Papers

2043  Ab initio calculation on the effect of substituents in the alkylation mechanism by nitrogen mustards at N-7 of guanine

Ab initio calculation of some DNA binding drugs, nitrogen mustards, has been reported for studying the effect of substituents in the alkylation reaction. The substituents do not affect the formation of aziridinium ion of most drugs but for bendamustine and some model drugs of nitrogen mustards with ethyl and ethoxy group substituents, the energies of forming the aziridinium ion are high.

P K Bhattacharyya & C Medhi*

2049  On the dehydrogenation of 1- and 2-propanols on Cu (111) surface: A UBI-QEP based approach

The method of unity bond index-quadratic exponential has been employed to investigate the energetics of routes to adsorption and decomposition of 1- and 2-propanols on Cu(111) plane. A mechanism based on the formation of surface alkoxide groups and elimination of β-hydrogen to yield exclusively the corresponding aldehyde-ketone is confirmed on the basis of the energy criteria.

F Gobal* & A Eftekhari

2055  Aromatization of methane under non-oxidative conditions over molybdenum containing molecular sieves with MFI & MEL topologies

Molybdenum containing molecular sieves with MFI and MEL topologies have been synthesized hydrothermally and characterized using XRD and BET surface area. The activity of these catalysts for the conversion of methane to benzene has been examined at 958 K, under non-oxidative conditions. The hydrothermally synthesized Al and Mo containing molecular sieves are found to be efficient for the above reaction.

P S Raghavan

2060  Esterification of isoamyl alcohol using solid acid catalysts

Catalytic activity of different solid acids obtained by calcination of hydroxides of Al, Si, Zr and Ti as well as their sulfated forms has been reported in liquid phase esterification of isoamyl alcohol with propionic acid. The major product of the catalytic reaction has been found to be isoamyl propionate. The yield (%) of the ester has been found to depend on the textural properties, total surface acidity and surface area of the catalysts.

N Nagaraju* & S Z Mohamed Shamshuddin

2066  Methacrylonitrile-vinylidene chloride-butyl acrylate terpolymers: Monomer sequence determination by one- and two-dimensional NMR spectroscopy

Methacrylonitrile-vinylidene chloride-butyl acrylate terpolymers of different compositions have been prepared by bulk polymerisation and their compositions determined from quantitative assessment of the respective \( ^{13}C(\text{H}) \) NMR spectra. The complete \( ^{1}H \) and \( ^{13}C(\text{H}) \) NMR spectra of terpolymers have been assigned without ambiguity with the help of 2D HSQC NMR spectroscopic techniques.

A S Brar*, D R Pradhan & Sunita Hooda
2073 Studies of osmotic coefficients and volumetric behavior on aqueous solutions of β-cyclodextrin at 298.15 K

Dilip II Dagade, Rahul R Kolhapurkar & Kesharsingh J Patil* The osmotic coefficient, solute activity coefficients and apparent molar volume are determined for β-cyclodextrin using the techniques of vapor pressure osmometry and digital densitometer in aqueous solutions at 298.15 K. Using the partial molar volume data at infinite dilution and B*2 value, the contribution due to solute-solvent and solute-solute interactions in terms of attractive and repulsive components are estimated. The results are discussed in terms of hydrophobic hydration and hydrophobic interaction.

2081 Coenzyme B12 model studies: Equilibria and kinetics of axial ligation of trifluoroethyl(aquo)cobaloximes by N donor ligands

D Sudarshan Reddy, M Bhoopal, N Navaneetha & S Salyanarayana* The kinetics of substitution of aqua ligands from cis-diaqua-bis-(bipyridyl) ruthenium(II) complex by glutathione (reduced; GSH) have been studied spectrophotometrically as a function of [glutathione], [Ru(bipy)2(H2O)2]2+ and temperature at pH 4.8. From the data a reaction mechanism involving SN2 path has been suggested.

