-b] pyridine-3-carbonyl] -2,4difluoro-phenyl}-amide with empirical formula is $C23H18CLF2N3O3$.

In this work, simple, rapid, economical, sufficiently precise and accurate, reproducible, and fully validated UPLC (Ultra Performance Liquid Chromatography). method with good detection limits for estimation of vemurafenib in urine samples has been developed.

For calibration graph, efavirenz was used as an internal standard. For vemurafenib and efavirenz, selectivity factors was found as 1.204. The asymmetry and capacity factors were obtained as 1.100 and 7.532 for vemurafenib.

Both two compounds were well separated in a total duration of 1.50 min, with good peak resolutions, sharpness and symmetry.

In order to check the applicability of the method to biological materials, the recovery studies performed for drug quantitation in human urine were done by means of the calibration graph method, achieving for each analysis the specified percent recoveries. Blank urine samples were spiked with studied drug. After five repeated experiments, the mean percentage recovery for urine sample was 97.924, with RSD% values of 0.5583.

Keywords: Vemurafenib, UPLC, Method Validation

**Scientific Research Projects Unit (BAP-2016/MF004) of Usak University.*

STUDY OF FORCED DEGRADATION BEHAVIOR OF THE MUTATED BRAF INHIBITOR VEMURAFENIB BY LC-MS

AYŞE ÖZDEMIR[a], SENEM ŞANLI[a]

[a]UŞAK UNIVERSITY

*ayse.ozdemir@usak.edu.tr

Abstract:

Introduction: In the present study, comprehensive stress testing of mutated BRAF inhibitor Vemurafenib was carried out according to ICH guideline Q1A(R2).

Materials and Methods: Each sample was prepared in triplicate. Degradation studies were attempt to stress condition of acid (0,1 M HCl), alkaline (0,1 M NaOH) hydrolytic conditions, UV light, oxidation and heat in oven (75 0C) [1].

Results: For acidic, alkaline, and oxidative degradation, solutions were prepared by dissolving raw material of Vemurafenib in DMSO. From this solution, aliquot amounts were diluted with HCl, NaOH and 3%-30% H2O2 to achieve a concentration of 10 µg mL−1 for each solution. In addition, samples of drug substance in the solid state were irradiated with UV radiation at 254 nm for 6 h and 24 h for photolytic stress condition. The products formed under different stress conditions were investigated by LC–MS.

Conclusions: The drug was found to be highly stable to acidic degradation as compared to that of hydrochloric acid. Vemurafenib was almost degradeted by NaOH. In 3% hydrogen peroxide at 100 °C the drug was found to be stable to degradation as negligible degradation was seen after exposing drug to 30% hydrogen peroxide. The drug was found to be stable against photochemical and thermal degradation. Based on the results, a more complete degradation pathway for the drug could be proposed.

Keywords: Vemurafenib, UPLC, Method Validation

Scientific Research Projects Unit (BAP-2016/MF004) of Usak University.

CU (I) HALIDE CATALYZED ELECTROPHILIC AMINATION OF DIARYLCADMIUM REAGENTS WITH ACETONE O-(4-METHOXYPHENYLSULFONYL)OXIME

ZIKRULLAH AHMET BARIT[a]

[a]ANKARA UNIVERSITY

*zikrullahahmet88@gmail.com

Abstract:

Electrophilic amination of an easily available organometallic reagent is a useful method for the preparation of aryl amines which are used for the synthesis of biologically active molecules and preparation of other useful materials. For this reason, electrophilic amination is an active research area and many papers related to amination of organomagnesium,-zinc and -copper reagents appeared in the literature [1].

According to our literature research, to date the only work on the electrophilic amination of organocadmium reagents in the literature was published by our group. We observed that, diarylcadmium reagents do not react with ketoximes under catalyst free conditions. They can react only in the presence of CuCN as copper (I) catalyst and give the corresponding functional group bearing aryl amines in good to high yields [2].

As a continuation of this work, we have presented here the results of the reaction of diarylcadmium reagents with a different ketoxim in the presence of copper (I) halides catalysis instead of CuCN at room temperature.

