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Opto-Electronic Properties of Ternary Chalcopyrite $A^{I}B^{III}C_2^{VI}$ and $A^{II}B^{IV}C_2^{V}$ Semiconductors

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(received January 6, 2012; revised August 17, 2012; accepted September 12, 2012)

Abstract. An investigation has been carried out for various crystal parameters like homopolar gap (E_h), heteropolar gap (E_c), average gap (E_g) and refractive index (n). These estimated values are used to calculate the ionicity of ternary chalcopyrite semiconductors. Based on the complex crystal chemical bond theory, the Moss formula which is for one type of bond only has been extended to calculate the refractive index (n). The estimated refractive index is used to evaluate the ionicity of ternary chalcopyrite semiconductors. The results have been compared with the literature ones. The calculated values are in fair agreement with previous reported values.

Keywords: refractive index, energy gap, ionicity, ternary chalcopyrite semiconductors

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Microwave Assisted Knoevenagel Condensation: Synthesis and Antimicrobial Activities of Some α-Cyanoacrylates

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(received June 6, 2012; revised August 14, 2012; accepted November 13, 2012)

Abstract. A series of α-cyanoacrylates (**1-9**) were prepared by Knoevenagel condensation of ethyl cyanoacetate with corresponding aromatic aldehydes in presence of ammonium acetate (NH_4OAc) using microwave irradiation under solvent free condition. The reactions were completed in 20-60 sec with excellent yield. These compounds were screened for their antibacterial activities against five pathogenic organisms: *Bacillus cereus, Staphylococcus aureus* (ATCC 6538)*, Vibrio cholerae*, *Shigella dysenteriae* (AE 14396) and *Salmonella typhi* (AE 14612) and antifungal activity against two organisms: *Aspergillus flavus* and *Saccharomyces cerevisiae* using disc diffusion method and poisoned-food technique, respectively. Some of them were found to possess significant activity, when compared to standard drugs.

Keywords: Knoevenagel condensation, microwave irradiation, α-cyanoacrylates, antimicrobial activity

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A Comparative Study of the Chemical Composition of *Entada pursaetha* and *Pentaclethra macrophylla* Seeds and Seed Oils

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(received April 19, 2012; revised October 6, 2012; accepted November 13, 2012)

Abstract. The proximate, physicochemical, mineral element and fatty acid composition of seeds and seed oils of *Entada pursaetha* and *Pentaclethra macrophylla* have been analysed and compared in order to establish any similarities/differences in their chemical composition and to evaluate the possibility of their suitability for nutritional or industrial purposes. The proximate analyses of the seeds showed that the oil yield of *P. macrophylla:* 40.21 mg/100 g is by far greater than that of *E. pursaetha*: 4.26 mg/100 g but the carbohydrate content is *vice versa* (*E. pursaetha*: 45.36 mg/100 g; *P. macrophylla*: 3.84 mg/100 g). The protein content of both seeds is high (23.19-33.00 mg/100 g) and is greater than those of high protein animal sources like beef, oyster, pork and marine fishes. The physicochemical properties of the oils are comparable with those of conventional oils and suggest the suitability of these oils as edible oils. Results of the analysis for the mineral element contents of the flour of both seeds showed that potassium is the most prevalent mineral present in the two seeds followed by magnesium for *P. macrophylla* and phosphorus for *E. pursaetha*. Analysis of the oils for fatty acids indicates that both oils contain more of unsaturated fatty acids than saturated ones. This is of great nutritional significance.

Keywords: *Entada pursaetha, Pentaclethra macrophylla*, comparative study, composition, fatty acid, seed oils

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Parameters of Biosorption and Bioaccumulation of Cr (VI) Ion from Aqueous Solutions by *Aspergillus niger*

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(received November 29, 2011; revised June 12, 2012; accepted June 20, 2012)

Abstract. Biosorption and bioaccumulation of Cr (VI) ion by *Aspergillus niger* were investigated in a batch system. Growth conditions for this strain were optimized using potato dextrose broth (PDB). The effects of some important parameters such as initial metal concentrations, temperature and inoculum concentration on biosorption capacity were also studied. In batch biosorption studies, *A. niger* removed 93.02% Cr (VI) ion at 30 °C at pH 6.0 and biosorbent dose of 1.0×10^3 spores/cm^3 solution containing 25 mg/L Cr (VI) ion at 100 rpm agitation. Biosorption equilibrium was established in 150 min and the kinetics of the process fitted well with pseudo second order kinetic model. The biosorption process was best explained by Langmuir isotherm.