2087 Kinetics and mechanism of substitution of aqua ligands from cis-diaqua-bis-(bipyridyl) ruthenium(II) complex by glutathione in aqueous medium

A Goswami & K De* Notes

2091 Solid solutions of strontium-calcium hydroxyapatites containing arsenate

P N Patel* & S Panda Homogeneous solid solutions of strontium-calcium hydroxyapatite containing arsenate, Ca10−nSr1n(PO4)10−n(AsO4)8−n(OH)2, with fixed n = 1, have been prepared over the entire compositional range by co-precipitation in aqueous media. The infrared spectra and lattice constants of the solid solutions have been found to vary linearly with composition between those of the pure end members.

2094 Synthesis and characterization of terpolymer of α-terpineol, styrene and methylmethacrylate: A kinetic study

Sarika Yadav & A K Srivastava*
Effect of ultrasound on the redox reactions of iron (II) and (III)

The phenomenon of cavitation, generated through ultrasound, is found to facilitate both oxidation and reduction reactions of iron. Under ultrasonic field a solution of Fe(II) oxidizes to Fe(III) and forms a pink coloured complex of \([\text{Fe(SCN)}_6]^{3-}\), whereas Fe(III) reduces to Fe(II) and complexes with \(K_3[\text{Fe(CN)}_6]\) to form a prussian blue solution. A possible mechanism for inter-conversion has also been discussed.

Pankaj* & Manju Chauhan

Ultrasonic behaviour and study of molecular interactions of substituted azole in N,N-dimethylformamide at different temperatures and concentrations

Ultrasonic velocity and density measurements of 2-(4-amino-5-mercapto-[1,2,4] triazol-3-yl)- phenol in N,N-dimethylformamide have been carried out at 303, 308, 313 and 318 K in the concentration range \(2 - 10 \times 10^{-3}\) mol dm\(^{-3}\). Different acoustic properties like apparent molal volume, apparent molal compressibility, intermolecular free length, specific acoustic impedance and relative association have been determined. These parameters have been interpreted in terms of solute-solvent and solute-solute interactions.

Deepali P Gulwade*, M L Narwade & K N Wadodkar

Kinetics and mechanism of acid assisted reduction of unsymmetrical chelate complex \([\text{Co}^{II}(\text{Am})(\text{endibigH})_2(\text{ClO}_4)_2]\) (where Am = amino acid and endibigH = ethylenedibiguamide)

Asim Kumar Majee, D D Chaturvedi, Abhishek Srivastava, Abhinav Agarwal, R M Naik* & P C Nigam

Mechanism of oxidation of \(p\)-nitroaniline by ammonium metavanadate in sulphuric acid medium: A kinetic approach

The kinetics of ammonium metavanadate oxidation of \(p\)-nitroaniline in sulphuric acid medium has been followed spectrophotometrically. The reaction follows second order kinetics being unity in each of the reactants. The stoichiometry of the reaction has been found to be 1:1. The effect of various parameters viz., [oxidant], [substrate], [\(H^+\)], ionic strength, dielectric constant and added micelles have been investigated and the thermodynamic parameters have been evaluated. A suitable mechanism consistent with the experimental results has also been proposed.

Madhavi Verma* & Chetna Tekchandani

Silyl nitrogen compound: Part XV — Reactions of nonmetal halides with silylated tosylhydrazines

S K Vasisht* & Anuradha Sharma
Synthesis, characterization, biological and thermal properties of some new Schiff base complexes derived from 2-hydroxy-5-chloroacetophenone and S-methyldithiocarbazate

M = Mo(II), Co(II) and Ni(II)

J T Makode & A S Aswar*

Cation-π interactions. Synthesis and crystal structure of complexes [K(B18-C-6)NCS and [K(DB18-C-6)2Hg(SCN)4]

Yuchua Zhu, Jianmin Dou*, Dacheng Li & Daqi Wang

Synthesis, characterisation and biological activities of ruthenium(II) Schiff base complexes

M Periyasamy, K P Balasubramanian & V Chinnusamy*

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