We observed that, in the electrophilic amination reaction of diarylcadmium reagents with ketoximes the catalytic activity of copper (I) halides is higher than that of CuCN and they allowed the synthesis of functionalized aryl amines in higher yields compared to CuCN at room temperature.

All reactions involving organocadmium reagents were performed in flame-dried glassware with standard syringe / cannula techniques under an atmosphere of dry, oxygen-free argon. Arylamines as the final products were isolated as their N-benzoyl derivatives and these known compounds were identified from their melting points and 1H NMR spectrums.

Acknowledgements: We would like to thank the Ankara University Research Fund for their financial support (grant no. 18L0430003).

References

[1]. T. Daşkapan; Arkivoc. 2011, v, 230.
[2]. Daşkapan, T., Korkmaz, A. Synth. Commun. 2016, 46(9), 813-817.

Keywords: Organocadmiums, Amines, Copper Catalysis, Amination, Ketoximes

CU (II) CATALYZED ELECTROPHILIC AMINATION OF DIARYLCADMIUM REAGENTS WITH ACETONE O-(4-METHOXYPHENYLSULFONYL)OXIME

ZIKRULLAH AHMET BARIT[a]

[a]ANKARA UNIVERSITY

*zikrullahahmet88@gmail.com

Abstract:

Because of high covalent character of C-Cd bond, organocadmium reagents show low reactivity toward many functional groups. For this reason, they are suitable reagents for the reactions which aim to synthesis of functional group-bearing useful organic compounds.

Our works showed that, the reactivity of organo cadmium reagents is too low to react with ketoximes which are sp2-Nitrogen containing aminating reagents. On the other hand, we observed that, Cu (I) catalysis helped organocadmium to react with ketoximes to give corresponding primary aryl amines in good to high yields [1].

In this work, we investigated the catalytic activity of a Cu (II) salt, Cu(SCN)2, in the electrophilic amination reaction of diarylcadmium reagents with acetone O-(4-methoxyphenylsulfonyl)oxime. Amination reaction took place at room temparature under mild reaction conditions and gave corresponding primary arylamines in good yields. These results show that, Cu(SCN)2 can be an alternative catalyst for the amination of diarylcadmium reagents with ketoximes.

All reactions involving organocadmium reagents were performed in flame-dried glassware with standard syringe / cannula techniques under an atmosphere of dry, oxygen-free argon. Arylamines as the final products were isolated as their N-benzoyl derivatives and these known compounds were identified from their melting points and 1H NMR spectrums.

Acknowledgements: We would like to thank the Ankara University Research Fund for their financial support (grant no. 18L0430003).

References

[1]. Daşkapan, T., Korkmaz, A. Synth. Commun. 2016, 46(9), 813-817.

Keywords: Organocadmiums, Amines, Copper Catalysis, Amination, Ketoximes

This study is supported by Ankara University Research Fund (grant no. 18L0430003).

THERMALLY REDUCED GRAPHENE OXIDE: SYNTHESIS AND CHARACTERIZATION

OSMAN EKSIK[a]

[a]ISTANBUL TECHNICAL UNIVERSITY

[*]eksikos@itu.edu.tr

Abstract:

Graphene is a single layer of graphite sheet; one atom thick sp2-bonded carbon atoms organized on a plane. It has extremely interesting electrical properties, which offers various applications in a number of nanometer scale devices.

In this study, we focused on production of few layer reduced graphene oxide. We investigated the production, characterization methods of graphene oxide (GO) and reduced graphene oxide (RGO). Primarily graphite was transformed into graphene oxide structure by using Hofmann methods which are suitable for large-scale production of graphene oxide. Obtained graphene oxide samples reduced by thermal method. GO and RGO were characterized by FT-IR, SEM, XRD, XPS, BET and Raman spectroscopy. FT-IR spectroscopy showed characteristic peaks belonging to the functional groups of GO (OH, C=O, C-OH). XRD analysis of the GO structure, it was observed that the GO interlayer spacing d-distance increased from 0.36 nm to 0.83 nm. From theese results, it is understood that GO is synthesized successfully. The XPS elemental analysis shows that GO with oxidation level C:O ratios is approximately 1.47. Reduced graphene oxide with C:O ratios up to 8,15. SEM images of thermally reduced graphene shows that transparent wrinkled RGO structures were obtained. RGO samples raman spectroscopy revealed that new sp2 structures were formed and the amount of regular structure increased. The BET surface area of RGO is about 600 m2 g−1 and the material consists of small mesopores (2–50 nm).