Keywords: bioaccumulation, *Aspergillus niger,* equilibrium, kinetic model, Langmuir isotherm

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Adsorptive Removal of Methylene Blue Dye by Melon Husk: Kinetic and Isothermal Studies

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(received February 10, 2012; revised May 4, 2012; accepted May 30, 2012)

Abstract. The adsorption capacity of methylene blue (MB) dye from aqueous solution onto raw melon husk (RMH) was investigated under various experimental conditions. Surface studies of RMH were investigated by fourier transform infrared (FTIR) and scanning electron microscopy (SEM). Batch studies were performed to evaluate the effect of various experimental parameters such as contact time, initial concentration of MB dye and dosage of RMH on the efficiency of the sorption process. Optimum conditions for MB dye removal were found to be at an adsorbent dosage of 8.0 g/L of solution for an equilibrium time of 120 min. Lagergren, Elovich and Morris – Weber equations were employed to study kinetics of sorption process. The sorption process was very rapid at the initial stage as 80% of the dye was removed within the first 5 mins. The kinetics of the adsorption followed pseudo second order model with R^2 values ranging from 0.999 to 1 for all initial dye concentrations studied. Equilibrium isotherms for the adsorption of MB dye on RMH were analysed by Freundlich, Langmuir and Temkin isotherm models and the goodness of fittings were inspected using linear regression analysis (R^2) and sum of square error (SSE). The equilibrium data were well described by Langmuir and Temkin equation at all range of operating parameters.

Keywords: melon husk, kinetics, isotherm, methylene blue dye, adsorption

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Distribution of Metals in Urban Street Dusts of Benin City, Nigeria

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(received January 31, 2012, revised November 17, 2012; accepted December 5, 2012)

Abstract. Dust samples were collected from 30 sites within Benin city, Nigeria, during the month of December, 2006 - March 2007 and analysed for Cu, Cr, Ni, Cd and Pb using atomic absorption spectrophotometry. The samples were divided into 3 categories, including a control. Results showed that the dust samples contained significant levels of the metals studied compared to the control site. The mean values for Cu, Cr, Ni, Cd and Pb were 16.83 mg/kg, 55.40 mg/kg, 5.91 mg/kg, 3.17 mg/kg, and 182 mg/ kg, respectively, for the high traffic density. The mean concentrations of Cu, Cr, Ni, Cd and Pb were 11.98 mg/kg, 52.21 mg/kg, 6.89 mg/kg, 3.92 mg/kg and 167.34 mg/kg, respectively, for the medium traffic areas, while mean concentrations of Cu, Cr, Ni, Cd and Pb in the low traffic areas were 10.46 mg/kg, 58.7 mg/kg, 8.06 mg/kg, 3.49 mg/kg and 142.53 mg/kg, respectively. These values suggest that motor vehicles and electricity generating sets formed the major sources of these metals in the dust samples. The values of metals in the dust samples in these areas were compared with the results of investigations in other countries and these values at various zones of Benin city were found similar, which indicates that Benin city can be considered as one big urban centre with high population and traffic density.

Keywords: heavy metals, contamination, dust, vehicular emission; electricity generating sets

Pak. j. sci. ind. res. Ser. A: phys. sci. 2013 **56** (3) 176-179

Determination of Physicochemical Parameters of Sugar Mill Effluents

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(received February 27, 2012; revised July 9, 2012; accepted July 31, 2012)

Abstract. A study on the determination of physicochemical parameters of sugar mills effluents has been carried out. In this scenario samples were taken from various parts of mills including mill house, process house, spray pond, compositive main drain colony and compositive main drain after lagoon. These samples were then subjected to analysis of some important physicochemical parameters such as pH, total dissolve solids (TDS), total suspended solids (TSS), biochemical oxygen demand (BOD), chemical oxygen demand (COD) and oil and grease. The results of all the effluent samples show that values of all the parameters are above the range fixed by national environmental quality standards (NEQS).

Keywords: sugar mill effluent, physicochemical parameters, environmental quality standards

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Short Communication

Application of Enzymatic Bating Agent on Leather

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[c]Pakistan National Accreditation Council, Islamabad, Pakistan

(received September 17, 2012; revised December 18, 2012; accepted February 6, 2013)

Abstract. Protease activity of *Aspergillus niger* was investigated for leather bating by solid state fermentation using wheat bran as substrate at a suitable concentration and was found to be 1200 units. The optimum conditions regarding temperature, time and speed of agitation for enzyme leaching were found to be 37 °C, 2.5 h and 12 rpm, respectively. The leather produced with such materials was compared with that produced using a widely applied commercial bating material with regard to quality, strength and softness. This leather was of good quality having no difference from the leather produced by using imported bating material.

Keywords: protease, *Aspergillus niger*, wheat bran

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