ICACCHE

International Conference on Applications in Chemistry and Chemical Engineering

BOOK OF ABSTRACTS

11 - 15 October 2017 **Sarajevo**

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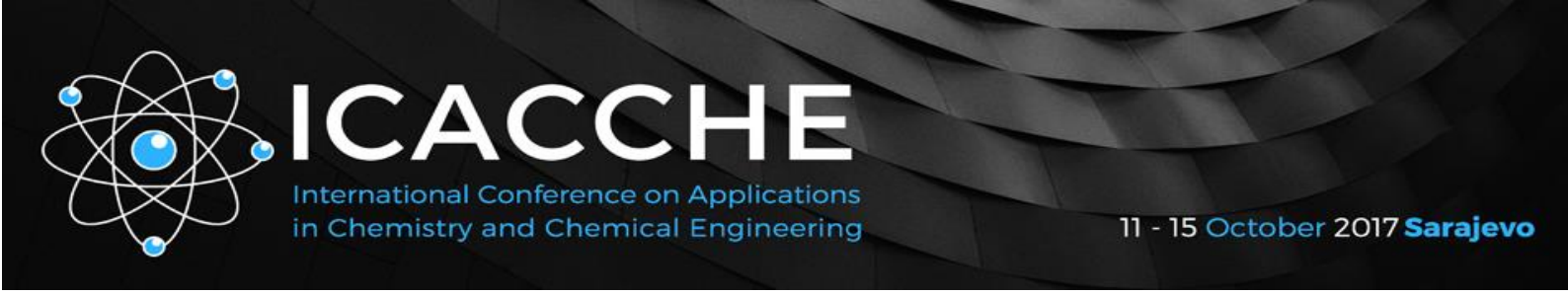

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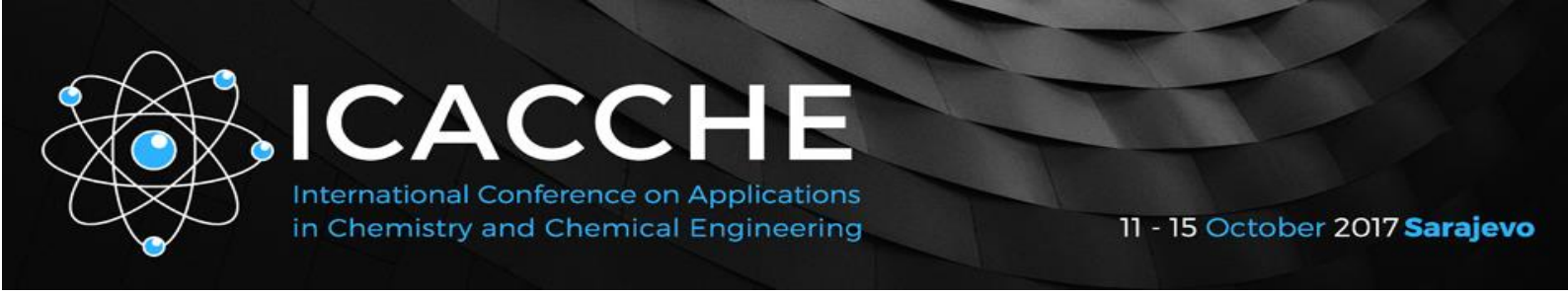

BOOK OF ABSTRACTS OF THE INTERNATIONAL CONFERENCE ON APPLICATION IN CEHMISTRY AND CHEMICAL ENGINEERING (ICACCHE) 11-15 OCTOBER 2017, SARAJEVO

Edited by
Prof. Dr. Ömer Şahin

Published, 2017

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WELCOME TO ICACCHE 2017

On behalf of the organizing committee, we are pleased to announce that the International Conference on Application in Chemistryand Chemical Engineering (ICACCHE-2017) is heldfrom October 11 to 15, 2017 in Sarajevo - BOSNIA-HERZEGOVINA. ICACCHE 2017 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

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MODELING THE GROWTH OF SACCHAROMYCES CEREVISIAE IN PYRITE ASH

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Abstract:

Application of several growth models to survival of sulfur tolerant Saccharomyces cerevisiaein pyrite ash is studied under different experimental conditions. The experiments were carried out by following the pyrite ash minerals of FeS, CuS, CuSO4, PbS and PbSO4 using X-ray powder diffraction (XRD) analysis. Among the models most of them have given appropriate results for the explanation of S. cerevisiaegrowth. The sulfur elimination in the process was monitored through (XRD) analysis and particular sulfur consumption was recorded.

Keywords: Growth Modeling, Saccharomyces Cerevisiae, Pyrite Ash

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PHOTOCATALYTIC HYDROGEN PRODUCTION FROM WATER UNDER SUN LIGHT

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Abstract:

Photocatalytic and photoelectrochemical water splitting under irradiation by sunlight are great practical interest for developing a sustainable energy system. Various nanoscale designs such as nanowires, nanotubes, heterostructures and nanocomposites have been explored to increase the energy conversion efficiency of photoelectrochemical water splitting and for an economical use of water and solar energy. Among various semiconductors, metal sulfides and chalcogenides with a variety of superior properties including appropriate bandgaps for visible-light absorption are highly active photocatalysts for water reduction to form H_2 under sunlight irradiation[. Additionally, efficient interfacial charge transfer is essential in graphene-based semiconductors to realize their superior photo activity. Here, we synthesized CdZnS-based photocatalysts including graphene and derivatives and tested in photocatalytic reactor systems for the production of H_2 from water under solar light and visible irradiation. To enhance the activity and stability of photocatalysts, they were loaded with different noble metals such as Pt and Ni. The results show that photocatalysts including graphene and derivatives have the best performance when band gap, solar energy conversion efficiency and hydrogen production rates are considered. Moreover, loading noble metal to nanocomposite, increase remarkable photocatalytic activity and efficiency.

Keywords: Photocatalytic Hydrogen Production, Photocatalysts, Graphene.

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ELECTRODE MODIFICATIONS, CHARACTERIZATIONS AND ELECTROCHEMICAL APPLICATIONS OF METALLOPHTHALOCYANINES

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Abstract:

Metallophthalocyanines (MPcs) have superior properties such as fast electron transportation, high thermal conductivity and flexibility, chemical and thermal stability. MPcs with different substituents were modified with different techniques such as Langmuir-Blodgett (LB), click chemistry (CC) and click electrochemistry (CEC), electropolymerization, dip coating, cast film deposition, spin coating and spray deposition for using various applications. Before any modification, MPc complexes were investigated with voltammetric and in-situ spectroelectrochemicals techniques for determine mechanisms, redox properties and optical behaviors like color change. MPcs having redox active metal center and containing electropolymerizable groups such as amino, triazole were electrochemically polymerized and tested for different applications such as electrochromism, pesticide sensor, sensor, catalyst for hydrogen evolution reaction (HER), oxygen evolution reaction (OER), oxygen reduction reaction (ORR) and photo anode or photo cathode. As well as, modified electrodes with phthalocyanines bearing terminal alkynyl substituents by using CC and CEC techniques were tested for practical usages as effective electrocatalysts in hydrogen evolution reaction (HER). In scope of these, modified electrodes were obtained via CEC technique and tested as electrocatalyst for OER in water splitting reaction. Modified electrodes significantly decreased the over-potential, increased the current density of OER, and illustrated suitable redox activity and conductivity for the practical applications.

Keywords: Metallophthalocyanines, Click Electrochemistry, Electrocatalyst, Oxygen Evolution Reaction.

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THERMAL ANALYSES OF TURKISH LIGNITES DURING COMBUSTION

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Abstract:

In this study, two Turkish lignite samples from Kütahya-Tunçbilek and Adıyaman-Gölbaşı region were subjected to combustion through heating from ambient temperatures to temperatures of 200ºC, 450ºC, and 800ºC for Kütahya-Tunçbilek lignite and 200ºC, 400ºC, and 600ºC for Adıyaman-Gölbaşı lignite a horizontal tube furnace under dry air atmosphere. These temperatures were selected from Differential Thermal Gravimetry graphs of both lignites. Ultimate, proximate and calorific value analyses were performed on the original samples and residues obtained from combustion process. After that, all original and thermal treated samples were subjected to combustion in a thermal analyzer under dry air atmosphere to burn the remaining carbon in samples. According to the data obtained from the analyses, the effect of temperature on the combustion efficiency, composition of the compounds of lignite samples were investigated and discussed.

Keywords: Lignite, Energy, Combustion, Thermogravimetry

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REMOVAL OF INORGANIC COMPONENTS OF CORN WASTE BY DIFFERENT WASHING METHODS

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Abstract:

Nowadays fossil fuel reserves are running out and alternative sources are being explored. Biomass is a promising alternative. Turkey is also suffering from energy problems. Therefore, firstly raw materials for biomass energy were searched as an alternative energy source in Turkey. In order to supply the increasing energy and food needs in Turkey, corn production increased by 52% during the 2016-2017 harvest period. The remaining parts of the corn biomass are removed by stubble burning here. This situation causes environmental pollution, also energy loss which can be obtained from the biomass. Also, inorganic constituents of the ash in biomass fuels negatively affect the quality of the fuel. In this study, the parameters required for the elimination of inorganic compounds and the burning of waste corn stalks under appropriate conditions were determined. The remaining corn waste stalk after the harvest obtained from Adana, Turkey was preferred. These wastes were dried in a laboratory medium at 60°C for 2 days with drying oven. After washing the samples with different methods (hand-spraying, flushing and soaking), the calorific values and the proximate analysis were performed. The changes in the inorganic constituents (K, Na, Cl, Ca, Si, Al, Fe, Mg, P, S) as a result of the washing processes were determined in the ICP device. Thermal analysis of the samples washed with different methods has been carried out. Also, ash was produced in the horizontal tube furnace. XRD analyses of ashes were carried out and the changes were examined. The appropriate method has been identified.

Keywords: Inorganics

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STUDIES ON THE SYNTHESIS OF SOME NEW FLAVONE SULFONAMIDE COMPOUNDS AS ANTICANCER AGENTS AND HDAC6 INHIBITORS

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Abstract:

Histone deacetylases (HDAC) can affect many vital regulatory processes, including gene expression, mRNA stability, protein interactions, protein stability, and enzymatic activity via the removal of acetyl groups attached to lysine residues in histone and non-histone proteins. HDAC6 which is the one of the non-histone deacetylase has become a target for treatment of serious diseases like cancer, Alzheimer and autoimmune disorders. HDAC6 is responsible for deacetylation of non-histone cytoplasmic proteins such as microtubule (α/β tubulin), Hsp90 (heat shock protein 90), cortactin and chaperon. İnhibition of HDAC6 results in the loss of microtubule stability and function and causes increased protein aggregation. Using these disadvantages as an advantage in favor of cancer treatment, histone deacetylase 6 inhibitors (HDAC6i) are valuable pharmacological targets.

In this study, in the light of anticancer properties of histone deacetylase6 inhibitors, flavon sulfonamide compounds have been synthesized. The structural evaluation of the synthesized compounds was based on the 1H NMR, Mass and elementary analysis data. Their docking studies are shown that they have enough interactions for the enzyme inhibition. Synthesized new flavone compounds are under investigation within the scope of anticancer properties and histone deacetylase6 inhibitory activities.

Acknowledgement: This work was supported by Research Organization of Ankara University, Turkey (No: 17L0237003).

Keywords: Flavone, Sulfonamide, Histonedeacetylase (HDAC), Histonedeacetylase Inhibitors (Hdacis), Anticancer, Synthesis.

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A STUDY ON SYNTHESIS OF NOVEL THIAZOLYL THIAZOLIDINEDIONE OR RHODANINE DERIVATIVES AS ANTICANCER AGENTS

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Abstract:

Thiazolidinedione (TZD) and rhodanine analog compounds have become a very important group of heterocyclic compounds in drug design and discovery. The PPAR-gamma (PPAR-γ) activating TZD medications are a class of drugs used to improve lipid and glucose metabolism in type-2 diabetes. More interestingly, numerous compounds containing the TZD ring have been developed as potential anticancer agents (1). Rhodanines have been reported to possess antibacterial, antifungal, antiviral, antimalarial, insecticidal, herbicidal, antitumor, anti-inflammatory and cardiotonic activities (2). Besides, rhodanine derivatives are still broadly evaluated for their anticancer activity against different cancer cell lines, often exhibiting selective toxicity against normal cell lines (3).

Thiazoles are ubiquitous building blocks in medicinal chemistry and can be found in numerous natural products (e.g., epothilone) and biologically important compounds including the anticancer drug dasatinib (4).

Inspired by the biological importance of these ring systems, we described the synthesis of a new series of thiazolyl-2,4-thiazolidinediones / rhodanines as lead structures in developing anticancer agents.

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Keywords: 2,4-Thiazolidinedione, Rhodanine, Thiazolyl-2,4-Thiazolidinediones, Thiazolyl-Rhodanines, Anticancer Activity, Anticancer Agent

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SUPERCRITICAL WATER GASIFICATION OF RED KIDNEY BEAN SHELLS BY USING ALKALI CATALYSTS

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Abstract:

Hydrogen and methane production by supercritical water gasification (SCWG) of red kidney bean shells which structure is lignocellulosic biomass, was investigated in these experiments. Red kidney bean shells(RKBS) which is not possible to recycle were chosen as model waste compounds. The experiments were performed in 100 ml shaking autoclaves. The studies were carried out without and with alkali catalysts as KOH and NaOH at four different temperatures (300, 400, 500, 600 °C). First of all, feedstock was dried at room temperature and then biomass samples were grounded in a crush mill until the particle size of biomass reached below 1 mm. Elemental analysis of RKBS was performed using an elemental analyzer (CHNS-932 by Leco, MI-USA). The air was removed from the system with an inert gas stream (nitrogen) later than putting the 1.2 g of RKBS and 15 ml water into the autoclave. Desired temperature was reached with heating the internal temperature of reactor with 6 K min-1 and held at this temperature for 1 h. The experiments were carried out at 300°C, 400°C, 500°C, 600°C with and without 10 wt % catalyst. Formation of gaseous products, water-soluble organics, coke and tars were observed using solid, liquid and gas analysis devices (GC, GC-MS, HPLC, TOC and TOC-SSM) in liquid and solid products. Temperature have positive effect on the gasification performance for hydrothermal gasification of RKBS but liquid and solid product decreased. Both of the catalysts type enhance gasification yield by decreasing residue yield. It was found that CO_2, H_2 and CH_4 was investigated at most, also there were trace amount of CO ve C_2-C_4 hydrocarbons. The highest gaseous product and hydrogen, methane yields were observed when using KOH as catalyst.