Keywords: Graphene, Synthesis Of Graphene Oxide, Hofmann Method

[*]*This study is supported by Scientific Activities Support Program of Istanbul Technical University*

THE EFFECT OF SOLUTION DIELECTRIC ON THE CAPACITANCE OF POLY(EDOT) COATED CARBON FIBER

HACER DOLAŞ[a], A. SEZAI SARAÇ[b]

[a]HARRAN UNIVERSITY
[b]ISTANBUL TECHNICAL UNIVERSITY

[*]hacerdolas@hotmail.com

Abstract:

Since the pioneering work two decades ago, conducting polymers have become an increasingly expanding research field and have marked a milestone towards the upcoming era of plastic electronics. Among others, poly-3,4-ethylene dioxythiophene (PEDOT) [1] is a very promising candidate for electrochromic applications. This originates from the fact that it shows good electrochemical stability, a small electronic bandgap, and significant differences in spectral absorption for the reduced and the oxidized states [1, 2]

Electropolymerization is the method of choice as the polymer growth process can be conveniently controlled by the electric charge or the electrochemical potential and an adherent film is obtained on the electrode surface.

Electrochemical impedance spectroscopy is an effective approach to quantify the electron-transfer resistance (Ret) of the electrochemical reactions produced at metal-electrolyte interfaces [3].

In this study, it was investigated how the used solution in electropolymerization changed the capacitance of poly(ethylenedioxythiophene), PEDOT, coated carbon fiber, because of that it was thought that solution composition affected the electrochemical reactions produced at metal-electrolyte interface. For this reason 2.5mM EDOT was electropolymerized in solutions with different dielectric constant. The solutions were obtained by mixing of the different ratio of Acetonitrile (ACN)-Water (H2O)When the obtained data were evaluated it was seen that the dielectric constant of used solution changed the capacitance values. The highest values were obtained at 70.

References:

1. G. Heywang, F. Jonas, Poly(alkylenedioxythiophene)s—new, very stable conducting polymersAdv. Mater., 4 (1992), p. 116
2. L. Groenendaal, F. Jonas, D. Freitag, H. Pielartzik, J.R. Reynolds, Poly(3,4-ethylenedioxythiophene) and Its Derivatives: Past, Present, and Future, Adv. Mater., 12 (2000), p. 481
3. Bard AJ, Faulkner LR. Electrochemical Methods: Fundamental and Applications, Wiley, Newyork, USA:1980

Keywords: PEDOT, Electrochemical Polymerization, Impedance. Capacitance, Dielectric Constant

IODOBENZENE DIACETATE (IBD) CATALYZED 2-ARYLBENZOXAZOLES: SYNTHESIS AND CHARACTERIZATION

NECLA BEKTAŞ[a], DEMET GÜRBÜZ[a]

[a]ISTANBUL TECHNICAL UNIVERSITY

*bektasn@itu.edu.tr

Abstract:

ESIPT (Excited State Intramolecular Proton Transfer) which gives dual fluorescence emission for single photo excitation makes hydroxy substituted benzoxazoles important. Because keto–enol tautomerism is formed by the proton tranfer and resulting emissions strike as fluorescence. Due to the their fluorescent nature, metal complexes of benzoxazoles can be used as sensor for the metal detection [1].

In addition to their fluorescent nature, benzoxazoles are important for some biological processes. For example, antioxidant benzoxazole molecules may prevent the formation of cancer, diabetes and aging by stopping the oxidative chain reaction or minimizing the formation of free radicals and they also form treatment methods for these diseases [2-5].

In this study, some 2-(5-bromobenzo[d]oxaxol-2-yl)phenol derivatives were synthesized by a two-step reaction. In the first step, a condensation reaction occured between 2-amino-4-bromophenol and the corresponding 2-hydroxybenzaldehyde derivative in ethanol to produce schiff base. In the second step iodobenzene diacetate (IBD) were chosen as oxidative reagent in the intramolecular cyclization to generate benzoxazole ring skeletons. All schiff bases and benzoxazole compounds characterized by FT-IR, UV-Visible and 1H-NMR spectroscopic techniques. According to the results, all the synthesized benzoxazole derivatives exhibited a high fluorescent property.

