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FTIR - A Didactic Approach for the Study of Humic Acid - Chromium Chelation During the Environmental Remediation

Zakiuddin Ahmed[a]*, Syed Arif Kazmi[b], Mateen Muhammad Khan[a], Gulzar Hussain Jhatial[a] and Nadir Buksh[a]

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(received December 15, 2011; revised April 12, 2012; accepted May 17, 2012)

Abstract. The present study uses infra-red spectroscopy as a didactic approach to characterize the chromium-humic acid interaction. Shifts of the characteristic carboxylate peaks in the IR spectrum of humic acid upon its interaction with chromium are noted. These changes have been interpreted to conclude that binding of chromium to humic acid is through these groups. An analytical grade humic acid was used for this study. It was also concluded that at the moderate pH i.e 8.5 all the waste chromium ions were cleared from waste water controlling the water pH.

Keywords: IR study, humic acid, chelation, chromium binding

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Characteristics Assessment of Cooking Oil and Vanaspati Ghee

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(received February 27, 2012; revised June 26, 2012; accepted July 4, 2012)

Abstract. Various physico-chemical characteristics of commercial cooking oil and vanaspati ghee of different brands collected from local market have been analyzed. All the characteristic parameters were analyzed using AOCS method, while fatty acids composition of samples were determined using gas chromatography (GC) coupled with flame ionization detector (FID). Physico-chemical characteristics of all cooking oils seem comparable with each other, however, vanaspati ghee samples showed different physico-chemical characteristics due to presence of high amount of *trans* fat. There is direct relation between physico-chemical characteristics such as moisture and impurities, iodine value, unsaponifiable matter, saponification value, refractive index, density and colour.

Keywords: physico-chemical parameters, fatty acid composition, GC-FID, cooking oil

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Density Functional Theory Studies on Electronic Properties of Thiophene S-oxides as Aromatic Dienophiles for Reactivity Prediction in Diels-Alder Reactions

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(received May 30, 2011; revised November 30, 2011; accepted December 27, 2011)

Abstract. The reactivity of thiophene S-oxides was discussed with special emphasis on the use of thiophene S-oxides as dienophiles in Diels-Alder type reactions. The ω values obtained for thiophene S-oxide (TO) with electron-donating group ($-CH_3$) increased the nucleophilicity power whereas substitution with electron-withdrawing groups (such as $-NO_2$ and $-CO_2CH_2CH_3$) increased the electrophilicity power, indicating an increase of reactivity towards a nucleophiles. The higher the value of Δω the more favourable the D-A process, therefore apart from (4+2) addition reactions of these TO as diene with the typical dienophiles like 1,2-dicyanoethene and 1,2-dicyanoethne, it could be possible for TO with strong electron withdrawing substituents to serve as dienophile, e.g. heterocycles 1e and 1f. Also, from the value of Δω heterocycle 1d could involve in (4+2) addition reactions with heterocycles 1e and 1f.

Keywords: thiophene S-oxide, reactivity, global properties, density functional theory

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Studies on the Composition of Effluent Wastes of Kot Lukh-pat Industrial Estate (0-400 M), Pakistan

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(received October 2, 2010; revised June 7, 2011; accepted June 9, 2011)

Abstract. The quality of wastewater effluents in the Kot Lukh-pat Industrial Estate main drain, stretched from 0 to 1.1 km ahead was studied. Samples were collected during June and September, 2008 along first 400 m and quality parameters like pH, conductance, TSS, TDS, COD, BOD, chlorides and sulphides were determined. In most of the samples COD, BOD and S^{2-} remained above the recommended limits of National Environmental Quality Standards (NEQS) of Pakistan, while chlorides and TSS were found to be below the limits. The effect of temperature and pH on the quality of wastewater was noted in most of the samples because, it affects the solubility of oxygen, volatile compounds and growth of microbes. The decrease in oxygen content caused by high temperature can shift the microbial community from aerobic to anaerobic and also causes life threatening conditions for the aquatic life in the water body that receives the wastewater. Increase in pH causes the increased efficiency of microbes which consume the organic compounds in wastewater. This study pointed out the alarming condition of the wastewater.

Keywords: wastewater, environmental management, Kot Lakh-pat Industrial drain, COD, BOD

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Forbidden Transitions for Low-Lying Levels in Atomic Boron

Gülay Günday Konan[a], Betül Karaçoban[a], Güldem Ürer[a], Leyla Özdemir[a]* and Osman Ağar[b]
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(received October 18, 2011; revised April 30, 2012; accepted May 2, 2012)

Abstract. The multiconfiguration Hartree-Fock in the framework of the Breit-Pauli Hamiltonian (MCHF+BP), relativistic Hartree-Fock (HFR), and multiconfiguration Dirac-Fock (MCDF) calculations of the wavelengths, oscillator strengths, and transition probabilities for the magnetic dipole (M1) and electric quadrupole (E2) forbidden transitions between low-lying levels in the atomic boron have been performed. The data for the analysis of forbidden lines in the spectrum is important for the study of the plasma in astrophysical objects and fusion devices. The data for forbidden transitions obtained from this study have been compared with experimental and other theoretical data available in the literature. Moreover, a discussion of these calculations for the boron atom (B I) has been given in view of the MCHF+BP, HFR and MCDF methods.