Keywords: Red Kidney Bean Shell, Biomass, Waste, Supercritical Water Gasification, Hydrogen

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SYNTHESIS OF BROMOSUBSTITUTED ISOINDOLE-1,3-DIONE DERIVATIVES: BROMINATION OF (3AS,5S,7AR)-5-HYDROXY-2-ALKYL/ARYL -3A,4,5,7A-TETRAHYDRO-1H-ISOINDOLE-1,3(2H)-DIONE

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Abstract:

N-substituted isoindole or norcantharimide derivatives have been found to have highly efficient biological activity and anticancer effects. Therefore, In recent years much effort has been done on the synthesis of N-derivatives of isoindole or norcantharimide. Recently, we have developed a versatile synthetic approach for the synthesis of new norcantharimide derivatives considering their biological properties . In this study, we synthesized a new class of isoindole derivatives. For this purpose, the key compounds 1-3 (5-hydroxy-2-alkyl/aryl-3a,4,5,7a-tetrahydro-1H-isoindole-1,3(2H)-dione) were synthesized from 3-sulfolene as in the literature. Then, the compounds 4a-6a (2-bromo-4-alkyl/aryl tetrahydro-1aH-oxireno[2,3-f]isoindole-3,5(4H,5aH)-dione) and 4b-6b (4,5-dibromo-6-hydroxy-2-alkyl/aryl hexahydro-1H-isoindole-1,3(2H)-dione) were obtained via addition of molecular bromine to the double bond of compounds 1-3. Result products 4a-6a and 4b-6b were synthesized in a ratio of 1:1 and purified by column chromatography.

Keywords: Bromination, Norkantharimide

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Γ-LACTONE SYNTHESIS-FUSED N-SUBSTITUTED NORCANTHARIMIDE

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Abstract:

Cantharidine and its analogues norcantharidine and norcantharimide are very important in that they show biological activity.

Derivatives of norcantharimide are also known to be potential anticancer agents. It is possible to find many scientific studies about these compounds in the literature due to these biological properties. Recently, we have developed synthesis of new class norcantharimide derivatives and investigated their some biological properties. In this study, we synthesized γ-lactone-fused N-substituted norcantharimide compound. For this purpose, 2-ethylhexahydro-1H-cyclobuta[f]isoindole-1,3,5(2H,3aH)-trione (1) was synthesized from 3-sulfolene as in the literature. Then, γ-lactone (6-ethylhexahydro-2H-furo[2,3-f]isoindole-2,5,7(6H,7aH)-trione) was synthesized via the oxidation of the compound 1 with H2O2.

Keywords: Norkantharimide, Γ-Lactone

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WATER RESOURCES AND TRAVERTINE OCCURRENCES AROUND SEYDISEHIR (KONYA-TURKEY)

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Abstract:

In the studied area, there are elate of water sources. Some of them are probably heated by the Miocene Erenler Dağı volcanics, while hot water emerges as some of them are cold water sources.While the autochthonous carbonates in the region refer to the reservoir rocks, Seydisehir Formation, which has a very impermeable feature, also assumed the role of covering layer. All of these waters around Seydişehir are of karstic origin and provide the drinking water requirement for cold waters (Beldibi, Kuğulu, Pınarbaşı).

The current hot waters in the region have about 1,5 lt/s, average pH of 6.91-7.92. Welding temperatures range from approximately 20-32°C on the surface and 36°C to 41°C deep (Kavak village drilling data). The total mineralization is between 2218 and 3529 mg / l and the concentrations of $CaCO_3$ (Ca++: 5,6 mg / lt -16.1 mg / lt), (HCO_3)- (350-1651 mg /lt), Cl- (220,5mg/lt), Na+ (293 mg / l), K+ (310 mg / l), Fe++ (2,5 mg / contains microorganisms. "Ca-Mg-Na (SO_4) -HCO_3" type water. Although it is classified as " low mineral hot water (acroterm) " according to the classification of International Hydrogeologists Association (AIH), but it is not used for medical treatment and other purposes, especially for central heating, greenhouse heating, greenhouse cultivation, or for the other purpose. Depending on the hot waters mentioned in the region, many types of travertine have been formed in different types and these must be protected as geological heritage.

Keywords: Seydisehir, Hot And Mineral Water Source, Ilica Hill, Acroterm, Traverten, Çaltepe Formation, Total Mineralization

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GEOLOGICAL AND MINERALOGICAL PROPERTIES OF THE GAZIPAŞA (ANTALYA-TURKEY) GALENA BEARING BARITE DEPOSITS

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Abstract:

Barite ore deposits are located to the north of Gazipaşa (Antalya) in the south of the Central Taurus Mountains. The ore is in Paleozoic (Permian-Devonian) meta-clastic rocks alternating with methacarbonates. Ore masses are generally stratiform, locally, lenses, and sometimes veins. The barite forming the main ore mineral is associated with galena, pyrite, chalcopyrite, sphalerite, tennantite-tetrahedrite, sericite, limonite, anglezite, covellite, azurite and malachite minerals in minor proportions.

Ore deposits and some structural and textural features indicate a sedimentary form, but the presence of thick ore veins and intercalation of sandstones, intensive silicification, the presence of barite-bearing dolomitized limestones, minerals such as galenite, pyrite, chalcopyrite in paragenesis, suggest that mineralization is not only related to sedimentary processes but also to hydrothermal processes.

Keywords: Keywords. Barite, Galena, Gazipaşa, Hydrothermal Process, Corresponding Author E-Mail: Mmkaradag@Selcuk.Edu.Tr, Mehmet Muzaffer

ICACCHE
International Conference on Applications in Chemistry and Chemical Engineering
11 - 15 October 2017 Sarajevo

DETERMINATION OF THE PHENOLIC PROFILE AND ANTIOXIDANT ACTIVITY OF THE PLANT 'TANACETUM ERZINCANENSE'

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Abstract:

Introduction: Many studies of different species of Tanacetum plant have revealed many bioactive properties of these plant species such as antioxidative, antimutagenic and anti-carcinogen.

Aim: In this study, it was aimed to determine the antioxidant activities and phenolic contents of methanol and ethylacetate extracts obtained from Tanacetum erzincanense plant which is defined as a new species and endemic to Erzincan, Turkey.

Materials and Methods: The airel parts plant material was collected in Mantarlı villages in Çayırlı-Erzincan, Tukey and dried in a dark room. After dry, the airal parts of the plants were ground to fine powder, their extractions were performed by ethylacetate and methanol solvents, respectively. The antioxidant capacities of the extracts were evaluated by DPPH, ABTS, FRAP, CUPRAC and metal chelating capacity tests. Total phenolic amounts of the extracts were determined by Folin-Ciocalteu methods. Phenolic profiles of the extracts were identified by Q-TOF/LC-MS.

Results: Methanol extract displayed higher scavenging capacity against DPPH and ABTS cation radicals than ethyl acetate extract, and both extracts showed lower activity than BHT and BHA standards but close to α-tocopherol and trolox. Methanol extract was found to have higher power to reduce Iron (III) ions and Copper (II) ions than the standards. In addition, both extracts were observed to chelate iron ions in a similar manner to standards. Total phenolic content of methanol extract was much higher than that of ethylacetate extract. As a result of Q-TOF / LC-MS analysis, it was determined that the plant contains abundant amounts of chlorogenic acid, quinic acid, tuberonic acid, emodic acid, lezonoric acid, quercitrin, luteolin, genistein, koparin, cosmosin, cefamandol and tamarixcetin.

Conclusion: Due to its high phenolic substance content and its antioxidant capacity, T. erzincanense plant and/or its extracts can be considered as pharmaceutical and natural therapy in the fight against oxidative stress.

Keywords: Tanacetum Erzincanense, Antioxidant Activity, Fenolics, Cromatography

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A NEW TECHNIQUE FOR THE MEASUREMENT OF MIXING TIME

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Abstract:

Mixing is defined as "the reduction of inhomogeneity in order to achieve a desired process result". Mixing process has an important role in almost all industrial systems. Agitated liquid units are the most commonly encountered systems in the mixing operations with a wide range of applications. One of the indications for the degree of mixing in these units is the mixing time. The mixing time can be measured by applying a tiny pulse on a homogeneous agitated system and then measuring and recording the history of the medium until the system attains to a new homogeneity. The pulse can be a temperature, concentration, or a colouring agent, and generates a measurable tiny change in the physical properties of the system without causing a considerable change of the system properties.

Electrochemical limiting diffusion current technique (ELDCT) has been widely employed for the measurements of mass transfer, shear stress, fluid velocity, and turbulent fluctuations. The aim of the present work is to search whether the application of the ELDCT for the measurement of the mixing time in stirred vessels is possible, and to establish a new technique for the mixing time measurements in the systems consisting of liquid contents. A stirred tank was designed according to the standards, and stirring speed, vane number, stirrer diameter, vane angle and liquid viscosity were chosen as parameters. Local mixing times and average mixing times was measured by using a local sensor, one of the baffle as sensor for average readings.

Comparisons with the results obtained from conductivity measurements showed that ELDCT can be practical, fast, simple and flexible mixing time measurement technique.

Keywords: Mixing Time, Stirred Tanks, Electrochemical Limiting Diffusion Technique

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HYDROTHERMAL SYNTHESIS OF COPPER (I) COMPLEX OF 2-BENZOYLIMIDAZOLE

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Abstract:

The synthesis of new copper (I) complex with 2-Benzoylimidazole as a ligand is reported. [Cu_2(2-Benzoylimidazole)2] complex was synthesized by the reaction of 2-Benzoylimidazole oxime with $Cu(NO_3)_2$ under hydrothermal reaction conditions. Single-crystal X-ray diffraction, melting point determination, elemental analysis (C.H.N.S), infrared spectroscopy, magnetic susceptibility, molar conductance techniques were used to characterize the structural formula of the complex. The photoluminescence properties of the complex have been carried out.

Keywords: Copper(I) Complex, 2-Benzoylimidazole, Hydrothermal Synthesis, Crystal Structure

Acknowledgements: This research is supported by Afyon Kocatepe University, Scientific Research Project Commission, Project number: 13.FENED.07.

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SYNTHESIS, CHARACTERIZATION, INVESTIGATION OF BIOLOGICAL ACTIVITY OF Cu(II) COMPLEX WITH 4-(IMIDAZOL-1-YL)PHENOL

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Abstract:

A Cu(II) complex of 4-(Imidazol-1-yl)phenol has been prepared. The structure has been determined using Single-crystal X-ray diffraction, melting point determination, elemental analysis (C.H.N.S), infrared spectroscopy, magnetic susceptibility, molar conductance techniques. 4-(Imidazol-1-yl)phenol on reaction with copper(II) salt produce Cu(II) complex $[Cu(L)4(NO_3)_2]$ where L=4-(Imidazol-1-yl)phenol. The complex exhibit distorted octahedral geometry to mononuclear Cu(II). The Cu(II) complex was screened for anticancer activities (MCF-7, HeLa and MRC-5). Other biological activities of Cu(II) complex are currently being investigated.

Keywords: Cu(II) Complex, 4-(Imidazol-1-Yl)Phenol, Crystal Structure, Anticancer Activity

Acknowledgements: This research is supported by Afyon Kocatepe University, Scientific Research Project Commission, Project number:17.KARİYER.18

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ACID TREATED AND BI ELECTRODEPOSITED GRAPHITE FELT ELECTRODES FOR FE/CR REDOX FLOW BATTERIES

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Abstract:

Renewable energy is hot research area for decades due to the fossil based energy source depletion. Electrical energy generated from renewable energy sources (wind, solar etc.) is not stable and intermittend so storage of the produced electrical energy is needed to prevent fluctuations. Redox flow batteries are advanced novel electrical energy storage systems that can store electricity efficiently. Among the flow batteries, Fe/Cr flow batteries are promising electrical energy storage systems due to low cost and easy to find active components and widely available industrial applications.

Electrolyte solution distribution and electrochemical properties of electrodes are fundamental parameters affecting the battery performance. A decrease in cell resistances, transport and ohmic limitations can be obtained with the development of electrode materials. With the improvement in the flow battery cell, optimal power density, efficiency and better system performance can be achieved. Chemical modifications like surface functionalization is a beneficial approach for the improvement of electrochemical properties of carbon materials. Oxygen containing groups could be introduced onto carbon electrodes by acid treatment.

In this study, mixed H_2SO_4 and HNO_3 are used for acid treatment of graphite felt electrode with the help of positive interaction of the two acid and electrodeposited Bi on graphite felt is used to suppress H2 evolution on chromium side. Acid treatment is done for 5h under reflux. After the acid treatment felt is washed with deionized water and dried at room temperature. Bi is electrodeposited during charge of the battery. Introduction of functional groups such as hydroxyl, carbonyl and carboxyl and surface morphology can be detected by FT-IR spectroscopy and SEM respectively. The electrochemical characterizations on Fe/Cr flow battery are on progress and results will be obtained by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS).

Keywords: Energy Storage, Fe/Cr Flow Battery, Graphite Felt, Acid Treatment, Bi Deposition

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HOLLOW GLASS MICROSPHERES REINFORCED SULFONATED POLYETHERSULFONE COMPOSITE MEMBRANESFOR H_2/O_2 PEM FUEL CELLS

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Abstract:

Nafion is mostly used perfluorosulfonated polymer membrane in PEM fuel cells which has high proton conductivity, chemical stability and mechanical strength. Due to its decreasing proton conductivity at high temperature, fuel crossover and high cost, it is necessary to develop new membranes to improve workability of PEM fuel cellsunder high temperature.There is an increasing interest in the development of various polymers that can replace Nafion. Using aromatic polymers as a polymer electrolyte in PEM fuel cells is seen as thebest approach owing to their low cost and easy processability.Among the aromatic polymers, although PES has been attracted owing to its chemical and mechanical strength it has low proton conductivity. Therefore, PES must be sulfonated to improve the proton conductivity of membrane.

Hollow glass microsphere (HGM) consists of stiff glass shell and inert gas inside.This structure provides some unique properties such as light weight, low electrical conductivity, low density and high stiffness. On the other hand, using HGM as an additive material for fuel cell membranes reduce fuel permeability and increase the water retention capacityof the membranes. Thus, the proton conductivity of the membrane can be increased at elevated temperatures.

Sulfonated PES (sPES)/HGM composite membranes are prepared using solvent casting method. sPESis dissolved in dimethylacetamide (DMAc). HGMs are fuctionalized by NaOH solution and the required amounts of HGM-OH(%1, 3, 5) are added to sPES solution. The sPES/HGM blend is poured onto petri dish and dried in vacuum oven.

In this study, proton conductivity, water uptake and gas/fuel (H_2/O_2 or air) permeability of membranes will be determined. After structural characterizationsof composite membranes, they are going to be used in H_2/O_2 PEM fuel cell and their performance tests will be conducted.