References:

[1]. Patil, V., Padalkar, V., Sekarn, N., 2015, Environment-sensitive benzoxazole based fluorescein derivatives: Synthesis and application to the design of ON–OFF fluorescent chemosensors for microenvironment, Journal of Luminescence, 158 (2015) 243–251.

[2]. Abdelgawad, M.A., Lamie, P., Ahmed, O.M., 2016, Synthesis of New Quinolone Derivatives Linked to Benzothiazole or Benzoxazole Moieties as Anticancer and Anti-Oxidant Agents, Medicinal chemistry, Volume 6(10): 652-657.

[3]. Parveen, S., Al-Alshaikh, M., Panicker, C.Y., El-Emam, A., Arisoy, M., Arpaci, O., Alsenoy, C.V., 2016, Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial and antimicrobial studies of 5-ethylsulphonyl-2-(p-aminophenyl)benzoxazole, Journal of Molecular Structure, 1115, 94-104.

[5]. Gomathi, A., Vijayan, P., Viswanathamurthi P., Suresh, S., Nandhakumar, R., Hashimoto T., 2017, Organoruthenium(II) compounds with pyridyl benzoxazole/benzthiazole moiety: studies on DNA/protein binding and enzyme mimetic activities, Journal of Coordination Chemistry, Vol . 10, 1645–1666.

Keywords: Benzoxazole, Schiff Base, Fluorescence

OPTIMIZATION OF THE ENZYMATIC SYNTHESIS OF GOLD NANOPARTICLES

LELA PINTARIĆ[a], ANA VRSALOVIĆ PRESEČKI[a], IVA REZIĆ[a]

[a]UNIVERSITY OF ZAGREB, FACULTY OF TEXTILE TECHNOLOGY

*lelapintaric@gmail.com

Abstract:

Use of metal and metal oxide nanoparticles (NPs) such as gold, silver, zinc and iron oxide, in various fields of research, including textile, pharmaceutical, packaging and food industry, is increasing daily. Application of those NPs can result in new or in improvements of existing functional properties of products such as their antimicrobial activity and hydrophobicity. Therefore, it is of high importance to develop ecologically, energetically and economically acceptable methods of NPs synthesis that doesn’t include the use of toxic chemicals. One of them is an enzymatic synthesis in which enzymes, as completely biodegradable proteins, are employed as catalysts and reducing agents.

Gold nanoparticles (Au-NPs) are commonly used as therapeutic, antibiotic, antifungal and antimicrobial agents when added to coatings, nanofibers and textiles. In this research, Au-NPs synthesis by using enzyme urease was optimized by using the Design of Experiments (DoE) method. Reaction kinetics and mechanism was measured spectrophotometrically. Synthesized Au-NPs were characterized by Nanoparticle Tracking Analysis (NTA) method and scanning electron microscope with energy dispersive spectroscopy (SEM-EDS).

According to the obtained DoE model, Au-NPs of smaller size will be produced when synthesis reaction is conducted with higher initial metal salt concentration, temperature and stirring rate, as well as with lower concentration of potassium carbonate which stabilizes the pH of the reaction. The results showed that Au-NPs with size in range of 120 and 260 nm were successfully synthesized using an eco-friendly enzymatic method. Therefore, in the following research, this reaction will be up-scaled and synthesized Au-NPs will be used to modify polymer materials foreseen as antimicrobial medical textiles.

Keywords: Nanoparticles, Gold, Enzyme, Optimization

ORGANIC SYNTHESIS IN GLYCEROL-BASED SOLVENTS

ADI WOLFSON[a], DORITH TAVOR[a]

[a]SAMI SHAMOON COLLEGE OF ENGINEERING

*adiw@sce.ac.il

Abstract:

In the past two decades a variety of green solvents have been proposed. However, their implementation in industrial processes is still limited due to their tedious and non-sustainable synthesis, lack of experimental data and familiarity, operational restrictions and high cost.

