

Controlled synthesis of CuO box shaped nanoparticles and their application in nitrophenol reduction

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Abstract : Box shaped copper(II) oxide particles with an average diameter of ~100 nm were synthesized by warming Cu(OH)₂ in cyclodextrin at ~80–90 °C. The tunable size, gram level preparation and characterization of the single crystalline CuO nanoboxes were demonstrated. The procedure involves the use of common copper compounds as precursor and unmodified cyclodextrin as capping agent for box shaped nanoparticles. The optical absorption spectrum provides a band gap of 3.05 eV for the prepared CuO nanoparticles. A possible mechanism that accounts the growth of these nanostructures has been described. The synthesized CuO nanoparticles were exploited as catalyst for the reduction of 4-nitrophenol.

Keywords : CuO NP, cyclodextrin, catalysis, 4-nitrophenol.

Syntheses and characterization of coordination compounds of N-(2-mercaptoethyl)-4-(3'-carboxy-2'-hydroxyphenyl)-2-azetidinone

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Abstract : A dioxane solution of N-(2-mercaptoethyl)-3-carboxy-2-hydroxybenzylideneimine, LH₃ (I) on reacting with chloroacetyl chloride in the presence of triethylamine, undergoes cyclization to form N-(2-mercaptoethyl)-4-(3'-carboxy-2'-hydroxyphenyl)-2-azetidinone, L'H₃ (II). A MeOH solution of L'H₃ reacts with Mn^{II}, Co^{II}, Ni^{II}, Cu^{II}, Zn^{II}, Cd^{II}, Zr^{IV}, MoO₄²⁺ and UO₂²⁺ ions to form the complexes [M(L'H).MeOH]₂ (where M = Mn^{II}, Co^{II} or Ni^{II}), [Cu(L'H)]₂, [M'(L'H)] (where M' = Zn^{II}, Cd^{II}, MoO₄²⁺ or UO₂²⁺) and [Zr(OH)₂(L'H)]₂. The compounds have been characterized on the basis of elemental analyses, molar conductance, molecular weight, spectral (IR, UV-Visible) studies and magnetic susceptibility measurements. L'H₃ behaves as a dibasic tridentate OON donor ligand in [Cu(L'H)]₂, while it acts as a dibasic tetradentate OONS donor ligand in rest of the compounds. The complexes [M(L'H).MeOH]₂ (where M = Mn^{II}, Co^{II} or Ni^{II}), [Cu(L'H)]₂ and [Zr(OH)₂(L'H)]₂ are dimers, and the complexes [M'(L'H)] (where M' = Zn^{II}, Cd^{II}, MoO₄²⁺ or UO₂²⁺) are monomers. The dimeric complex [Cu(L'H)]₂ exhibits subnormal magnetic moment and is involved in antiferromagnetic exchange, while all other complexes are magnetically dilute. The octahedral structure for Mn^{II}, Co^{II}, Ni^{II}, MoO₄²⁺ and UO₂²⁺ complexes, square planar structure for Cu^{II} complex, tetrahedral structure for Zn^{II} and Cd^{II} complexes, and pentagonal bipyramidal structure for Zr^{IV} complex have been suggested.

Keywords : Azetidinones, mercapto, dimetallic coordination compounds, paramagnetism, infrared spectra, UV-Visible spectra, coordination compounds.

One-pot syntheses and characterizations of $[\text{Cd}(\text{diik})_3](\text{ClO}_4)_2$ [diik = *N,N'*-carbonyldiimidazole] and $[\text{Cd}(\text{imH})_6](\text{ClO}_4)_2$ [imH = imidazole] : 2D supramolecular sheet structure in $[\text{Cd}(\text{imH})_6](\text{ClO}_4)_2$ through N–H...O hydrogen bonds

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Abstract : The details of synthesis and characterization of two mononuclear coordination compounds $[\text{Cd}(\text{diik})_3](\text{ClO}_4)_2$ (1) [diik = *N,N'*-carbonyldiimidazole] and $[\text{Cd}(\text{imH})_6](\text{ClO}_4)_2$ (2) [imH = imidazole] are described. The compounds are characterized on the basis of microanalytical, spectroscopic and physicochemical results. Structure of 2 has been solved by X-ray diffraction measurement. Structural analysis shows that cadmium(II) centre in 2 has a centrosymmetric octahedral geometry with a CdN_6 chromophore ligated through six N atoms of six imH ligands. The mononuclear units in 2 are packed through N–H...O hydrogen bonds leading to a 2D sheet structure in *ac* plane. Compounds 1 and 2 display intraligand $^1(\pi-\pi^*)$ fluorescence at room temperature.