Keywords: Hollow Glass Microsphere, Polyethersulfone, PES, Composite Membrane, PEM Fuel Cell

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THE STRUCTURAL AND THERMAL PROPERTIES OF PLA COMPOSITES BASED ON SILICA DERIVED FROM RICE HUSK AND POLYETHYLENE GLYCOL

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Abstract:

Most of the plastic materials used in the packaging industry are petroleum-based. These plastics such as polyethylene (PE), polystyrene (PS), polyethyleneterephthalate (PET) do not decompose in soil for many years and lead to increase environmental pollution and CO_2 in the atmosphere. There have been various approaches to eliminate environmental pollution caused by plastics. Today, the best approach is seen as using of biodegradable polymers.

Among the biodegradable polymers, polylactic acid (PLA) has attracted attention due to having properties such as biodegradable, environment friendly, biocompatible, easily processable, transparent, high modulus and strength. Although PLA has these advantages, it can not be used in many applications due to its gas barrier properties, thermal stability, fragile and cost. The physical, thermal or mechanical properties of PLA can be improved by several methods, such as modification, addition of additives or polymer blends.

Rice husk is an agricultural by-product during the rice milling process. Ash content of rice husk is mainly consist of silica. It can be used as an additive material to improve the gas permeability and thermal properties of materials.

In this study, composite films are prepared using solvent casting method. PLA, PEG and silica obtained from rice husk are dissolved in chloroform under continuous stirring. The blend is poured into a petri dish and dries in oven. In this study, the thermal and structural properties of the prepared composite films were determined by SEM (Scanning Electron Microscope), FTIR (Fourier Transform Infrared Spectroscopy), TGA (Thermogravimetric Analysis). Water absorption capacity and gas (O_2, N_2, CO_2 and air) permeability of films were also investigated. According to results of analysis as the silica content increases, the thermal degradation temperature and water absorption capacity of films increase.

Keywords: PLA, Polymer Composites, PEG, Silica, Biodegradable Polymer, Polymer Blends

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IN VITRO EFFECTS OF ACTIVE COMPOUNDS FROM ARUM ELONGATUM STEVEN SUBSP. DETRUNCATUM (C.A. MEY. EX SCHOTT) RIEDL ON BOVINE LIVER GLUTATHIONE REDUCTASE

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Abstract:

Arum is distinguished a large area from east to west Turkey where local people were collected it as spring plant. It was consuming by local people in the food after arum was dried or boils. So, the antioxidant effects of Arum on Glutathione reductase activity, an antioxidant enzyme, were researched. Firstly, Glutathione reductase was purified from bovine liver by affinity column chromatography and purification rate and specific activity of the enzyme were calculated as 1832 fold and 141 EU/mg.protein respectively. Moreover, the subunit molecular weight of the enzyme was determined 55 kDa by means of SDS-PAGE. Later, natural fatty acids of Arum elongatum plant were isolated by column chromatography and seven substances (from R1 to R7) were obtained. The structure analysis of all substances was evaluated by GC-MS and NMR method. These compounds were understood to be the mixture of fatty acid, except R7. R7 is β-Sitosterol and Campesterol. Only three from these substances were affected on GR activity. R6 was shown competitive inhibition when R4 had non-competitive inhibition on GR activity. But, R1 has a role as an activator on GR activity. I50 values of R4 and R6 were calculated as 0.193 mg/mL, 3.98 µg/mL respectively.

Keywords: Arum Elongatum Subsp. Detruncatum, Fatty Acid, Glutathione Reductase, Isolation, Purification.

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ENRICHMENT OF ZONGULDAK (TURKEY) BITUMINOUS COAL FOR CASTING INDUSTRY

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Abstract:

Casting sand is used in precision casting industry and contains coal dust in important ratio. The use of coal dust in the sand is indispensable for obtaining a smooth casting surface. The coal should have a low ash ad high volatile matter. In this study, raw material was taken from Zonguldak-Kurtköy region. The bituminous coal was formed in the Alacaağzı formation in Zonguldak (Turkey) and is a Namurian aged bituminous coal. A study has been carried out to convert it into a feature that can be used in the casting industry. The bituminous coal produced from coal mine contains high ash (40% ash). For this reason, a number of coal preparation and enrichment experiments have been carried out to reduce the ash content to 7%. Enrichment experiments were performed at different size ranges. Ash of bituminous coal above 0.5 mm in size was reduced by physical method (float-sink). That of below 0.5 mm in size was removed by physicochemical (flotation) method. The physical and chemical properties of the obtained low ash products were found to be suitable for the casting sector.

Keywords: Casting Sand, Bituminous Coal, Enrichment, Floatation, Physical Method

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LEARNING RELATIONAL PATTERNS FOR MUTAGENIC COMPOUNDS

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Abstract:

Graph databases provide simple yet effective mechanisms to model complex real life problems and are equipped with powerful querying tools to extract patterns from data. In this work, we focus on modeling mutagenic and non-mutagenic compounds and propose a method to extract relational patterns (concept descriptors) that define characteristics of both types of compounds. For this purpose, we modeled 125 mutagenic and 63 non-mutagenic compounds within Neo4j environment such that drugs and properties are represented as vertices and edges are labeled after the relations that hold between a drug and its property. In order to obtain generalized rules we further enhanced the graph with generalized version of the categorical attributes and discretized version of the continues attributes. To extract the relational patterns, we implemented a substructure-matching algorithm via traversal method of Neo4j database management system and those substructures with at least 0.1 support and 0.7 confidence value are considered valid relational patterns. The proposed method was able to find 8 relation patterns that cover 100% of the mutagenic compounds. Among those, there are very general relational patterns such as mutagenic(A,true):-atm(A, B, c, 22, [-0.128,-0.106]) logp(A, C), lumo(A, D), inda(A, E), ind1(A, F) (covering 83.2%), as well as specific relational patterns such as mutagenic(A,true):-atm(A, B, h, 3, [0.122,0.144]) logp(A, C), lumo(A, [-2.292,-2.138]), inda(A, E), ind1(A, F) (covering 1.1%). When compared to the state of the art methods, the proposed method was able to find several relational patterns reported in the literature in a reasonable time.

Keywords: Chemical Data Modeling, Mutagenicity, Neo4j, Substructure Matching

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THE ENHANCEMENT OF ORGANIC SOLAR CELL PERFORMANCE BY INTERFACIAL MONOLAYERS

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Abstract:

The effects of interfacial layers has been investigated on the performance of TiO_2 based inverted type organic solar cells. TiO_2 buffer layer was used as electron transporting layer between ITO and PC61BM active layer. A series of benzoic acid derivatized self-assembled monolayers with electron donating groups were used to modify the interface between TiO2 buffer layer and [6,6]-phenyl C61 butyric acid methyl ester (PC61BM) layer with the device structure of ITO/ TiO_2/SAM/ PC61BM:P3HT/MoO3/Ag . The work function and surface energy of TiO2 buffer layer can be changed by a self assembled monolayer (SAM). The solar cell parameters of fabricated devices without SAMs were lower than that of the modified ones. The power conversion efficiency (PCE) of i-OSCs devices with bare TiO_2 electrodes enhanced from 2.00% to %2.43% with SAM treated TiO2 electrodes. The open circuit voltage (Voc) of the organic solar cell also improved by the use of SAM molecules. The Voc values increased from 0.57 V to 0.61 V. The change of surface energy was determined by the contact angle tecnique. The contact angle values were obtained higher than bare unmodified surfaces. These results show that that using an interfacial layer, SAM, between organic and inorganic layers is an useful alternative method to improve the performance of organic solar cell.

Keywords: Organic Solar Cell, Monolayer, Benzoic Acid

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PREPARATION AND CHARACTERIZATION OF ACTIVATED CARBONS FROM AGRICULTURAL WASTE

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Abstract:

The activated carbons are predominantly amorphous and have a large internal surface area and pore volume at an exceptional level. Activated carbon can be produced by chemical activation or physical activation. Carbon-containing materials such as lignite, peat, coconut shells and fruit stones can be selected as raw materials. Due to the wide variety of properties of activated carbon, there is no comprehensive terminology or standardization. The activated carbons can be characterized by appearance, surface area, pore size and pore size distribution, or typical applications. Activated carbons are generally characterized by appearance such as powder, granules or cylindrical or spherical pellets. The activated carbon contains not only carbon but also oxygen, nitrogen, sulfur and hydrogen in small quantities chemically bonded to various functional groups such as carbonyl, carboxyl, phenol, lactone and ether groups. Activated carbon is a versatile adsorbent that is a major industrial concern and is used in a wide range of applications involving the removal of species by adsorption from fluids or gas basically to provide for the purification or recovery of chemicals.

In this study, production of activated carbons was carried out by chemical activation method from vine-trimming waste and the surface properties of these activated carbons were investigated. For this purpose, firstly, the waste was carbonized at 400°C. And then, the obtained chars with KOH were activated at carbonization temperatures of 500, 600 and 700°C. The char/KOH ratio was taken as 1/1. In addition, by taking char/KOH ratio of ½ and 1/3, activated carbons were produced from char at a carbonization temperature of 700°C. Surface properties of the activated carbons were investigated by nitrogen adsorption at -196°C.

Keywords: Activated Carbon, Vine-Trimming Waste, KOH Activation

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CARVACROL PROTECTS AGAINST CYCLOPHOSPHAMIDE-INDUCED TESTIS TOXICITY IN RATS: BIOCHEMICAL EVALUATION

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Abstract:

Cyclophosphamide (CP) is an effective drug widely used in the treatment of clinical cancer and non-malignant diseases. But, the use of CP causes cytotoxicity in one or more tissues. This study aims to investigate the possible protective effects of carvacrol (Cr) on testicular toxicity, an important component of thyme and known as antioxidant properties. For this study, 35 male rats were categorized into 5 groups, each of them including 7 members. Blood samples was obtained from each animal for the evaluation of biochemical markers such as glutathione (GSH), catalase (CAT), malondialdehyde (MDA), superoxide dismutase (SOD) , total oxidant Total oxidant (TOS) and total antioxidant levels (TAS) examination. Assessing serum samples, Cr has an important role in protecting against CP-induced testicular damage. Our data also show that Cr is a highly effective antioxidant with cell-protective properties. We therefore believe that Cr can help reduce the side effects of anticancer drugs in terms of chemotherapy protocols.

Keywords: Cyclophosphamid, Carvacrol , Biochemical Markers, Cell-Protection, Rats

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EVOLUTION OF BORIC ACID CRYSTAL SIZE DISTRIBUTION AND SHAPE IN A CMSMPR CRYSTALLIZER-THE EFFECT OF RESIDENCE TIME, STIRRING SPEED, FEED FLOW RATE AND AMOUNT OF SUPERSATURATION

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Abstract:

In industrial crystallization processes, Crystal size Distribution (CSD), crystal size and the shape of crystal are important characteristics for both process efficiency and further use of the crystals. In this study, the effect of residence time, stirring speed, feed flow rate and amount of supersaturation on the CSD as well as the shape of boric acid crystals were investigated in a CMSMPR (Continuous Mixed-Suspension Mixed-Product Removal) crystallizer. The CSD and kinetic data were determined experimentally using CMSMPR crystallizer running at steady state. Sieve and light microscope analyzes were performed to determine the effects of important parameters (residence time, stirring speed, feed flow rate and amount of supersaturation) for the crystallization process of boric acid. The population density of nuclei, the nucleation rate and the crystal growth rate of boric acid were determined from the experimental population balance distribution when the steady state was reached.

Keywords: Boric Acid, CMSMPR, CSD, Crystallization

Acknowledgement: This work was supported by the Eti Mine Enterprises, Turkey [ETIMINE, project number: 400.02(TGD.2014/3)].

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DETERMINATION OF BORAX PENTAHYDRATE CRYSTAL SIZE DISTRIBUTION AND SHAPE IN A CMSMPR CRYSTALLIZER-THE EFFECT OF SUPERSATURATION, FEED FLOW RATE AND STIRRING SPEED WITH TIME

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Abstract:

In this study, the effect of residence time, stirring speed, feed flow rate and amount of supersaturation on the CSD as well as the shape of borax pentahydrate crystals were investigated in a CMSMPR (Continuous Mixed-Suspension Mixed-Product Removal) crystallizer. In industrial crystallization processes, Crystal size Distribution (CSD) and the shape of crystal are important characteristics for both process efficiency and further use of the crystals. The CSD and kinetic data were determined experimentally using CMSMPR crystallizer running at steady state. Sieve and light microscope analyzes were performed to determine the effects of important parameters (residence time, stirring speed, feed flow rate and amount of supersaturation) for the crystallization process of borax pentahydrate. The population density of nuclei, the nucleation rate and the crystal growth rate of borax pentahydrate were determined from the experimental population balance distribution when the steady state was reached.

Keywords: Borax Pentahydrate, CMSMPR, CSD, Crystallization

Acknowledgement: This work was supported by the Eti Mine Enterprises, Turkey [ETIMINE, project number: 400.02(TGD.2014/3)].

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THE EFFECT OF HIGH FREQUENCY COLD PLASMA OBTAINED IN VARIOUS PARAMETERS, ON THE ELECTROCHEMICAL ACTIVITY OF Co-Cr-B BASED CATALYSTS

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Abstract:

In this study, the catalytic activity of Co-Cr-B based catalysts reduced from $CoCl_2.6H_2O$ is investigated under Alternating Current cold plasma obtained in various applying frequency parameters. Co-Cr-B catalyst reduces by the known procedure, was put into a special reactor and then exposed to the cold plasma obtained in various applying frequency conditions. Each sample of Co-Cr-B catalysts was treated by AC plasma obtained in various applying frequencies separately. In the presence of a plasma-treated catalyst, the hydrolysis reactions complete within shorter time intervals than in the presence of untreated catalysts. In the period of 20 minutes, the best chosen cold plasma-treated Co-Cr-B catalyst produces 785 ml Hydrogen gas whereas the untreated catalyst produced 600 ml in the same hydrolysis reaction conditions. The experimental results show that the frequency of applying the voltage of plasma is very effective on the catalytic activity of catalysts.

Keywords: Cobalt-Chrome-Boride Catalyst, AC Cold Plasma, Hydrogen Generation, Sodium Borohydride

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11 - 15 October 2017 Sarajevo

VIBRATIONAL SPECTRA AND ASSIGNMENTS OF STRAINED CYCLIC ALLENES INVESTIGATED BY THEORETICAL METHODS

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Abstract:

Recently, strained cyclic allenes have been received considerable interest by organic and computational chemists. Their synthesis and trapping is quite difficult. Due to that, our knowledge about the cyclic allenes are based on the results of computational methods developed in recent years besides the experimental studies. The geometries of studied molecules were prepared by Gauss View 3.0 computer program. The theoretical calculations have been done by using GAUSSIAN03W computer program. At start, the results of DFT, ab-initio and semiempirical methods were compared with the experimental results. Especially, it was found that both geometrical results and vibrational results given by B3PW91/cc-pVTZ method are consistent with the experimental results, whereas the only geometrical results given by HF/6-311+G(d,p) are consistent with the experimental ones. Later, the vibrational frequencies of 1,2-cyclobutadien, 1,2-cyclopentadien, 1,2-cyclohexadien, 1,2-cycloheptadien, 1,2-cyclooctadien, 1,2-cyclononadien cyclic allenes were calculated by using B3PW91/cc-pVTZ methods. Especially, the values of C=C=C symmetrical strecthing frequencies for these molecules were found to be 1322, 1436, 1434, 1441, 1449, 1452 cm^{-1}, respectively. When examined these values, the value of C=C=C symmetrical strecting vibrational frequency increases as the ring size incorporated by the allene unit increases.