Recently, we presented the use of glycerol-based solvents as alternative sustainable reaction mediums in both catalytic and non-catalytic organic synthesis. Glycerol is the main by-product from the conversion of oils and fats in oleochemical production. Moreover, in the past decade, its price has substantially decreased due to an increase in supply from the production and use of fatty acid derivatives in the food, cosmetics, and drugs industries and in biodiesle synthesis. The renewable origin, beneficial physicochemical properties and reusability of glycerol-based solvents, enabled improved product yield and selectivity as well as easy product separation and catalyst recycling. Furthermore, their high boiling point and polarity make them perfect candidates for non-conventional heating and mixing techniques such as ultrasound- and microwave-assisted reactions. Finally, in some reactions, such as catalytic transfer-hydrogenation or transesterification, they can also be used simultaneously as both solvent and reactant.

In our ongoing efforts to design a viable protocol that will facilitate the acceptance of glycerol-based solvents as sustainable solvents, pure glycerol and triacetin as well as various glycerol-triacetin mixtures were tested as sustainable solvents in several representative organic reactions, such as nucleophilic substitution of benzyl chloride to benzyl acetate, Suzuki-Miyaura cross-coupling of iodobenzene and phenylboronic acid, baker’s yeast reduction of ketones, and transfer hydrogenation of olefins. It was found that reaction performance was affected by the glycerol/triacetin ratio, as the solubility of the substrates in the solvent determined product yield. Thereby, employing optimal glycerol/triacetin ratio resulted in maximum product yield. In addition, using glycerol-based solvents enabled easy and successful separation of the products and recycling of the catalysts.

Keywords: Green Chemistry, Catalsyis, Solvents, Glycerol

TOXICITY AND ANTIBACTERIAL ACTIVITY OF CIPROFLOXACINE IN CONVENTIONALLY TREATED URBAN WASTEWATER BEFORE AND AFTER OXIDATIVE TREATMENT

BOUDRICHE LILYA[a], IRENE MICHAEL-KORDATOU[b], STELLA MICHAEL[b], POPI KARAOLIA[b], AMEL BOUDJEMAA[a], DESPO FATTA-KASSINOS[b]

[a]CRAPC RESEARCH CENTER
[b]UNIVERSITY OF CYPRUS

[*]boudriche.lilya@gmail.com

Abstract:

Antibiotics are among the pharmaceuticals most commonly detected in the aquatic environment, their presence and accumulation in wastewater, even at low concentrations, may contribute at long-term to the development of multi-resistant bacterial strains potentially causing serious problems of public health and imbalance of microbial ecosystems. The limitation of conventional treatment processes to remove such microcontaminants motivated the development of more powerful processes for the treatment of urban wastewater like the advanced chemical oxidation processes (AOPs).

This study aimed at evaluating the degradation of the antibiotic ciprofloxacin (CIP) in urban wastewater effluents, using uv-c-driven oxidation processes with H2O2 as oxidant. Various concentrations of H2O2 were examined for the process optimization. The complete degradation of CIP was achieved within 15 min of treatment under the optimum concentration of H2O2 which it was found to be 10 mg L-1. The phytotoxicity and ecotoxicity of the treated samples was investigated against one plant species and a crustacean, respectively. At the end of the process the phytotoxic effect was eliminated. In addition, this study demonstrated the ability of the UV-C process to reduce the toxicity towards D. magna since the immobilization of the organisms was significantly reduced comparatively to the untreated wastewater. The antibacterial activity of the treated samples was investigated and a total inactivation of CIP-resistant Escherichia coli within 2 min of treatment was recorded.

Keywords: Antibiotics, Ciprofloxacin, UV-C/H2O2, Toxicity, Antibiotic Resistance

ICACChE
2nd International Conference on Applications in Chemistry and Chemical Engineering
10 - 14 October 2018 Belgrade

INFLUENCE OF PH AND RADICALS IONS ON THE REMOVAL OF SULFAQUINOXALINE FROM AQUEOUS MEDIA USING UV/NA2S2O8

BOUDRICHE LILYA[a], ZAHRA SAFAEI[b], DEEPIKA RAMASAMY[b], MIKA SILLANPÄÄ[b], AMEL BOUDJEMAA[a]

[a]CRAPC RESEARCH CENTER
[b]LAPPEENRANTA UNIVERSITY OF TECHNOLOGY

*boudriche.lilya@gmail.com

Abstract:

Sulfonamides are a group of antibiotic drugs widely used in veterinary medicine. After animal medication, they are excreted in high percentages of the administered amount, either as active substance or as acetyl conjugate. In manure, these sulfonamides are persistent, inducing environmental contamination.