Keywords : Cadmium(II), imidazole, synthesis, superstructure, luminescence.

1-Aryl substituted-3-(2'-chlorophenyl)-5-(3''-phenyl-4''-oxo-(3''H)-quinazolin-2''-mercaptoacetyl)formazans as insecticidal agents

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Abstract : Synthesis of some novel formazans have been carried out by the reaction of 2-mercapto-2-(methylamido-2'-chloro-*N*-benzylidene)-3-phenyl-4-oxo-(3*H*)-quinazoline with diazotised solution of aromatic amines in pyridine and screened for their insecticidal activity against *Tribolium confusum*.

Keywords : Formazans, insecticidal activity, *Tribolium confusum*.

Quantum chemical study of the structures, stability and vibrational spectra of the nitrous acid complexes with B₂O₂ and C₂N₂ molecules

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Abstract : *Ab initio* calculations at the SCF and MP2 levels with 6-311G basis set have been used to investigate the structures, stability and vibrational spectra of the binary complexes B₂O₂-HONO(*trans*) and B₂O₂-HONO(*cis*) alongwith complexes of C₂N₂-HONO(*trans*) and C₂N₂-HONO(*cis*). Full geometry optimization was made for the complexes studied here. It was established that the complexes B₂O₂-HONO(*trans*) is more stable by 2.40 kcal/mol than the complex B₂O₂-HONO(*cis*) and C₂N₂-HONO(*trans*) is more stable by 2.48 kcal/mol than C₂N₂-HONO(*cis*). The accuracy of the *ab initio* calculations have been estimated by comparison between the predicted values of the vibrational characteristics (frequencies and infrared intensities) and the available experimental data. It was established that the molecules, used in the present work, are well correlated. The changes in the vibrational frequencies of B₂O₂, C₂N₂ and *trans*, *cis*-nitrous acid upon formation of hydrogen bond respectively showed that the complexes B₂O₂-HONO(*trans*) and B₂O₂-HONO(*cis*) have geometry in which the OH group interacts with B₂O₂ molecules forming a single hydrogen bond. Similar study was also observed for C₂N₂ and HONO complexes.

Keywords : Complexes, B₂O₂, MP2 method, nitrous acid, C₂N₂.

Polyelectrolyte-dye interactions : Study of interaction between Sodium Carboxymethylcellulose and Acridine Orange

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Abstract : The interaction between Sodium Carboxymethylcellulose (NaCMC) and a fluorescent cationic dye, Acridine Orange (AO) has been investigated by spectrophotometric and spectrofluorometric methods. The polymer induces metachromasy in the dye as evidenced from the considerable blue shift in the absorption maximum of the dye. The interaction constant and thermodynamic parameters of polymer-dye interactions have been determined by the absorbance and fluorescence measurements. The effect of additives such as alcohols and urea on the reversal of metachromasy has been studied. The data has been used to determine the stability of the metachromatic complex and the nature of binding.

Keywords : Sodium Carboxymethylcellulose, Acridine Orange, metachromasy, polyelectrolyte, stoichiometry, thermodynamic parameters.

H-bonding interactions between simple DNA base cytosine and formamide molecules (model of protein unit) : A density functional theory study

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Abstract : The molecular geometry of complexes C-F_n (n = 2–7) of cytosine with formamide molecules was calculated within the density functional theory using the B3LYP function at 6-31G(d) basis set level. It was found that the interaction with formamide molecules forming a locked chain around cytosine results in significant changes in its intramolecular geometry. An obvious effect of hydrogen-bonding cooperativity can be seen during the complex process. The most interesting geometrical change of cytosine upon the complex is the shortening of bond C4–N7 resulting from the strengthening of the conjugation between the π system of the cytosine ring and the lone pair of the nitrogen atom. The significant elongation of C1–O8 bond and the presence of weak C–H...O hydrogen bonds are also revealed.

Keywords : DNA, H-bonding, formamide, cytosine, density functional theory.