Keywords: Allene, Strain, Reactive Intermediate, Computational Organic Chemistry, DFT, Ab-Initio, Semiemprical Methods, IR Spectroscopy

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THE EFFECT OF COLD PLASMA OBTAINED IN VARIOUS PARAMETERS, ON THE ELECTROCHEMICAL ACTIVITY OF Co-B BASED CATALYSTS

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Abstract:

In this study, the effect of Alternating Current cold plasma obtained in various applying voltages or various frequency parameters, on the catalytic activity of Co-B based catalysts reduced from $CoCl_2.6H_2O$ is examined. Co-B catalyst reduces by the known procedure, was put into a special reactor and then exposed to the cold plasma obtained in various conditions. The catalytic activity of Co-B catalysts was measured by the way of hydrogen generation volume from hydrolysis of the NaBH4 method. The catalysts were treated by AC plasma obtained in various applying voltages and different frequencies separately. In the presence of a plasma-treated catalyst, the hydrolysis reactions complete within shorter time intervals than in the presence of untreated catalysts. Paying attention to the period of 20 minutes, the best chosen cold plasma-treated Co-B catalyst produces 700 ml Hydrogen gas whereas the untreated catalyst produced 575 ml in the same hydrolysis reaction conditions. The experimental results show that plasma applying voltage and frequency of applying voltage are very effective on the catalytic activity of catalysts.

Keywords: Cobalt-Boride Catalyst, Cold Plasma, Hydrogen Generation, Sodium Borohydride

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THE USE OF Ni-Cr-B CATALYST IN THE HYDROLYSIS OF SODIUM BOROHYDRIDE AND DETERMINATION OF ITS KINETICS

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Abstract:

In this study Ni-Cr-B catalyst was synthesized for using in the hydrolysis of sodium borohydride. It was determined that the mole fraction of the Ni-Cr-B catalyst determined in this study was 0.95. Catalytic activity was found to increase as the amount of Cr in the catalyst decreased. The characterization of the synthesized catalyst was determined by SEM, EDX, XRD, BET and FTIR devices. In the sodium borohydride hydrolysis experiments, the effects of sodium hydroxide amount, sodium borohydride amount, catalyst amount and temperature parameters were investigated. The catalyst was found to be more effective in the presence of 1% NaOH. It has been found that as the amount of sodium borohydride increases, the rate of starting hydrogen production decreases and also decreases with increasing amount of catalyst. It has been determined that the hydrogen initial production rate increases greatly with the increase of the temperature. The rate of hydrolysis reaction of sodium borohydride carried out in the presence of Ni-Cr-B catalyst was determined to be 0.35. Likewise, by using the reaction rate constants at different temperatures, it was determined that the activation energy calculated by Arhenius equation is 55 kJ.mol^{-1}. As a result, optimum production conditions have been determined for a new catalyst to be used for the hydrolysis of sodium borohydride.

Keywords: Ni-Cr-B Catalyst, Sodium Borohydride, Hydrolysis, Kinetics

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SYNTHESIS AND CHARACTERIZATIONS OF PURE AND LA-DOPED CDS NANOPARTICLES

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Abstract:

Successive ionic layer adsorption and reaction (SILAR) technique was used to synthesize pure and La doped CdS nanoparticles (NPs) onto glass substrates. The structural, optical and morphological properties were examined by x-ray diffraction (XRD), ultraviolet visible (UV-Vis) spectroscopy and scanning electron microscopy, respectively. In addition to these characterization measurements, photovoltaic properties of NPs were investigated. The solar cell efficiency of NPs were compared each other. Consequently, it was observed that both pure and La doped CdS NPs can be used as promising materials for solar cell devices.

Keywords: Nanoparticles, La Doped Cds, Photovoltaic And Silar

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SYNTHESIS, CARECTERIZATION AND CATALYTIC APPLICATION OF TWO DIFFERENT PD-PEPPSI COMPLEXES

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Abstract:

Pd-NHC complex systems show high catalytic activity especially in C-C and C-heteroatom coupling reactions such as Heck-Mizoraki, Kumada, Negishi, Suzuki-Miyaura, Sonogashira [1]. The first work for NHC-palladium PEPPSI complex (Pyridine-Enhanced Precatalyst Preparation Stabilization and Initiation) was developed by Organ et al. which palladium is bound to an NHC with two halogen atoms and is easy to liable pridyne ligand.[2].

Suzuki-Miyaura cross-coupling reaction is mostly used to synthesize substituted biphenyls and polyolefins and can be described as a coupling of boronic acid derivatives with mesylate, halide or triflate using a palladium catalyst in the presence of a base [3].

In this work, new NHC-palladium pyridine (Pd-PEPPSI) complexes that contained two different benzimidazole derivative ligands were synthesized. The structures of these synthesized complexes were analyzed by spectroscopic methods and the complexes were used as catalysts in Suzuki-Miyaura Cross-Coupling Reaction. It has been observed that Pd-PEPPSI complexes that provided 100 % yield efficiency are active catalysts in Suzuki-Miyaura cross-coupling reaction.

RESOURCES:

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Keywords: N-Heterocyclic Carbene, Benzimidazole, Cross-Coupling Reaction, Peppsi

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SYNTHESIS AND CATALYTIC ACTIVITY OF SUPPORTED Ni (II) SCHIFF BASE COMPLEX IN NABH4 HYDROLYSIS

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Abstract:

Chemical hydrides have received much attention as potential hydrogen storage materials because of their high hydrogen capacities. Among chemical hydrides, sodium borohydride ($NaBH_4$) is given a big attention, due to its 10.8% theoretical hydrogen storage capacity, stable in alkaline solution, non-flammable, non-toxic in nature [1].

Schlesinger et al. made a detailed study on the hydrolysis reaction of $NaBH_4$ for hydrogen generation [2]. Catalyst plays a so important role in increasing the generation rate of hydrogen. Ni, Co based catalysts and noble metals are common catalysts for the hydrogen pro-duction from $NaBH_4$.

In this research, we used the Schiff base-Ni complex which we previously synthesized [3] to support on Eupergit C polymer and it was used as a catalyst for H_2 production from $NaBH_4$ hydrolysis. Polymer-Ni catalyzed $NaBH_4$ hydrolysis reaction was investigated depending on some parameters, like concentration of $NaBH_4$, NaOH, temperature, amount of catalyst. In addition the catalyst and products were characterized with some analysis technique.

As a result of this work, it observed that polymer supported Ni (II) complex catalyst has a high activity with 7200 mL H_2. g^{-1} cat..min^{-1} maximum reaction rate and 26200 j.mol^{-1} activation energy in $NaBH_4$ hydrolysis reaction.

RESOURCES:

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Keywords: Catalysis, Schiff Base, Complex, Hydrolysis

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EFFECT OF CHROMIUM ON THE PROPERTIES OF CADMIUM SULFIDE QUANTUM DOTS

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Abstract:

Un-doped CdS and Cr doped CdS quantum dots (QDs) have been prepared by the co-precipitation method at room temperature using the mercaptoethanol as a capping agent. I-V measurements were carried out for Cr doped CdS QDs for the first time in this study, showed that Cr doped CdS QDs can be utilized as sensitizers to improve the performance of solar cells. In addition to the photovoltaic properties; structural, optical, and magnetic properties of Cr doped CdS QDs have been investigated. Study (XRD) on the structural properties showed that CdS and Cr doped CdS QDs have cubic (zinc blende) structure and the particle size of Cr doped CdS QDs becomes smaller than un-doped CdS QDs. Optical absorption revealed that the absorption Cr doped CdS QDs are blue shifted compare to un-doped CdS QDs. The M-H measurements indicated that unlike un-doped CdS QDs, Cr doped CdS QDs show ferromagnetic behavior at room temperature. Consequently, the results indicate that Cr doped CdS QDs can be suitable material for photovoltaic and spintronic applications.

Keywords: Doped Semiconductors, Quantum Dots, Photovoltaic Properties

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EFFECT OF MANGANESE ON THE PROPERTIES OF SB2S3

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Abstract:

Mn-doped Sb2S3 thin films have been deposited onto glass substrates by chemical bath deposition (CBD) tecnique. 5 wt% of Mn was used as a dopant. The experiment was carried out at room temperature. The synthesized thin films were annelead at 350°C under N_2 for 1 hour. The structural, optical and photovoltaic properties of annealed Mn- doped Sb2S3 were characterized, respectively. The obtained data show that the annealed Mn- doped Sb2S3 thin films can be used as promosing materials to enhance the efficiency of solar cell devices.

Keywords: Mn Doped Sb2S3 Thin Films, Chemical Bath Deposition Method, Solar Cell Efficiency

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INVESTIGATION ON THE MALACHITE GREEN ADSORPTION WITH PLASMA TREATED BENTONITE ADSORBENT

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Abstract:

Environmental pollution is one of the most important problems affecting human health today. As a result of industrial processes, pollutants are becoming more complicated and threaten human health. In today's industry, waste water is generated as a result of the production process and these are discharged to the receiving environment through a series of treatment processes. Environmental scientists and engineers are continuously conducting studies to develop the most appropriate processes for the treatment of wastewater. The most economical and practical ones are adsorption. The most used adsorbent active carbon in adsorption, but the price of active carbon is quite expensive. For this reason, researchers have tried to find adsorbents that are cheap, natural and economical. For this purpose, bentonite clay with large amounts of reserves in our country can be used as adsorbents. On the other hand, the adsorption capacities of the materials such as dyes and heavy metal are at a certain level. One of the methods used for increasing the adsorption capacities is surface modification of the material used. One of the most recent surface modification methods is the cold plasma method. In this study, plasma treated bentonite clay was used as adsorbent. In the study, 80% plasma power, N_2 plasma gas and 10 minute plasma application time were used for the optimum bentonite adsorbent. The malachite green adsorption on the adsorbent obtained from the plasma treated bentonite clay was investigated as a function of the dye concentration, adsorbent amount and pH. Freundlich and Langmuir isotherms were applied to malachite green adsorption data.

Keywords: Keywords Bentonite, Plasma, Adsorbent, Malachite Green, Adsorption

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REMOVAL OF METHYLENE BLUE DYE WITH PLASMA TREATED SEPIOLITE ADSORBENT

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Abstract:

In our age, industrial wastewater has become an important source of contamination of surface waters as well as urban wastes and sewage waters. "Wastewater" is used for all the waters that are taken in the cities and after the use of the industry. Different methods are applied for the removal of environmental wastewater. One such process is the adsorption process using adsorbents prepared from suitable materials. On the other hand, the adsorption capacities of the materials such as dye and heavy metal are at a certain level. One of the methods used for increasing the adsorption capacities is surface modification of the material used. One of the most recent surface modification methods is the cold plasma method. Because the plasma process requires very small quantities of chemicals, it can replace wet chemical processes. Waste water or chemical waste does not come into play in plasma processes. In this study, plasma treated sepiolite clay was used as adsorbent. In the study, 80% plasma power, CO_2 plasma gas and 10 minute plasma application time were used for the optimum sepiolite adsorbent. The methylene blue adsorption on the adsorbent obtained from the plasma treated sepiolite clay was investigated as a function of the adsorbent amount and pH. Freundlich and Langmuir isotherms were applied to methylene blue adsorption data.

Keywords: Sepiolite, Plasma, Adsorbent, Methylene Blue, Adsorption

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OPTIMIZATION WITH Cr (VI) ACTIVATED CARBON ADSORPTION AND SURFACE RESPONSE METHOD

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Abstract:

In this study, Cr (VI) adsorption was carried out using activated carbon obtained from beech wood. Adsorption process was modeled by Surface Response Method in Design Expert package program and the effects of process time, process temperature and solution initial concentration parameters on adsorption capacity were investigated. It was determined that the Cr (VI) adsorption was consistent with the quadratic model equation and regression equation was obtained. An ANOVA table was constructed with the quadratic model and it was determined that the most effective parameter on the adsorption capacity is the solution initial concentration. It was also found that the adsorption capacity increased with the increase of parameters such as treatment time, treatment temperature and solution initial concentration. Moreover, It was determined that the value of the adsorption capacity obtained from the regression equation is very close to the value determined experimentally.

Keywords: Actived Carbon, Cr (VI) Adsorption, Numerical Modeling, Anova

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INVESTIGATION OF SODIUM BOROHYDRIDE HYDROLYSIS OF Co-Ni-B CATALYST DEVELOPED IN MICROWAVE ENVIRONMENT

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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 Co-Ni-B catalyst was increased in the microwave environment, and the effect of this catalyst on the hydrolysis of sodium borohydride was investigated. The effects of some parameters such as different gases, treatment time, concentrations of $NaBH_4$, concentrations of NaOH, temperatures, microwave power, on the catalytic activity of Co-Ni-B 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 as 0.33 and 38.4 kJ/mol, respectively.

Keywords: Microwave, Sodium Borohydride, Co-Ni-B, Catalyst, Hydrogen Energy.

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PRODUCTION OF LITHIUM TETRABORATE TETRAHYDRATE BY SPRAY DRIER METHOD AND DETERMINATION OF PRODUCTION CONDITIONS

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Abstract:

The crystallization process, which is a surface process, consists of the step of diffusing the substance from the crystal surface in an oversaturated solution and the step of depositing the substance from the surface into the crystal network. Each of these stages is under the influence of different forces and factors. The various impurities present in the solution medium affect the crystal's exterior appearance and particle size distribution as the pH of the medium and the hydrodynamic conditions of the environment in which the crystallization is carried out are affected. It is aimed to determine the industrial production conditions of lithium tetraborate tetrahydrate. Since Lithium Tetraborate Tetrahydrate is prone to oversaturation, the production was carried out using the Spray Dryer system. When the input air temperature of 230°C was used, the product was found to be in the product trihydrate structure in the TG-DTA and boroxide analysis results. When 170°C drying air was used, the obtained structure was determined to be between tetra and trihydrate. On the other hand, it has been determined that it is possible to produce 5% -20% of Lithium Tetraborate Trihydrate using Spray Dryer.