Radical-based advanced oxidation processes (AOPs) have gained much attention for antibiotics degradation. In the recent years, a great scientific interest is being placed on the sulfate radical based-advanced oxidation processes due to their high efficiency in degrading a wide range of recalcitrant microcontaminants in aqueous matrices, including pharmaceuticals.

The present work evaluates the feasibility of UV-C driven advanced oxidation process induced by sulfate radicals in degrading sulfaquinoxaline (SQ-Na) sodium in water.

The results show that sulfaquinoxaline was decomposed at 90% within 5 hours of irradiation under the optimum concentration of sulfates anions. The SQ-Na decay exhibited a pseudo-first-order kinetics when the initial sulfate radical anion concentration varied from 0 to 240 mg/L.

The decomposition of sulfaquinoxaline via UV/sodium persulfate process was strongly favorable under acidic conditions but was slowed down at inherent pH (6.8) and almost inhibited under alkaline conditions (pH 9).

The contribution of SO.-4 alone, andboth radicals HO., SO.-4 on SQ-Na degradation was found to be 69% and 81%, respectively.

UV/sodium persulfate was more efficient than UV/H2O2, meaning that sulfate radical anion generation has made UV/persultafe a kinetically effective process in removing sulfaquinoxaline from water.

Keywords: Sulfaquinoxaline Sodium, UV-C, Degradation, Ph Effect, Ions Efficiency

GRAPE MARC ACTIVATED CARBON IMPREGNATION BY ANATASE-TIO2 NANO-PARTICLES: DEGRADATION OF RB5 AZO DYE WITH INSTANTANEOUS REGENERATION OF PHOTOCATALYST HYBRID

BELAYACHI HANANE[a], BELAYACHI AMEL[a], BOURAHLA SARRA[a], NEMCHI FADELA[a], BELHAKEM MOSTEFA[a]

[a]UNIVERSITY OF MOSTAGANEM-ALGERIA

[*]belayachi.hanane@hotmail.fr

Abstract:

Adsorption onto activated carbon (AC) and oxidation using photocatalyst are widely used technics to remove dyes from waste water. The aim of this work is to increase the removal capacity of activated carbon by combining AC and titanium dioxide ($TiO2$) in a Photocatalytically Regenerative Activated Carbon.

Anatase titania were deposited on powder activated carbon made from grape seeds (AGS) by impregnation/mixing method and then the composite photocatalyst was employed for the removal of reactive black 5 from aqueous solution. The TiO2/AGS was characterized by BET, MEB, XRD and optical absorption spectroscopy. The BET surface area and the pore structure of composite photocatalyst (TiO2/AGS) and activated grape seeds (AGS) were evaluated from nitrogen adsorption data at 77 K in relation to process conditions. Our results indicate that the photocatalytic activity of TiO2/AGS was much higher than single phase titania. The adsorption equilibrium of reactive black 5 from aqueous solutions on the examined materials was investigated. Langmuir, Freundlich, and Redlich– Petersen models are in good agreement with the experimental equilibrium data. The degradation kinetics fitted well to the Langmuir-Hinselwood pseudo first order rate low. The photo catalytic activity of TiO2/AGS was much higher than virgin TiO2. COD removal was measured at regular intervals to quantify the mineralization of the dye. Above 96% mineralization was observed. These results suggest that UV-irradiated TiO2 immobilized on activated carbon may be considered as an adequate process for the treatment of diluted colored textile waste water.

Keywords: Photocatalytic, Activated Carbon, Composite.