Ultrasonic and viscometric investigation of albumin protein in aqueous solution

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Abstract : The ultrasonic wave is an efficient powerful and reliable method for various investigations including those of solution dynamics, molecular interactions, miscibility and compatibility of protein in aqueous solution. Ultrasonic velocities and related acoustic parameters were calculated as a function of concentrations of albumin protein in water with a resonance method at frequencies of 3 MHz and 10 MHz. Viscosity (η) of aqueous protein solution was measured by suspended Ubbelohde viscometer. The comparative result of ultrasonic velocities (u), density (ρ), relaxation time (τ), adiabatic compressibility (β_s) and acoustic impedance (z) were studied as a function of the concentrations. The mode of compatibility interaction and miscibility of albumin protein in water were investigated. It was found that the acoustic sound wave perturbed at 3 MHz which explained the weak interaction of water molecule with the segmental motion of albumin protein chains. The interactions of the acoustic result of albumin protein may lead to the development of biomedical active molecules.

Keywords : Ultrasonic velocity, compatibility, relaxation time, acoustic impedance.

Study on electronic-spectral aspects with special emphasis on symmetry change around Pr^{3+} ion in solution of organic oximes

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Abstract : The change in symmetry around (stereo-environment) the doped Pr^{3+} ion in various solutions of some organic oximes has been studied for various electronic spectral parameters. The parameters viz. Slater-Condon (F_K), Lande parameter (ζ_{4f}), intensity of hypersensitive band, bonding parameter ($b^{1/2}$), Judd-Ofelt parameter (T_λ) and Racah parameter (E^k) for Pr^{3+} doped in solution of organic oximes have been studied.

Keywords : Doped systems, stereo-environment.

Synthesis of poly-styrene based nickel phosphate membrane : Evaluation of membrane parameters and to test the membrane potential theories

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Abstract : The fabrication of polystyrene-based nickel phosphate membranes at different pressures with varying amounts of material has been described. In order to understand the mechanism of transport of ions and to evaluate various membrane parameters controlling the transport phenomena, the membrane potential measurements were carried out using different concentrations of 1 : 1 electrolytes solutions. Teorell-Meyer and Sievers (TMS) method was used for the estimation of membrane parameter in the form of thermodynamically effective fixed charged density of membranes. The data were then utilized to calculate theoretical membrane potential values using extended TMS theory. Bi-ionic potential (BIP) measurements were reported keeping the same concentration of ionic species on the two sides of the membranes. On the other hand, Toyoshima and Nozaki method was used for the evaluation of theoretical values of bi-ionic potential (BIP) at the same concentration of ionic species on two sides of the membrane, utilizing the membrane parameters evaluated using the values of membrane potential. The close agreement between theoretical and observed values in both cases not only proved the existence of the membrane but also confirm the applicability to examine the validity of the theory utilized to the membrane electrolyte systems. Scanning electron microscope (SEM) monographs of the membrane have also been presented.

Keywords : Membrane potential, membrane bi-ionic potential, charge density, scanning electron microscope (SEM), polystyrene based nickel phosphate membrane.

Voltammetric behaviour of *o*-nitrophenol in aqueous methanol medium at various electrodes

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Abstract : Voltammetric curves of *o*-nitrophenol in aqueous methanol medium for acidic, basic and neutral ranges using B.R. buffer for various concentrations (0.05, 0.1, 0.15, 0.2 mM) and scan rates were obtained. The prominent three reduction peaks corresponding to 3e⁻ change of *o*-nitrophenol was characterized at 0.1 mM concentration in neutral medium at scan rate 90 mV/s. The reversibility of the reaction was also studied by the cyclic voltammetry.

Constant current electrolysis of 0.02 mM *o*-nitrophenol in neutral medium gives *o,o'*-dihydroxyazobenzene at stainless steel (type 316) cathode and counter electrode of same size and material at constant current 1.8 ampere respectively, as a major product which were confirmed by spectral and chemical analysis.

Keywords : Electrochemical reduction, *o*-nitrophenol, cyclic voltammetry, constant current electrolysis, SS cathode.

Thermodynamic parameters of micellization and transfer of amino acids from water to aqueous linear alkyl benzene sulphonate

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Abstract : The solution properties of linear alkyl benzene sulphonate (LABS) in water in presence of amino acids have been investigated conductometrically. The critical aggregation concentration (cac) and critical saturation concentration (csc) were determined. It has been observed that at low concentration of surfactant amino acids interact with hydrophilic head group of surfactant molecules and form molecular aggregate/micelle like structure.

Keywords : cac, csc, cmc, gsp, surfactant, micelle, micellization, conductance, linear alkyl benzene sulphonate, LABS.