Keywords: Crystallization, Spraydrier, Lithium Tetraborate Tetrahydrate, TG-DTA

Acknowledgement: This work was supported by Turkish Scientific and Technological Research Center (TUBITAK) (No: 108M043)

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EFFECT OF PROCESSING TIME ON HIGH TEMPERATURE CARBONIZATION OF TEA PLANT WASTES

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Abstract:

In this study, carbonization of tea plant wastes, which was done at relatively low temperatures and durations, was carried out at higher temperatures and was examined the effect of the transaction time on the carbonization process. The sample to be carbonized was placed in a crucible with the screw and processed in a muffle type furnace at different temperatures of 400-800°C for 30-2160 minutes. The carbon and sulphur content in the sample treated at 1400 minutes at 800°C was 94.68% and 0.03%, respectively, while the heat value of the same sample was 8823 cal/gr. In the samples subjected to the carbonization process, it was determined that as the temperature increased, the sulphur ratio decreased by 92% in parallel with the increase of the carbon ratio.

Keywords: Tea Plant Waste, Carbonization

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REMOVAL OF WATER FROM RAW BIODIESEL BY SUNFLOWER HULLS

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Abstract:

Following completion of transesterification reaction in the biodiesel production biodiesel is seperated from the glyceride by gravitational settling. Biodiesel is then washed with water in order to remove the impurities such as basic catalyst, excess methanol and soap. But, water content of the biodiesel increases during the washing cycles, which should be removed before using it as a diesel fuel substituent in a diesel engine. Vacuum evaporation of the water content of this crude biodiesel is the most common route applied in the process. This is a time and energy consuming step in the biodiesel production.

In this study, sunflower hulls were used to remove the water content of the raw biodiesel obtained from sunflower oil. Hulls were crushed, separeted by size and mixed with raw biodiesel at specified eperimental conditions. Sunflower hulls (shells) had already some water content as a result of open atmosphere by a ratio of 6.85 %. In order to increase their water adsorbtion capacity sunflower hulls were dried at 100±4°C and atmospheric pressure for different periods ranged from 1 to 3 hours in an ordinary laboratory oven. Dried sunflower hulls behaved as an effective water adsorbant for the raw biodiesel samples. A small amount of the shells (less than 1% (w/w) of hulls was enough to adsorb an important percent of water in the biodiesel. As a result, it is safely suggested that most of the water content of raw biodiesel samples could be removed by using dried sunflower shells as a water adsorbtion agent which makes it suitable for using as a diesel fuel substituent.

Keywords: Biodiesel Washing, Purification, Water Content, Sunflower Hulls

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REMOVAL OF BORON FROM AQUEOUS SOLUTION USING TANNINS FROM TURKISH ACORNS (VALONIA)

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Abstract:

In this study, valex which has natural tannens was produced from Turkish acorns (valonia) by extraction process and adsorption of boron from aqueous solutions onto tannic acid (TR) resin was investigated.

Valonia is obtained from the corn cup of the oak which grows in Asia Minor. The tannins content of valonia is about 35%. Bioadsorbent tannin used in this study was obtained from Artu Chemical-Turkey.

The extraction method used in the production of valex was the classic method. Valonia was firstly broken into small pieces 2-6 mm in size with crasher. The pieces of valonia were then extracted in hot water at 80-90°C. The obtained valonia solution was acidic (pH: 3-3.5). The solution with tannin was mixed with distilled water and centrifuged to remove inert materials. Then, evaporated in vacuum evaporator for more concentrated solution. The solution was feed spray drayer at 190-200°C hot-air temperature and finally, valex was obtained for using on boron removal.

The adsorption experiments were performed by batch equilibration method. Firstly, sorbent was prepared from valex. Then, the stock solution of boron containing 1000 mg/L was prepared and this was used for adsorption experiments. The batch adsorption experiments were carried out by mixing 1 g sorbent with 50 mL of 8 ppm as initial boron concentration. The contents were shaken at 35°C, 24 hours thoroughly using a shaker rotating at a speed of 250 rpm.

The solution was then filtered and the residual boron concentrations were measured using the ICP. The solid phase was also characterized by using FTIR and SEM. The results showed that boron can be removed from aquesous solution by tannins by yield of 88%.

Keywords: Boron Removal, Tannins, Bioadsorbents, Turkish Acorns

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THE USE OF NiPB CATALYST IN THE HYDROLYSIS OF POTASSIUM BOROHYDRIDE

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Abstract:

In this study, the NiPB catalyst synthesized by reduction of $Ni(NO_3)_2.6H_2O$ and NaH_2PO_4 with $NaBH_4$ was used for the hydrolysis of potassium borohydride. When NiPB catalyst was synthesized, the B/P ratio was determined and the best ratio was found as 1/7. The effects of the amount of KOH, the amount of KBH4, the amount of catalyst and the temperature parameters on the hydrolysis of the synthesized catalyst were investigated separately in the studies used in the hydrolysis of potassium borohydride. According to the experimental results obtained, it was determined that the presence of potassium hydroxide at different concentrations in the hydrolysis medium was effective on the hydrolysis and 2.5% of the KOH percentage of the catalyst worked best. According to the results obtained in the behavior of NiPB catalyst in the presence of different potassium borohydride in the solution, it was determined that the reaction rate did not change with the amount of KBH_4 increased, that is, the reaction rate was independent in the concentration. It was determined that the temperature was very effective over the rate of potassium borohydride hydrolysis. The hydrolysis of potassium borohydride in prensence of different quantities of NiPB catalyst, it was determined that the amount of catalyst increased the rate of the reaction, that is, the reaction was catalyst controlled. As a result, it has been determined that the NiPB catalyst can be used in the hydrolysis of sodium borohydrite for fuel cell aplication.

Keywords: KBH4, Catalyst, Hydrolysis

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DFT STUDIES ON EFFECTS AND RING-OPENING MECHANISM OF MONOSILACYCLOPROPYLIDENOIDS

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Abstract:

Density functional theory (DFT) calculations have been carried out for the ring–opening of 1-bromo-1-lithiosiliranes and 2-bromo-2-lithiosiliranes to LiBr complexes of 2-silaallenes and 1-silaallenes, respectively. The solvent effect has been investigated on the models using both implicit (CPCM) and explicit solvation models. The activation energy barriers of the solvated models are found to be little higher than results of gas phase computations. Note the fact that the electron–withdrawing groups impede the reaction, whereas electron–donating substituents lower the barrier to 1–silaallene and 2–silaallene formation. Moreover, the ring opening of dimer is also computed for the ring-opening mechanism with the energy barrier of 3.7 kcal/mol at B3LYP/6-31+G(d,p) level of theory.

Keywords: Silaallene, Silylenoid, DFT, Reactive Intermediate

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EXPERIMENTAL AND COMPUTATIONAL STUDY OF THE VIBRATIONAL SPECTRA OF OXO-THIACROWN ETHERS

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Abstract:

The syntheses of some constructional isomers of thio-oxocrown ethers; B1 (1,4-dithio-12-crown-4), B2 (1,7-dithio-12-crown-4), under mild conditions, were reported in detail. The synthesized ligands were fully characterized by FT-IR, 1H-NMR and GC-MS spectroscopy. Vibrational assignments and analyses of the fundamental modes of title compounds were performed using the observed FTIR data recorded in the solid phase. The vibrational frequencies determined experimentally are compared with those obtained theoretically from DFT calculations. We also performed DFT calculations to explain their geometrical properties, charges and frontier molecular orbitals.

Keywords: Crown Ether, DFT, FT-IR

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ALL-SOLID-STATE BATTERY MANUFACTURED ON SI WAFER

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Abstract:

The commercial type batteries consist an electrolyte in liquid or gel forms. These type electrolytes create size limitations because of the electrolyte types. A traditional battery of nano dimension cannot be manufactured with these electrolytes. Nowadays, a new type battery has been improved with all-solid-state electrolyte. All-solid-state battery is a new type rechargeable battery system. This type battery is proper for the nano technological application because of the very small size manufacturing. All-solid-state batteries are manufactured with physical vapour deposition system. In this study, an all-solid-state battery on Si Wafer has been deposited by two different physical deposition systems. Si Wafer is widely used in many nano technological applications such as photovoltaic, sensors, LED and etc. These are thermionic vacuum arc (TVA) and RF magnetron sputtering method. These deposition systems work in high vacuum conditions. Electrochemical test and surface imaging results are presented. According to results, nano dimension rechargeable battery is possible with a new type design.

Keywords: All-Solid-State Battery, Si Anode, Afm

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ENERGY AND EXERGY ANALYSES OF ROCK SALT REFINING PLANT

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Abstract:

Thermal intensive processes can be directed to a more efficient use of energy through a better analysis and/or design where existing processes can be improved or new processes can be developed to increase the efficiency of energy consumption, and thus decrease the amount of energy consumed.

Salt (sodium chloride) is mainly produced from rock salt and seawater. Rock salt is mined and refined by dissolving and evaporative crystallization processes. Since a rock salt refining process is highly energy-intensive process, it should be directed to a more efficient use of energy through better process design and analysis, based on accurate exergetic analysis.

This work aims the energy and exergy analyses of the rock salt refining process presently in operation at MED-MAR salt factory in Çankırı, Turkey, to determine the energy and exergy efficiencies with exergy losses for system performance evaluation.

Keywords: Exergy Analysis; Salt Refining, Rock Salt.

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PROCESS SIMULATION OF BIOGAS CHEMICAL LOOPING COMBUSTION

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Abstract:

Chemical Looping Combustion is developed for converting of fuels to energy instead of the conventional combustion processes, both the capture and sequestration of CO_2 from flue gas can be achieved and an efficient combustion can be provided since the CO_2 capture&sequestration operation substantiates inherently in CLC without any energy penalty.

The purpose of this study is to do process simulations of raw biogas and biomethane chemical looping combustion processes. Avarage molar composition of raw biogas as 75% CH_4 and 25% CO_2 was supplied. Simulation model of biomethane combustion process has biogas upgrading unit. Hematite was used as an oxygen carrier. In this regard, the SimSci PRO/II process simulation software was employed as a simulation package for the required parametric studies and to compare energy consumption and production performances of processes.

Keywords: Chemical Looping Combustion, Biogas, Biomethane, Process Simulation

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OPTIMIZATION OF PRODUCTION OF BORIC ACID FROM COLEMANITE ORE WITH SO_2 GAS IN AQUEOUS MEDIUM

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Abstract:

Boric acid can be produced with processes based on the reactions between acids and boron minerals such as colemanite, tincal and ulexite. At the present time, sulphuric acid is used industrially most, although various mineral acids have been used for this purpose.

In this study, firstly, optimum conditions have been determined in dissolution of colemanite with sulphur dioxide in aqueous medium. And then, levels of impurities such as magnesium, calcium, sulphate and sulphite have been investigated in boric acid samples obtained in optimum conditions using a four stages process. A -150 µm ore, containing 81.25% colemanite and 18.75% gangue minerals from Espey, Kütahya,Turkey has been used in experiments in a 1 L-jacketted glass reactor. Chosen parameters are temperature(70-85°C), pH(3.5-4.5) and reaction time(90-150 min). Solid to liquid ratio was kept constant at 115 g/500 mL water, gas flowrate at 225 mL/min and stirring speed at 228 rpm. Optimum conditions have been found to be 4 for pH, 70°C for temperature and 60 min for reaction time. At these conditions, results of a 4-turning study have been evaluated with regard to magnesium, sulphate and sulphite impurities.

As a result, impurity levels of obtained boric acid samples have been found to be 200 ppm for magnesium, 1000 ppm for sulphate and 100 ppm for sulphite. When obtained boric acid is washed with 40 mL water for 40 g boric acid, impurities of magnesium, sulphate and sulphite drop off 20 ppm, 40 ppm an 30 ppm, respectively.

Keywords: Colemanite, Sulphur Dioxide, Impurity, Optimization

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MODIFICATION OF GLASSY CARBON ELECTRODE WITH GRAPHENE DERIVATIVES AND CONDUCTING POLYMER FOR APPLICATION IN ELECTROCHEMICAL BIOSENSORS

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Abstract:

Biosensors have attracted increasing attention due to their advantages including facile production, low cost, portability, short detection time and high selectivity. In order to enhance these properties of biosensors and consequently improve their potential applications, the researchers have been extensively studied different materials. Graphene is a two-dimensional one-atom thick layer of carbon and has been extensively studied material due to its unique electrical, optical and thermal properties [1]. Graphene oxide (GO) is the oxidized form of graphene, which contains some chemically reactive oxygen functionalities. The oxygen-containing groups on surface of GO greatly enhanced the surface ability to bind with other materials. Thus, various materials can be used to modify the GO surface and develop composites for different applications. Conducting polymers (CPs) have received significant attention both from scientists and engineers due to the ability to prepare polymer materials with similar electrical and optical properties to semiconductors or even metals [2]. CPs are also attractive materials for biosensor applications. It is expected that the combination of the excellent properties of GR and conducting polymer in composite structure will enhance their charge transport and electrocatalytic properties for electrochemical biosensor applications. In this study, the glassy carbon electrode was modified with conducting polymer of poly(3,4-ethylenedioxythiophene) and graphene oxide or reduced graphene oxide and then used in electrochemical biosensors for determination of ascorbic acid, uric acid and dopamine.

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Keywords: Graphene, Conducting Polymer, Electrochemical Biosensor

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SYNTHESIS OF THIOPHENE SUBSTITUTED PORPHYRIN DERIVATIVES AND THEIR APPLICATION IN ELECTROCHEMICAL BIOSENSOR

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Abstract:

Porphyrins have been widely studied materials due to their importance in biological systems and for many applications in solar cells, photodynamic therapy, biological electron-transfer systems, catalysis and sensors. Porphyrins and their metal derivatives are very suitable for electron transfer based applications and catalytic applications due to their large aromatic conjugated π-system and unique electrochemical properties. In order to improve their applications, porphyrin have been substituted with a variety of molecules. Among these, substitution with conjugated thiophene derivatives can enhance the conjugation of porphyrin macrocycle and add new functionalities. In this study, thiophene substituted porphyrin derivatives were synthesized and characterized. Then, the synthesized porphyrins were studied with electrochemical methods and their application in electrochemical biosensor was investigated.

-This work was supported by the Mehmet Akif Ersoy University Coordinatorship of Scientific Research Project with the Project number of 0369-NAP-16.

Keywords: Porphyrin, Thiophene, Electrochemical Biosensor

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MEP DIAGRAMS AND SOLVATION FREE ENERGIES OF THE C1-SUBSTITUTED 9-METHYL-BC ALKALOIDS

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Abstract:

Abstract: In order to calculate the quantum chemical parameters and stabilization energies of the βC alkaloids, the geometry optimization and frequency calculations have been performed using DFT with 3 basis sets in both the gas phase and the aqueous phase. It has been determined that as the solvent dielectric constant increases and as the basis set rises, each structure becomes increasingly more stable. In water phase, the solvation free energy changing is calculated as following order: D (10.513)> A (9.374)> C (9.214)> E (9.098)> B (8.564) in kcalmol-1 unit at B3LYP/6-311++G** basis set. It can be said that the stabilization energy ordering agrees with the aromaticity of the substituent group to attach to the C1 position. In according with the calculated electrophilicity index, the most electrophilic structure was the structure B which is quite compatible with the MEP diagrams. Hopefully, the calculated parameters will help to explain the process of action of existing drugs and are expected to provide useful information prior to the synthesis of future new ligands.