ENHANCED CATALYTIC ACTIVITY OF ZSM-12 FOR THE BENZYLATION OF BENZENE WITH BENZYL ALCOHOL

SEMA AKYALCIN[a]

[a]ANADOLU UNIVERSITY

*sdogruel@anadolu.edu.tr

Abstract:

Zeolites are used as heterogeneous catalysts in benzylation reactions. Although they have strong acidity, large surface area, and regular porous structure with good stability, they can show low catalytic activity caused by their microporous networks. In order to overcome the diffusion limitation, mesoporous zeolites can be prepared by desilication.

In this study, a series of mesoporous ZSM-12 zeolites were prepared by desilication at different operation conditions (NaOH solutions: 0.2-0.6 M; temperatures: 35-85°C; operating time: 15- 60 min) from the conventionally synthesized ZSM-12 zeolite. The parent and desilicated ZSM-12 samples were characterized by XRD, ICP-OES, N2 adsorption-desorption, and NH3-TPD. The catalytic performances of ZSM-12 and desilicated samples were evaluated for the benzylation of benzene (B) with benzyl alcohol (BA) under the same reaction conditions of 353 K, B/BA molar ratio of 56/1 and in the presence of 91 mg catalyst/0.75 mL BA for 4 h. The reaction products and unconsumed reactants were analyzed by using HP 7890 GC equipped with a FID detector and a HP-5 capillary column.

The conversion of BA over ZSM-12 was found to be 7.7 %. The desilicated ZSM-12 samples showed the better catalytic performance than the untreated ZSM-12 since the increase of external surface area and mesoporosity improve the ability of reactant transfer. The sample treated with 0.2 M NaOH at 85 °C for 60 min gave 89.5 % conversion of BA. DPM selectivity also increased in the presence of desilicated samples.

Keywords: Zsm-12, Desilication, Benzylation

This study was supported by the Anadolu University Scientific Research Projects Commission under the Project No. 1410F412

THE DESIGN OF ORGANOHYBRID STRUCTURES

ELENA RODLOVSKAYA[a], VALERII VASNEV[a], BORIS IZMAILOV[a]

[a]A.N. NESMEYANOV INSTITUTE OF ORGANOELEMENT COMPOUNDS RUSSIAN ACADEMY OF SCIENCES

*rodlovskaya@mail.ru

Abstract:

One of the most actual problem in the field of informational nanotechnology is the development of photochromic recording media for three-dimensional optical memory with high information capacity. Usually these light-sensitive materials are developed by employment of thermally irreversible photochromic compounds, particularly 1,2-diarylethenes, in polymer binders [1]. Unfortunately, the information capacity (resolution) of these recording media is limited by diffusion and low content (up to 5 mass %) of photochromic compounds in a polymer matrix.

The present report on the synthesis and the spectral-kinetic study of photochromic three-dimensional silicone polymers (coatings) based on 1,2-dihetarylethenes with N-hydroxyethyl and N-allyl groups, polysiloxanes and polysilazanes. The polymers prepared contain photochromic moieties linked to the polymer chain by covalent bonds that allow achieving high concentration of photochromic units (up to 40%).

This work was supported by the Russian Foundation for Basic Research (Project 18-03-00892).

References

[1] E.N. Rodlovskayaa, B.A. Izmailov, V.A. Vasnev, L.I. Komarova, S.I. Luiksaar, M.M. Krayushkin V.A. Barachevskii, O.I. Kobeleva and T.M. Valova, Polymer Science, Ser. B, 2011, Vol. 53, Nos. 5–6, pp. 352–357.

Keywords: Photochromic Compounds. 1,2-Diarylethenes, Polymer Matrix

EFFECT OF Co-B-Ag CATALYST SODIUM BOROHYDRIDE HYDROLYSIS

M. SAIT İZGİ[a]

[a]SIIRT UNIVERSITY

*saitizgi@gmail.com

Abstract:

One of the chemical compounds with high energy density, which removes the problem of the storage of hydrogen from the clean energy sources, is sodium borohydride. The basic parameter that determines the hydrolysis of sodium borohydride, hydrogen production efficiency and reaction course is the catalyst. Energy sources are undoubtedly one of the greatest challenges facing humanity due to increasing concerns over a series of worldwide energy and environmental problems. In the past decades, research around nano scale interface technologies related to photovoltaic, batteries and fuel cells has brought fascinating breakthroughs in energy conversion and storage. In particular, hydrogen has become one of the most promising future energy resources due to concerns about global warming and the depletion of fossil fuels.Metal hydrides like sodium borohydride ($NaBH_4$) have attracted much attention worldwide as a source of high purity hydrogen for portable and stationary applications.