Keywords: boron, forbidden transitions, transition probabilities, oscillator strengths

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Synthesis and Thermopower of Vanadium-Doped Bismuth-Based (Bi-2223) High-T_c Superconductors

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(received June 6, 2011; revised August 15, 2012; accepted September 5, 2012)

Abstract. A superconducting sample with nominal composition of $Bi_{1.3}Pb_{0.4}V_{0.3}Sr_2Ca_2Cu_3O_\delta$ prepared by using solid-state reaction method. DC electrical resistivity of the sample determined by using a standard four-probe technique within a temperature range of 77-300 K. Zero electrical resistivity of the sample was found at a critical temperature ($T_{c,zero}$) of 108 ± 1 K. Whereas, the onset temperature ($T_{c,onset}$) was observed at 122 ± 1 K. Temperature dependent thermoelectric power (Seebeck coefficient) of the superconducting sample was measured with a newly developed and calibrated apparatus.

Keywords: $Bi_{1.3}Pb_{0.4}V_{0.3}Sr_2Ca_2Cu_3O_\delta$ superconductors, vanadium doping, thermoelectric power, electrical resistivity

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Investigation of Flash Cure Process for Finishing Cotton

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(received May 24, 2011; revised February 28, 2012; accepted March 7, 2012)

Abstract. Easy-care performance is imparted to cotton fabric by the formation of crosslinks between the adjacent cellulose chains. The most widely accepted crosslinking method is treatment with *N*-methylol resins using sequential pad-dry-cure technique. Flash cure technique is also used to complete the crosslinking by single stage dry/cure cycle. As a result better tear and tensile properties are attained without the undesirable effect on crease recovery property. Such a curing system can be used for energy conservation or to reduce energy consumption in resin finishing of cotton fabrics.

Keywords: crosslinking, *N*-methylol, flash curing, easy-care properties

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Effect of Fibre Length on the Physical and Mechanical Properties of Sisal / Polyethylene Composites

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(received April 4, 2011; revised November 30, 2011; accepted December 30, 2011)

Abstract. Composites of sisal fibres with polyethylene polymer chips were prepared at 50% fibre weight with varying lengths of the sisal fibres and the physical and mechanical properties of the composites were determined. The results of the physical properties show that moisture uptake of the composites initially increases from 0 to 60% as the fibre length increased from 0 to 5 mm and there after remained about the same. Density was observed to decrease initially at 5 mm and then steadily increased. The hardness and thickness was increased with increase in fibre length. Young's modulus, breaking load and breaking extension increased as the length of fibres in composite increased from 10 mm length, while work of rupture increased with increase in fibre length from about 5 mm.

Keywords: composites, sisal fibre, fibre length, physical properties, mechanical properties.

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Comparative Study of D-Slot and Straight Slot in Compact Spinning System under Mechanical Variables

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(received October 31, 2011; revised September 5, 2012; accepted September 12, 2012)

Abstract. The present research study was planned, to appraise the quality and properties of the compact yarn as influenced by hank roving, type of suction slots, spindle speed and spacer size. The basic properties of the compact yarn such as strength, elongation, unevenness and hairiness were analyzed as a function of compact spinning to control those protruding fibres which become the part of the yarn but have no role in the yarn formation and ultimately no contribution to yarn strength.

Keywords: suction straight and D slots, spindle speed, hank roving, spacers

Pak. j. sci. ind. res. Ser. A: phys. sci. 2013 **56** (1) 54-56

Short Communication

Synthesis and Photochromic Activity of a New Diarylethene Bearing Benzo[b]Thiophene Unit

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(received May 5, 2011; revised July 15, 2011; accepted September 26, 2011)

Abstract. The synthesis of new photochromic compound 3-[2-(3,5-*bis* methoxymethoxymethylthiophene-2-yl)-3,3,4,4,5,5-hexafluorocyclopent-1-enyl]-2-methyl-benzo[b]thiophene is reported. In multistep synthesis from 2,4-dibromothiophene, benzo[b]thiophene was synthesized. This product exhibited photochromic properties upon irradiation with ultraviolet and visible light.

Keywords: photochromism, photomemory, photocyclization, coupling reaction

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Short Communication

Alkyd Resin from *Ipomoea batatas* Lam.

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(received March 21, 2012; revised May 9, 2012; accepted May 16, 2012)

Abstract. A new alkyd resin has been isolated from the hexane extract of powdered sweet potato (*Ipomoea batatas* Lam.) peels. The proposed structure of the compound was established to be Poly 3-(2,4-dihydroxyphenyl) butanoate by means of data obtained from the FTIR, ^{1}H-NMR and ^{13}C-NMR spectra.

Keywords: *Ipomoea batatas*, Poly 3-(2,4-dihydroxyphenyl) butanoate, alkyd resin, renewable resin