Keywords: Beta Carboline Alkaloids, MEP Diagrams, FMO Analysis

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A COMPUTATIONAL STUDY ON THE NOR-HARMAN DERIVATIVES

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Abstract:

βC alkaloids have a wide effect on the central nervous system receptor due to its wide chemical and pharmacological, photochemical properties [1]. Nowadays, these group compounds are being studied more and more in many sciences due to antitumor activities [2]. DFT calculations have been conducted to predict of their stabilization energies in the gas phase and water phase performed with the three basis sets. The calculate solvation free energy of each structure increases as the basis set grows. Also, each structure exhibits a more stable structure in water phase than that of the gas phase. The Solvation free energy decreases as 1> 2> 3 for all basis sets in both the gas phase and water phase because the substituted groups on N9 position is different with each other. As the hydrophobic character of substituted group on position N9 increases the solvation free energy decreases. Some quantum chemical parameters such as electrophilic properties and chemical potentials have been determined as well as solvation energies and these parameters have been used to predict how these compounds will have chemical behavior on electrophilic/ nucleophilic reactions.

Acknowledgments

The authors wish to acknowledge the financial support of the Scientific Research Projects of Cumhuriyet University (Project No: EĞT-066). All calculations have been conducted at TUBITAK ULAKBIM, High Performance and Grid Computing Center (Tr-Grid)

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Keywords: FMO Analysis, Quantum Chemical Descriptors, Chemical Reactivity, Solvent Effect

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CHARACTERIZATION OF BURNING BEHAVIOUR AND STRUCTURAL COMPONENTS OF CORN WASTE

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Abstract:

Corn is one the most important agricultural products of Turkey. Accordingly, great deal of amount of wastes are formed that may be regarded as renewable and sustainable energy source. In order to decide the suitable procedure to take advantage of the energy potential of these huge waste energy source, different options should be properly investigated. From this point of view, burning method will be studied where corn wastes will be used as feedstock. For this purpose, the main macromolecular ingredients of corn waste such as lignin, cellulose, and hemicellulose will be isolated first and then these individual components will be subjected to burning test. That is, after the size of the corn waste was reduced through milling to 250 μm with grinder; hemicellulose, lignin and extractive substances of sample were determined and eliminated. Then, each ingredient as well as the parent sample were heated to 700°C with a heating rate of 40°C/min under dry air atmosphere by using of thermo-gravimetric analyzer. Combustion characteristics of structural components of the samples were investigated.

Keywords: Biomass, Corn, Combustion

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A KINETIC STUDY FOR OLIVE OIL RESIDUE PYROLYSIS: MODEL FREE APPROACHES

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Abstract:

In this study, olive oil residue (OOR) was selected as waste biomass resource to evaluate the thermal and kinetic behaviors during pyrolysis process. Having long coasts along the Aegean and Mediterranean seas, Turkey is rich in olive trees. Annually, about 1 million tonnes of olive is used in olive-oil production and approximately 450,000 tonnes of olive-oil residues are produced. Therefore, utilization of this oil rich residue could be a promising solution for the energy and chemical production. Pyrolysis experiments were carried out from room temperature to 900°C at 5, 10, 20 and 50°C/min heating rates in the presence of nitrogen. The obtained thermal data was used to calculate the kinetic parameters using Coats-Redfern, Friedman, Flylnn-Wall-Ozawa (FWO) and Kissinger-Akahira-Sunose (KAS) methods. Experimental and modelling studies showed that thermal behaviors of olive oil residue can be divided into three main regions which are i) moisture removal, ii) main decomposition of the structure (hemicellulose and cellulose degradation together with the start of the lignin degradation) iii) lignin decomposition.

Keywords: Pyrolysis, Biomass, Olive Oil Residue, Kinetic Analysis

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PANI-BASED HYDROGEL FOR GLUCOSE SENSING

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Abstract:

Biosensors have recently attracted much interest due to provide rapid and continuous measurement, high specificity, fast response time and ability to measure non-polar molecules that cannot be estimated by other conventional devices. They are commonly used in environmental monitoring, food freshness, bioprocess monitoring and especially the estimation of glucose, urea, cholesterol and lactate in whole blood. In this context, conducting polymers have emerged as a potential candidate for using as a transducer in biological sensors, since they have a lot of unique and attractive features such as availability of varied range of monomer types, cost effectiveness, strong biomolecular interactions, low detection limits and enhanced sensitivity.

The production of biocompatible, pH-sensitive conductive polymer which could be used in biosensor applications was aimed in this study. For this purpose, firstly photopolymerizable chitosan-grafted-glycidyl methacrylate (CTS-g-GMA) was obtained by grafting of glycidyl methacrylate onto the chitosan backbone. Following that, CTS-g-GMA was photopolymerized with poly(ethylene glycol)diacrylate (PEGDA) under the UV light. Aniline monomer was absorbed into the crosslinked polymeric network obtained in photopolymerization step. Then, it was transformed into conductive polyaniline (PANI) by using a proper initiator.

Obtained PANI-based biocompatible conductive polymer was characterized by FT-IR and SEM analysis. Thermal behavior and conductivity of the polymer were determined by TGA and four-point probe technique, respectively. Additionally, the produced polymer was tested within the scope of glucose sensitivity.

All the results showed that the production of PANI-based conductive polymer which could be used especially in glucose sensing applications was carried out successfully.

Keywords: Biosensor, Chitosan, Polyaniline, Conductive Hydrogel

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INVESITIGATION OF THE BIOSORPTION CONDITIONS REMAZOL BRILLIANT BLUE R DYESTUFF BY WASTE BIOMASS OF ARTICHOKE LEAVES

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Abstract:

Environmental problems and study of the solve these problems are rapidly increasing in everyday. Biosorption, a method for the purifications of the water contains organic and inorganic contaminations, is most important research subject. Biosprtion methods have a potential for the cleaning pollutant with efficiency on many pollutants. Biosorption method is effective, low-cost and harmless Uses of biosorbents are increasing. In this study, artichoke leafs used as a biosorbent material in removal of the pigments of the Remazol Brilliant Blue R in the wastewater. Artichoke is herbal and it grows in Mediterranean and Europe. Commercial artichoke outer leafs were used as biosorbent after the dried and milling of its. Optimization process of the removals of the Remazol Brilliant Blue R pigments were done. The results demonstrated that the used waste biomass of artichoke leaves was a low cost promising sorbent for the removal of Remazol Brilliant Blue R dyestuff wastewater.

This research activity was supported by Bilecik Şeyh Edebali Üniversity scientific research commission (grant number is 2016-01-BŞEÜ.04-06)

Keywords: Biosorption, Artichoke Leaves, Remazol Brilliant Blue R

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CORROSION PROTECTION OF STEEL BY ELECTRODEPOSITED POLY(N-METHYL CARBAZOLE) FILMS

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Abstract:

Poly(N-methyl carbazole) films were electrodeposited on 304 stainless steel electrode by electropolymerization of N-methyl carbazole monomer in tetrabutyl ammonium perchlorate containing acetonitrile solution using cyclic voltammetry technique. Poly(N-methyl carbazole) films were characterized by attenuated total reflectance-fourier transform infrared spectroscopy, scanning electron microscopy, thickness, conductivity and contact angle measurements. Corrosion performances of the uncoated and polymer coated stainless steel electrodes were evaluated in 1 M sulfuric acid solution using open circuit potential-time curves, potentiodynamic polarization and electrochemical impedance spectroscopy techniques. Poly(N-methyl carbazole) films were found to provide anodic protection to the stainless steel substrate and significantly reduce the corrosion rate of stainless steel in highly acidic corrosive test solution.

Keywords: Electropolymerization, Corrosion

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SYNTHESIS AND CATALYTIC PROPERTIES OF SCHIFF BASE CONTAINING METHYL 2-AMINO-5,5,7,7-TETRAMETHYL-4,5,6,7-TETRAHYDROBENZO[B]THIOPHENE-3-CARBOXYLATE AND ITS Pd(II) AND Ru(II) COMPLEXES

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Abstract:

Schiff bases derived from substituted salicylaldehydes and various amines and their metal complexes have been widely investigated because of their wide applicability. The large impact of the use of Schiff base ligands in metal complexes is evident from their utility in various catalytic reactions such as, hydrogenation of olefins and carbonyl groups, transfer of an amino group, photochromic properties, complexing ability towards some toxic metals, etc.. The work include the synthesis, spectroscopic characterization and as well as catalytic activities of Ru(II), and Pd(II) complexes with a novel Schiff base ligand derived from methyl 2-amino-5,5,7,7-tetramethyl-4,5,6,7-tetrahydrobenzo[b]thiophene-3-carboxylate and salicylaldehyde. Spectroscopic techniques including IR, UV–Vis, NMR, and mass analysis as well as elemental analysis and measurement were used to identify the products. In conclusion, based on continuing interest in developing more efficient and stable catalysts, we wanted to examine whether we could influence the catalytic activity of ruthenium complex for the transfer hydrogenation of ketones and we wanted to evaluate palladium complex under various conditions in Heck and Suzuki C-C crosslinking reactions of aryl and heteroaryl bromides with arylboronic acids.

Keywords: Catalysis, Pd(II) And Ru(II) Complexes, Carboxylate, Spectroscopic Techniques.

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H_2O_2 SENSING WITH A SELF IMMOLATIVE CHEMILUMINESCENT PROBE

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Abstract:

Hydrogen peroxide (H_2O_2) is widely used in various commercial, industrial, medical, environmental and personal hygiene applications. Very small quantities of Hydrogen peroxide, which is a colorless liquid at room temperature, exist as gaseous form in air. H_2O_2 is a strong oxidizing agent and it may cause burning when combined with organic compounds. The most industrial consumption of H_2O_2 is in the textile and paper industries as a bleaching agent. Moreover, it is widely used in water and wastewater treatment with ozone and UV light. In addition to these uses, hydrogen peroxide also plays a significant role in many biological processes. As a relatively mild reactive oxygen species (ROS), H_2O_2 is recognized as a messenger molecule in various signaling processes therewithal it is also included in many biological processes like biosynthesis, immune response and cell signaling. Additionally, in many enzymatic reactions, H_2O_2 is also produced as a byproduct. On the other hand, like other reactive oxygen species, excessive production of H_2O_2 can cause oxidative stress which brings about the development of many diseases such as Alzheimer's disease, Parkinson's disease, cardiovascular disease and Huntington's disease.

Herein, we designed and synthesized 1,2-dioxetane based self immolative chemiluminogenic probe for H_2O_2 detection. We wanted to incorporate a self immolative linker to trigger two chemiluminescence processes at the same time, in response to single H_2O_2 mediated deprotection event. Self-immolation of the probe was initiated with the deprotection of the boronate ester group leading to light emission. Our 1,2-dioxetane based probe has fulfilled the H_2O_2 detection in a highly selective manner. We believe that this study is likely to provide new insights into the development of chemiluminescence based H_2O_2 sensors and bright chemiluminescence of this probe or structurally related derivatives could provide a promising alternative.

Keywords: Hydrogen Peroxide, 1,2-Dioxetanes, Chemosensors, Chemiluminescence

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ESSENTİAL OILS OF YARROW (ACHILLEA) THAT WERE OBTAİNED USİNG MİCROWAVE EXTRACTION METHOD, DETERMINATION OF ANTIOXIDANT ACTIVITY

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Abstract:

In this study, the endemic yarrow plants (Achillea setacea) that grow naturally in the Sivas ecological conditions and endemic to the province of Sivas was used as material. Essential oil was obtained by microwave extraction method from plants collected from natural areas. The experiments were carried out in completely randomized design with three replications. Antioxidant activities using DPPH radical scavenging and β-caroten/Linoleic acid method of obtained yarrow essential oils were investigated. According to the obtained data, it has been determined that essential oils has significant antioxidant activity.

Keywords: Antimicrobial, Antioxidant, Essential Oil, Achilla Setace

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SOLID-LIQUID EQUILIBRIA (SLE) OF TERNARY SYSTEM $NaCl+Zn(H_2PO_2)_2+H_2O$ AT T=(313.15 AND 333.15 K)

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Abstract:

Phase diagrams have beneficial method for separating salts and production of important chemicals. According to thermodynamic equilibrium studies Van't Hoff was the first to report a stable phase diagram at 293.15 K via using the isothermal method.

Hypophosphite salts have been using in many applications such as hydrogen and anticorrosive commercial paint production.

In this study, the temperature dependence of simultaneous solubilities of $Zn(H_2PO_2)_2$, which has a vast of application areas, and NaCl were investigated.

Solubility of binary systems were determined 22.22% mass $Zn(H_2PO_2)_2$ and 27.25% mass NaCl at 313.15 K. The invariant point of these system is analyzed as 23.66% mass NaCl, 28.89% mass $Zn(H_2PO_2)_2$ and 47.45% mass H_2O. It is determined that NaCl and $Zn(H_2PO_2)2.H_2O$ in equilibrium with liquid phase.

Solubility of binary systems were determined 27.23% mass $Zn(H_2PO_2)_2$ and 27.04% mass NaCl at 333.15 K. The invariant point of these system is analyzed as 23.34% mass NaCl, 42.6% mass $Zn(H_2PO_2)_2$ and 34.06% mass H_2O. It is determined that NaCl and $Zn(H_2PO_2)2.H_2O$ in equilibrium with liquid phase.

Table and graphics were created using experimental data.

The results indicated that the solubility of $Zn(H_2PO_2)_2$ increased from 22.20% up to 28.89% at 313.15 K, while the solubility of NaCl decreased from 27.25% to 23.26% at the same conditions. The changings in the solubility of both salts at 333.15 K were as followings: 27.23-42.60% for $Zn(H_2PO_2)_2$; 27.04-23.34% for NaCl.

The solubility of $Zn(H_2PO_2)_2$ increased with the increase in the temperature, when the solubility of NaCl remained almost stable. This findings supports the fact that NaCl has a salting-on effect on the solubility of $Zn(H_2PO_2)_2$.

Keywords: $Zn(H_2PO_2)_2$, Phase Diagram, Solid-Liquid Equilibria, Ternary System

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SOLUBILITY BEHAVIOR OF Na^+, Zn^{2+}/ H_2PO_2-//H_2O TERNARY SYSTEM AT DIFFERENT TEMPERATURES

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Abstract:

Metal hypophosphites have been gaining importance among the inorganic compounds due to their some useful properties. The hypoposphites have been using in a various application areas such as in some chemical process being as reducing agent, anti-corrosive, flame retardant etc.

The most important demand in industry and recycling systems is to achieve the process under optimal conditions and economically.