In this study, Co-B-Ag catalyst was studied for hydrogen generation from the hydrolysis of the sodium borohydride solution. Then, the optimal metal ratio, the amount of catalyst, the concentration of different, and the catalytic activity at different temperatures were examined for sodium borohydride hydrolysis. The kinetic model of first order and according to the values obtained the activation energy was determined as 20.301 kJ/mol.

Keywords: Co-B-Ag, Hydrogen, Catalyst, $NaBH_4$, Hydrolysis

HYDROGEN PRODUCTION FROM HYDROLYSIS OF SODIUM BOROHYDRATE IN THE PRESENCE OF Ni-B-Ag CATALYST

M. SAIT İZGİ[a], ÖMER ŞAHİN[a]

[a]SIIRT UNIVERSITY

*saitizgi@gmail.com

Abstract:

As is known, the demand for energy is increasing with the increasing population in the world. In this context, sodium borohydride, which has the highest hydrogen carrier, is considered in this study. Effective, convenient and cheap catalysts (metal boron catalysts) are needed to use hydrogen obtained by alkaline sodium borohydride hydrolysis in PEM fuel cells.

In this study, the catalytic activity of Ni-B-Ag catalyst was increased in the microwave environment, and the effect of this catalyst on the hydrolysis of sodium borohydride was investigated. The concentrations of NaOH, catalyst amount and different temperature on the catalytic activity of Ni-B-Ag catalyst were investigated. Accordingly, the kinetic of the reaction which was hydrolyzed at different temperatures was subtracted to determine that the reaction order. Thus, the order of kinetic of the reaction and the activation energy were found.

Keywords: Sodium Borohydride, Ni-B-Ag, Catalyst, Hydrogen energy

EFFECT OF MİCROWAVE IRRİTATED Nİ-B-P CATALYST ON THE HYDROLYSİS OF POTASSİUM BOROHYDRİDE

M. SALİH KESKİN[a], M. SALİH AĞIRTAŞ[b], ÖMER ŞAHİN[a], M. SAIT İZGİ[a]

[a]SIIRT UNIVERSITY

[b]VAN YÜZÜNCÜ YIL UNIVERSITY

*saitizgi@gmail.com

Abstract:

Hydrogen can be produced using a wide variety of techniques without the emission of pollutants and greenhouse gases, and as technology improves, production costs are targeted to reach levels comparable to other sources. Nowadays, hydrogen is produced by catalytic conversion from natural gas or hydrolysis of water. However, these methods are not fast enough and flexible for portable PEM fuel cells. This work, Ni-B-P catalysts were synthesized from $Ni(NO_3)_2$. $9H_2O$ and $NaHPO_4$ compounds by using KBH_4 as chemical reducing agent at temperature range of 3–8°C. The microwave irradiation method utilized depends on different gas medium (N_2, Ar, CO_2), microwave power (0–1,000 W), and microwave applying time (0–20 min) to increase the catalytic activity of Ni-B-P catalysis used in the hydrolysis of KBH_4. It was found that the Ni-B-P catalyst with best catalytic activity for KBH_4 hydrolysis was produced under microwave conditions of N_2 gases for 10 min treatment time and 300 W applying power. Hydrolysis of KBH_4 is completed in 15 min by using Ni-B-P catalysis treatment optimum irradiation microwave conditions and it is completed in 18 min in the case of non-microwave treatment of Ni-B-P.

Keywords: Hydrolysis, KBH_4, catalyst. Microwave

ICACCHE

2nd International Conference on Applications in Chemistry and Chemical Engineering

SİİRT ÜNİVERSİTESİ 2007

INTERNATIONAL UNIVERSITY OF SARAJEVO 2004 IUS

TURKISH AIRLINES

ZENITH GROUP
www.zenithgroup.ba

EUROPE CONGRESS
www.europecongress.org

www.icacche.com