In this study, a process based on physicochemical methods has been proposed for the production and recycling of sodium and zinc hypophosphites.

Solubility of binary systems were determined 22.22% mass $Zn(H_2PO_2)_2$ and 57.03% mass NaH_2PO_2 at 313.15 K. The invariant point of these system is analyzed as 56.8% mass NaH2PO2, 1.62% mass $Zn(H_2PO_2)_2$ and 41.58% mass H_2O. It is determined that $NaH_2PO_2.H_2O$ and $Zn(H_2PO_2)2.H_2O$ in equilibrium with liquid phase.

Solubility of binary systems were determined 27.23% mass $Zn(H_2PO_2)_2$ and 61.13 % mass NaH_2PO_2 at 333.15 K. The invariant point of these system is analyzed as 37.94% mass NaH_2PO_2, 7.05% mass $Zn(H_2PO_2)_2$ and 55.01% mass H_2O. It is determined that $NaH_2PO_2.H_2O$ and $Zn(H_2PO_2)_2$ in equilibrium with liquid phase.

Table and graphics were created using experimental data.

The results revealed that when the solubility of $Zn(H_2PO_2)_2$ at 313.15 K decreased from 22.20% to the value of 1.62%, that of NaH_2PO_2 was decreased from 57.03% to 56.80%. The solubilities of $Zn(H_2PO_2)_2$ and NaH_2PO_2 at 333.15 K were decreased from 27.23% to 7.05%, and from 61.13% to 37.94% (the latter values are near the invariant points), respectively. Also the solubility of both salts has increased almost evenly with the temperature. As can be seen from the invariant point data at both temperatures, NaH_2PO_2 has a salting-out effect on $Zn(H_2PO_2)_2$.

Keywords: $Zn(H_2PO_2)_2$, Phase Diagram, Solid-Liquid Equilibria, Ternary System, NaH_2PO_2

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DETERMINATION OF CAROTENOIDS IN TWO ALGAE SPECIES FROM THE SALINE WATER OF KAPULUKAYA RESERVOIR BY HPLC

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Abstract:

Two local algae species, Chlorella sp., and Scenedesmus sp. Chlamydomonas sp. from a highly saline water body (Kapulukaya Reservoir) were isolated to analyze their carotenoid composition and content using HPLC method. The gradient solvent system of methanol–acetonitrile–water (84:14:2, v/v/v) and methylene chloride (100%), used for the extraction of carotenoids from the saponified cells, proved an acceptable separation as inferred from the retention factor (k) ranging between 0.75-7.76 and the separation factor (α) values greater than 1 detected. Resolution peaks assigned to carotenoids, 21 for Chlorella sp. extract and 22 for of Scenedesmus sp. extract were reached within the duration time of 45 min. Main carotenoids tentatively or positively identified were all-trans-lutein, 9-or 9'-cis-lutein, 13-or 13'-cis-lutein, cis-lutein, all-trans-α-Carotene, 9-or 9'-cis-α-Carotene, all-trans-β-Carotene, 9-or 9'-cis-β-carotene in both species except for all- trans-β-cryptoxanthin found only in Scenedesmus sp. Auroxanthin neochrome neoxanthin and cis-neoxanthin were commonly identified as epoxy-containing compounds. Quantitatively, Chlorella sp. was distinguished to have a greater amount of lutein and cis-isomers (2.74 mg/g), 77.89 % while Scenedesmus sp. were predominated by β-carotene and cis isomers as the major component being 80.72 % (5.76 mg/g) in total carotenoids (TC). In terms of total carotenoids, the species were considered to be efficient sources for further practical applications.

Keywords: Microalgae, Chlorella Sp., Scenedesmus Sp., Carotenoids, Hplc

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TWO PRONOUNCED CHLORELLA SPECIES FOR NEUTRAL LIPID AND CARBOHYDRATE PRODUCTION

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Abstract:

Microalgal lipids and carbohydrates are of broad interest in biotechnology world. The genus Chlorella holds several characterized and undefined specimens that have distinct features to be exploited for primer metabolite production. In this study, two Chlorella species isolated from a volcanic lake, Lake Narligöl (38°20'50"N 34°29'28"E) located in Ciftlik Province of Turkey, were evaluated for triacylglycerol and carbohydrate productions. The strains were identified based on morphological characteristics and genomic information and named as Chlorella vulgaris IMU12 and Chlorella vulgaris IMU17. Chlorella strains were grown in controlled and N-lacking 200ml Bold's Basal medium in 500ml flasks under the continuous light intensity of 250 µE/(m^2/s) in a temperature-controlled orbital shaker with a 120 rpm speed under 22°C temperature during 15 days of incubation period. A rapid decrease in growth was accompanied by decreased chlorophyll and protein contents in both strains. Increased carotenoid, neutral lipid and carbohydrate contents were also a similar response of both strains to nitrogen deprivation. However, as suggested by fluorescence and FT-IR measurements, increase in triacylglycerol content was most pronounced in C. vulgaris IMU12 while that was the case for increased carbohydrate production in C. vulgaris IMU17.

Keywords: Chlorella, Biodiesel, Triacylglycerol, Microalgal Carbohydrate

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MICROWAVE ASSISTED SYNTHESIS AND CHARACTERIZATION OF BENZO-THIO CROWN ETHERS

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Abstract:

Macrocyclic crowns containing sulphur, nitrogen atoms and aromatic ring demonstrate extraordinary selectivity properties with cations. Interior sides of these type of compounds have a hydrophilic interior cavity from electronegative atoms. Also outer parts have a flexible skeleton from nonpolar hydrophobic groups. Because of these cavity properties, crown ethers form complex with some of cations and neutral compounds. Additionally, oxacrown ethers to alkali metals, thiocrown ethers to heavy and precious metals are known to be interested [1-5].

New benzo thio crowns (U1-U7) were prepared from the corresponding 2,2'-dithiodibenzoyl chloride and dithiols-diols under reflux conditions (conventional heating) and microwave (MW) irradiation. In the reactions pyridine was used as a catalyst and high dilution was used as a method. These reaction routes were used for the synthesis of a series of benzo thio crown ethers. The synthesis of benzo-thio crown ethers under MW irradiation in comparison with conventional heating has some superior advantages. Microwave assisted synthesis has shorter reaction times, simpler reaction conditions, higher yields, and low rate of by-product.

After purification all synthesized compounds were characterized by FT-IR, 1H-NMR, 13C-NMR, LC-MS, and elemental analysis methods [6].

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This study was supported by Balikesir University Scientific Research Projects Unit (BAP) and presented as a master thesis at Balikesir University in Turkey.

Keywords: Thio-Crown Ether, Microwave-Assisted Synthesis, Oxa-Crown Ether, Selectivity Factor, Liquid-Liquid Ion Pair Metal Extraction

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EXPERIMENTAL AND THEORETICAL STUDIES ON THE FT-IR SPECTRA FOR BENZO-THIO CROWN ETHERS

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Abstract:

In this study two samples of original benzo thio and benzo oxa crown ethers were synthesized as described before and FT-IR spectra are investigated. Infrared spectrums show that these smallest rigid macrocyclic crowns are synthesized. While synthesizing benzo thio crown eter and benzo oxa crown ether, 1,2-mercaptoethanol's –S-H bonds were disappeared as similar as ethylene glycol's –O-H bonds. Furthermore, 2,2'-dithiodibenzoic acid dichloride has a –C(O)-Cl bond and after esterification this bond disappears. We also report the FT-IR spectra of some free benzo- thiacrown ethers with the help of theoretical methods. To predict in what conformation exist, for the vibrational analysis of both molecules and to assess the performance of the different computational methods for the accurate prediction of the vibrational frequencies of relatively large molecules, the computations have been done using the harmonic and anharmonic force fields using the 6-31+G(d) basis set and at the HF and B3LYP levels.

Keywords: Thio-Crown Ether, Oxa-Crown Ether, Liquid-Liquid Ion Pair Metal Extraction, Physical Organic Chemistry

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EFFECT OF ADDITIVES ON META-STABLE ZONE WIDTH FOR BORIC ACID CRYSTALLIZATION

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Abstract:

In this work, meta-stable zone has been investigated for boric acid crystallization at 20°C, 30°C, 40°C and 60°C by using different cooling rates and using some additives: calcium nitrate, magnesium chloride and sulfuric acid. Boric acid production is commonly uses precipitation from some boron minerals by crystallization. In these crystallization processes, meta-stable zone width was very important role because of processes often have gone through in the meta-stable zone. Processes have different crystallization temperatures in the present of different ions. These ions also find in the boric acid crystallization processes. In this work, calcium, magnesium and sulfate ions have used between 150-1800 ppm; 2000-12000 ppm and 5000-30000 ppm respectively. Effect of calcium, magnesium and sulfate ions at crystallization temperature has been found between in these limits.

Keywords: Crystallization, Meta-Stable Zone, Boric Acid, Additives

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INHIBITION EFFECT OF POMEGRANATE EXTRACT ON CALCIUM CARBONATE CRYSTALLIZATION

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Abstract:

In the processes, calcium carbonate ($CaCO_3$) has found in scale formation on heat exchanger pipes in evaporators. Cleaning processes in exchanger are expensive and hard. On the other hand, process must be stop when cleaning and maintenance. Therefore, production costs rise up. For this reason, inhibition of forming $CaCO_3$ crystal is very important. There are many ways to inhibition of crystallization. One of these ways is additives. Some additives are produced in laboratory, synthetic while others are natural. It is important to search for cheap and effective additives. Pomegranate fruit is produced and consumed much in Mediterranian Region. In this work, inhibition effect of pomegranate extract has been investigated by using Taguchi experimental design for $CaCO_3$ crystallization. Experiments have been carried out at 20°C, 25°C, and 30°C by using different amounts of pomegranate extract. Three type of pomegranate extract have been used: freshly squeezed, waited for one week, and commercial. It has been found that pomegranate extract is effective in hindering $CaCO_3$ crystal formation.

Keywords: Crystallization, Inhibition, Calcium Carbonate, Pomegranate

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FACILE SYNTHESIS OF SOPHISTICATED COMPOUNDS

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Abstract:

Syntheses can be classified as simple salts, nanomaterials, organic simple compounds, heterocyclic compounds, macrocyclic compounds and coordination compounds. The desired synthesis for all these classes is to be easy and cheap to obtained. There are important considerations that facilitate synthesis. These are: 1. kinetic and thermodynamically appropriate design. 2. caught of optimum conditions. 3. Synthesis tools used. Proper use of time and energy in synthesis is also a necessary criterion for success. When the appropriate conditions for synthesis are obtained, macrocyclic compounds such as phthalocyanine, porphyrin and complex compounds can be easily synthesized. In summary, the synthetic method have to be facile, fast, low reaction temperature, environmental friendly, and easy controlled preparation condition[1-2].

Easy synthesis serves less business and a lot of profit.

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Keywords: Keywords: Facile Synthesis, Appropriate Technique, Fast, Environmental Friendly

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SYNTHESIS TECHNIQUES CHANING DUE TO NANOCHEMISTRY AND TECHNOLOGY

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Abstract:

Organic and inorganic syntheses traditionally used in chemistry have innovated in classical synthesis methods to accommodate the intelligent materials and nanochemistry needed in today's technology. For normal syntheses, the starting materials are taken and the product is obtained by optimizing the temperature, solvent and ambient conditions in order to reach the synthesis of the desired product. With modern synthesis tools nano, intelligent or hybrid materials are obtained by laser, microwave, optical, thermal plasma, photochemical, photothermic or photothermochemical changes [1]. Analysis tools used in the characterization of synthetic products obtained using classical and modern methods also vary. In modern synthesis, advanced analytical techniques such as SEM, TEM, BFTEM, HRTEM, BET, AFM, OFET, XRD and FESEM analyzes are also used in addition to the NMR, IR, UV, Mass and Micro analysis techniques used in the structure elucidation. Today, computer calculations support synthesis [2]. It may play a more important role in design in the future.

Advances in synthesis methodology in chemical science provide a significant potential to improve the science of chemistry and find more applications.

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Keywords: Synthesis, Technique, Target Product, Classical Method, Modern Method.

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PHOTOCHEMICAL REACTIONS OF METAL CARBONLYS [$M(CO)_6$ (M=Cr, M_o, W), $Mn(CO)_3$ Cp] WITH 4-AMINO-3-HYDRAZINO-5-MERCAPTO-1,2,4-TRIAZOLE (AHMT) AND 3-AMİNO-5-MERCAPTO-1,2,4-TRIAZOLE (AMT)

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Abstract:

Four new complexes of M(CO)5(AHMT) [M= Mo(1), Cr (2), W (3)], and $Mn(CO)_3$ (AHMT) (4), where AHMT is 4-amino-3-hydrazino-5-mercapto-1,2,4-triazole have been synthesized by the photochemical reactions of metal carbonlys $M(CO)_6$ (M= Mo, Cr, W) and $Mn(CO)_3$ Cp with AHMT (1-4). In addition four more new complexes of M(CO)5(AMT) [M= Mo(5), Cr (6), W (7)], and $Mn(CO)_3$ (AHMT) (8), where AMT is 3-amino-5-mercapto-1,2,4-triazole (AMT) have been synthesized by the photochemical reactions of metal carbonlys $M(CO)_6$ (M= Mo, Cr, W) and $Mn(CO)_3$ Cp with AMT (5-8) .The complexes have been characterized by elemental analysis, FT-IR, 1H and 13C- NMR spectroscopy. The spectroscopic studies show that, AHMT complexes (1-3) and AMT complexes (5-7), behave as a monodentate ligand and coordinate via ring NH donor atom to the central metal atom in M(CO)5(AHMT) and M(CO)5(AMT) where M= Mo, Cr, W, and as a tridentate ligand coordinating via imine nitrogen donor atom, amino N donor atom and ring NH donor atom in $Mn(CO)_3$ (AHMT) and $Mn(CO)_3$ (AMT).

Keywords: Metal Carbonyl; Photochemical Reaction; Thiol; 1,2,4-Triazole

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THERMODYNAMIC MODELLING OF HYBRID SOLID OXIDE FUEL CELL AND GAS TURBINE SYSTEM

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Abstract:

Fuel cell-gas turbine systems have a great potential to reach high fuel-to-electricity efficiency from pure hydrogen or any hydrocarbon based fuels. This high efficiency provides energy conservation, low cost energy and low carbon emission. In addition, a fuel cell-gas turbine can also be considered as a sustainable system if biofuels are used. In this research, it will be investigated that hybrid solid oxide fuel cell and gas turbine (SOFC-GT) system by computer simulations (i.e. the help of Cycle Tempo which is a thermodynamic model software developed by Delft University) to obtain enough information before practically using this new high efficiency system as an alternative to conventional power plants. The hybrid system model's assumptions and initial parameters were input based on previous simulations and experimental studies. Model configurations and each operation parameters of the items were designed in order to reach a system have highest fuel-to-electricity efficiency. The system models were performed with steady state for constant electric energy demand. DC/AC converter ratio, compressors, turbines and generator efficiency were also considered in the simulation calculations. The study mainly aims to determine key factors (e.g. temperature, pressure, cycle configurations and items etc.) which limit the efficiency of fuel cell-gas turbine hybrid systems, and to understand the co-generation mechanism between fuel cells and gas turbines.

Keywords: Solid Oxide Fuel Cell; Hybrid Fuel Cell System,

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INVESTIGATION OF ANTIOXIDANT AND ANTIMICROBIAL PROPERTIES OF VERBASCUM THAPSUS

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Abstract:

Verbascum thapsus plant samples used in our study were collected in Mus province. The roots and leaves of the collected plant were dried and water and ethanol extracts were prepared by soxhalet extraction method. The antioxidant and antimicrobial properties of the extracts obtained were studied comparatively for root and leaf.

Antioxidant activities of plant extracts were examined using different in vitro methodologies such as total antioxidant activity, total reducing power, Cuprac method, DPPH• free radical scavenging, ABTS radical scavenging activity. Reduction capacities of leaf tissue for V.thapsus plant are as follows; BHA > V.thapsus (ethanol) > BHT > V.thapsus (water). The order for root tissue is as follows: BHA > BHT > V.thapsus (ethanol) > V.thapsus (water).

According to the study results, we found that the leaf samples had a higher reduction than the root samples and leaf ethanol extract had a higher reduction than standards. (% inhibition was 66,68% for v. Thapsus (ethanol) , 64,02% for BHA and 61,37% for BHT). Also, the ABTS radical scavenging capacity of all our samples is very high and very close to the standards.

The antimicrobial activities of the Verbascum thapsus extracts were determined by the hollow agar method. B. subtilis, S. aureus, B. megaterium, E. aerogenes, E. coli, P. aeroginosa, K. pneumonia, C.albicans, Y. lipolytica and S. cerevisiae was used as test microorganisms. Five antibiotics were used for positive control. V. thapsus root ethanol extract showed the highest antifungal activity against Y. lipolytica while the least activity against S. cereviciae. Leaf ethanol extract showed antifungal activity against Saccharomyces cereviciae while showing the highest antifungal activity against Y. lipolytica and C. albicans. It has been determined that none of the root and leaf ethanol extracts exhibit antibacterial activity.

Keywords: Antioxidant, Antimicrobial, Inhibition, Verbascum Thapsus

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INVESTIGATION OF ANTIOXIDANT ACTIVITIES OF ESKTRAKTS OBTAINED FROM LALLEMANTIA CANESCENS (L.) FISCH. & C.A. MEY. AND LALLEMANTIA PELTATA (L.) FISCH. & C.A. MEY. SPECIES

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Abstract:

There are three species of Lallemantia (Lamiaceae) genus in Turkey. In our work, plant material was collected in Bitlis province. The collected plant samples of Lallemantia canescens (Topajadarbaşı) and Lallemantia peltata (Kalkanbaşı) were dried and extracted with the soxhalat method. The antioxidant activities of the extracts obtained were investigated.

Antioxidant activities of plant extracts were examined using different in vitro methodologies such as total antioxidant activity by ferric thiocyanate, total reducing power by potassium ferricyanide reduction method, reduction capacity of cupric ions (Cu^{2+}) by the Kuprak method, 1,1-diphenyl-2-picryl-hydrazyl (DPPH•) free radical scavenging, 2,2'-azino-bis(3-ethylbenzthiazoline-6-sulfonic acid) (ABTS) radical scavenging activity. Compared with the standard antioxidants BHA, BHT and α-tocopherol, reduction capacities for L.canescens and L. peltata plants are as follows; BHA > L.peltata > BHT > α-tokoferol > L.canescens.

According to the results of the study,% inhibition was 70.77% for BHT, 66.35% for BHT, 62.11% for α-tocopherol and 61.86% for extraction. When we look at the results of ABTS•+ radical scavenging activity, we can say that all of them are close to each other and show very good activity. ABTS radical activities of plants and standards are listed as follows: BHT (%96,16) ≥ α-tocopherol (%96,15) ≥ BHA (%96,04) ≥ L.peltata (%95,86) ≥ L.canescens (%95,50).

Keywords: Lallementia Canescens, Lallamentia Peltata, Antioxidant Activity

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ACTIVATED CARBON PRODUCTION FROM SIIRT PISTACHIO SHELL USING DIFFERENT CHEMICAL ACTIVATING AGENT

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Abstract:

Actived carbon has a highly developed internal surface area and pore structure, and the adsorption capacity of organic and inorganic materials in the liquid phase defines a high group of substances. For this reason, activated carbon has a wide range of applications from industrial water treatment to gas adsorption. The most commonly used activated carbons are in the form of powder, granules and pellets produced by various methods. The price of actived carbon depends on the applied process to provide the desired adsorptive property. The most commonly used raw materials for actived carbon production are botanical originals (biomass) such as wood, coconut shells, and fossil-based materials that are carbonized or degradable (all types of ground coal, lignite). In this study, production conditions of actived carbon obtained by chemical activation using different concentrations (wt) (10%, 20%, 30%, 40%, 50%, 70%, 100%) of Na_2SO_3, KOH H_3PO_4, NaCl compounds from Siirt pistachio shells, was investigated. When producing activated carbon, parameters such as different impregnation times (24, 48, 72, 96 hours) and different temperatures (400, 500, 600, 700ºC) have been tried as well as these mass percentages. . The adsorption capacities, surface area and microstructure properties of the obtained activated carbons were compared with each other. However, this was done in the first place by looking at iodine numbers rather than BET analysis. The highest surface area values for activated carbon from Siirt pistachio shells were found to be 30 minutes carbonized at 600ºC with 24 h impregnation effect in the presence of chemical activators such as 70% Na_2SO_3, 30% NaCl, respectively. The iodine numbers of this activated carbon obtained from Siirt pistachio shell are 1103,63 mg / g, 908,05 mg / g, respectively.

Keywords: Activated Carbon Siirt Pistachio Shell, Number Of Iodine, Surface Area, Porosity

ICACCHE
International Conference on Applications in Chemistry and Chemical Engineering
11 - 15 October 2017 Sarajevo

ACTIVATED CARBON PRODUCTION FROM ACORN SHELL USING DIFFERENT CHEMICAL ACTIVATING AGENT

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Abstract:

Actived carbons are commonly used as adsorbents in separation processes due to their excellent adsorption ability for organic contaminants, which are usually associated with specific surface area, pore volume and porosity. Actived carbon can be obtained from municipal and industrial wastes, natural raw materials, and coal and derived fossil-derived materials. In this study, the outer shell part of the acorn was used as a raw material and was obtained by chemical activation using different concentrations (wt) (10%, 20%, 30%, 40%, 50%, 70%, 100%) of chemical activators (Na_2SO_3, KOH H_3PO_4, NaCl) The production conditions of activated carbon were investigated. In addition to examining the different mass percent parameters, different impregnation times of 24, 48, 72 and 96 hours and different temperature values of 400, 500, 600 and 700ºC have been tried. The activated carbon samples obtained in this study were compared based on adsorption capacities, surface area, microstructure properties. First, only iodine numbers of activated carbon samples are analysed. The highest surface area values for activated carbon from acorn shells were found to be 30 minutes carbonized at 600ºC with 24 h impregnation effect in the presence of chemical activators such as 70% Na_2SO_3, 50% H_3PO_4, respectively. Similary %30 NaCI was reached the highest surface area in the carbonization process with 24 h impregnation effect in 30 min at 400ºC. The iodine numbers of this actived carbon obtained from the acorn shell are 987,23 mg / g, 654,3 mg / g, and 707,81 mg / g, respectively.

Keywords: Activated Carbon, Acorn Shell, Number Of Iodine, Surface Area, Porosity

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11 - 15 October 2017 Sarajevo

CARBON MOLECULAR SIEVE PRODUCTION FROM SIIRT PISTACHIO SHELLS USING $ZnCl_2$

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Abstract:

The rapidly developing industry has been causing the pollutants of different properties to mix with the air, earth and underground water day by day. Greenhouse gas among industrial pollutants has significant role. Most of the greenhouse gases are stem from heavy industry. The aim of this work is to investigate the production of molecular sieves from Siirt Pistachio Shell. The Pistachio shells for the specified particle size were chemically activated with $ZnCl_2$ and then carbonized at different temperatures (400, 500, 600, 700ºC). After characterization of the obtained activated carbon, activated carbons with the highest BET surface area were tried to produce carbon molecular sieves by modifying the surface of benzene vapor at different temperatures (600, 700, 800ºC) and different burning times. The resulting molecular sieves were sent back to the BET analysis to check the porosity and surface area. In addition to the BET analysis, SEM images were also examined. Analyze results showed that porosities varied between 2 and 4 ºA. Similarly surface areas have not been significantly changed by BET analysis. The obtained carbon molecular sieves facilitate the elimination of polluting gases by means of suitable porosity radius. In addition, the carbon molecular sieves produced can also be used in gas purification fields.

Keywords: Siirt Pistachio Shells, Carbon Molecular Sieve, Gas Adsorbtion, Active Carbon

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CARBON MOLECULAR SIEVE PRODUCTION FROM ACORN SHELLS USING $ZnCl_2$

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Abstract:

Purification of substances such as natural gas has great importance in terms of usability. In gas purification processes, carbon molecular sieve plays a significant role. The purpose of this study is to investigate the production of molecular sieve from the acorn shell. The acorn shells for the specified particle size were chemically activated with $ZnCl_2$ and then carbonized at different temperatures (400, 500, 600, 700°C). After characterization of the obtained activated carbon, activated carbons with the highest BET surface area were tried to produce carbon molecular sieves by modifying the surface of benzene vapor at different temperatures (600, 700, 800ºC) and different combustion times. Molecular sieves were resent to the BET analysis to check porosity and surface area. In addition to the BET analysis, SEM images are also analyzed. Analyze results showed that porosities varied between 2 and 4 ºA. Surface areas have not been significantly changed by BET analysis. The obtained carbon molecular sieves can be used for the removal of impurities such as CO_2 in natural gas considering the porosity of the sieves, which is important for the elimination of gases. In order to see the selectivity of applying this carbon molecular sieve produced, applications should be done in gas chromatography. Thus, we can investigate the activity by applying the carbon molecular sieves used in the purification process of the gases.

Keywords: Acorn Shells, Carbon Molecular Sieve, Gas Adsorbtion, Gc

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11 - 15 October 2017 Sarajevo

INVESTIGATION OF KINETICS OF SODIUM BOROHYDRIDE HYDROLYSIS AT DIFFERENT TEMPERATURES

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Abstract:

In this study, the effect of activated carbon supported Co-B catalyst on sodium borohydride hydrolysis at low and high temperatures was investigated and kinetic was determined. We conducted this study because sodium borohydride hydrolysis kinetics are different at low (10-25°C) and high temperatures (30-50°C). Sodium borohydride hydrolysis experiments were carried out at 10, 15, 20, 25, 30, 40 and 50°C using activated carbon supported Co-B catalyst. Sodium borohydride hydrolysis was determined at low temperatures (10-25°C) and both reaction decay order and activation energy were determined as 0.34 and 53.3 kJ*mol^{-1}, respectively. At the same time, kinetics at high temperatures was also determined and the order of decay and the activation energy were found as 0.5145 and 55 kJ*mol^{-1}, respectively. Consequently, sodium borohydride hydrolysis was carried out at low and high temperatures.

Keywords: Hydrolysis, Kinetic, Sodium borohydride

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11 - 15 October 2017 Sarajevo

PREPARİNG La_1-xAxBO$_3$ (A=Fe, Ba; B=Fe, Mn) PEROVSKİTE NANOPARTİCLES BY SOL- GEL FOR MAGNETOCALORİC AND HYPERTHERMİA APPLİCATİONS

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Abstract:

Magnetic refrigeration (MR) at room temperature has emerged as a powerful technology to replace traditional cooling systems, which are mainly based on the compression or decompression of gases. MR depends on the magnetocaloric effect (MCE), which is an intrinsic property of all magnetic materials. Beside these materials, perovskite type are potential candidates for MR applications due to their large entropy-changes, high chemical stability and low cost. It is also contemplated that these perovskite materials may be used for hyperthermia applications. Hyperthermia is used to treat cancer by heating tumors to temperatures in the range of 41-47°C. In this process, heating mediators are injected into a tumor and are then heated by applying an external alternating magnetic field. The magnetic nano-particles have been used to convert radio-frequency electromagnetic energy into heat at the nanoscale. Thus, the magnetic nanoparticles are heated by the Neel–Brown relaxation. The resulting heating often called magnetic fluid hyperthermia (MFH) opens up new perspectives, especially for the destruction of tumor cells.

La_1-xAxBO$_3$ (A=Fe, Ba; B=Fe, Mn) perovskite structures were prepared by Sol-Gel method and their structural, magnetic, magnetocaloric and hyperthermia properties were investigated. The main goal of this study is provide a new perspective about both magnetic hyperthermia mediators and the magnetocaloric materials.

Keywords: Perovskite, Hyperthermia, Magnetocaloric Effect, Sol-Gel

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11 - 15 October 2017 Sarajevo

REMOVAL OF SULFATE ANİONS FROM BORAX SOLUTİON BY PUROLİTE A 400 MB

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Abstract:

Boron compounds have a wide range of usage in industrial areas all over the world. In the production of borax pentahydrate, a boron compound used much, tincal ore is first dissolved with the necessary amount of water or mother liquor containing about 18% $Na_2B_4O_7$ at 90-93°C. Then the saturated borax solution is separated from the undissolved particles by flocculation and filtration. Borax pentahydrate is then crystallized by cooling clear hot borax solution up to transition temperature (60.6–60.8°C) in batch or continuous type crystallizers. One of the most important problems encountered in the production of borax pentahydrate is a wide variety of impurities especially sulphate ions in crystallization solution.

In this study, Purolite A 400 MB, an ion echange resin was used to remove sulphate ions. This resin is a strong base type 1 anion exchange resin with gel polystyrenic matrix specially designed for use in mixed bed systems. and it has high operating capacity, excellent regeneration efficiency and good rinse characteristics.

In the experiments, temperature, borax concentration and sulphate concentration were chosen as parameters and the effects of these parameters on sulphate removal were investigated. The resin was packed into a water jacket glass column of internal diameter 2.5 cm and a lenght of 80 cm. A solution of borax containing sulphate was fed onto the top of column at the known flow rate using peristaltic pump. Eluate samples were collected at intervals and analyzed by ICP OES. .The results of analysis of samples collected showed that Purolite A 400 MB can efficiently remove sulphate anions in borax solutions.

Keywords: Borax, Sulphate, Ion exchanger

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