Synthesis and antimicrobial activities of some novel 4-substituted pyrazoline derivatives

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Abstract : A series of 5-aryl-3-isopropyl-4-[N-phenyl-aminocarbonyl]-4,5-dihydro-1H-pyrazoles were synthesized by the reaction between 3-aryl-2-isobutanoyl-N-phenyl-acrylamide with hydrazine hydrate in acetic acid as solvent gives acetyl pyrazoline. All the compounds have been evaluated for their *in vitro* biological assay like antibacterial activity towards Gram-positive and Gram-negative bacterial strains and antifungal activity towards *Aspergillus niger* at a concentration of 40 µg. The biological activities of synthesized compounds were compared with standard drugs.

Keywords : Pyrazolines, acetylpyrazolines, antimicrobial activity.

Synthesis and biological significance of pyrano pyrazoles from 8,9-dimethyl-3-acetoacetyl pyrano[3,2-c][1]benzopyran-2,5-dione

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Abstract : 6,7-Dimethyl-3-formyl-4-hydroxycoumarin 1 was treated with triacetic acid lactone 2 in heating methanol to afford 8,9-dimethyl-3-acetoacetyl pyrano[3,2-c][1]benzopyran-2,5-dione 3. The compound 3 was transformed to pyrano pyrazole derivatives 4a-c by treatment with nitrogen bases such as hydrazine hydrate, phenylhydrazine and hydrazinobenzothiazole. The structure of all compounds was established on the basis of spectroscopic studies and screened for their antibacterial and anti-inflammatory activities.

Keywords : 6,7-Dimethyl-3-formyl-4-hydroxycoumarin, 8,9-dimethyl-3-acetoacetyl pyrano[3,2-c][1]benzopyran-2,5-dione, triacetic acid lactone, pyrano pyrazoles, antibacterial and anti-inflammatory activities.

A green chemical approach for nitration of aromatic compounds

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Abstract : Photochemical aromatic nitration of anthranilic acid has been carried out in the presence of UV radiations and the formation of product has been observed spectrophotometrically. The effect of different variables like pH, concentration of nitrite ion, formate ion, anthranilic acid etc. was observed on the rate of the reaction. A tentative mechanism involving NO₂[•] radicals has been proposed for photochemical nitration of anthranilic acid.

Keywords : Photochemical nitration, aromatic, eco-friendly.

Antifungal flavonoids of *Melochia corchorifolia*

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Abstract : 5,7-Dihydroxyflavone, apigenin, kaempferol and quercetin has been isolated from aerial parts of *Melochia corchorifolia* and their structures established by spectral evidences. These flavonoids exhibited significant antifungal activity. This is the first report of these flavonoids in *M. corchorifolia* and their antifungal activity.

Keywords : *Melochia corchorifolia*, flavonoids, antifungal activity.

A simple spectrophotometric method for determination of antimony(III) with *N*-bromosuccinimide and methyl orange

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Abstract : In this study, a simple and sensitive spectrophotometric method for the determination of antimony(III) is described. It is based on the oxidation of antimony(III) with slight excess of *N*-bromosuccinimide (NBS) in acidic medium and the unconsumed (NBS) is determined with methyl orange (λ_{max} 500 nm). Beer's law is obeyed over the concentration range of 0.4–2.8 $\mu\text{g/ml}$ for antimony(III). The molar absorptivity and Sandell's sensitivity were found to be $3.43 \times 10^4 \text{ L mol}^{-1} \text{ cm}^{-1}$ and $0.0035 \mu\text{g cm}^{-2}$ respectively. The method has been successfully applied for the determination of Sb^{III} in water, soil and biological samples.

Keywords : Spectrophotometric determination, antimony(III), NBS, methyl orange.

Biosorption of chromium(VI) by some algae

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Abstract : In the present study, biosorption of chromium(VI) from aqueous solutions was studied on two algae species *Synechococcus* sp. and *Asterocapsa* sp. in living condition with variation in initial metal concentration. The algae species were cultured in BG 11 medium, which was supplemented with 1–4 mg L^{-1} of chromium(VI), and were harvested after 15 days of incubation. The total chlorophyll content and percent removal was determined. The maximum removal was 36% for *Synechococcus* sp. and 37.5% for *Asterocapsa* sp. The results suggest that both species could be used as bioadsorbent for removal of metal. The results also suggested that in living conditions, *Synechococcus* was found more suitable for removal of chromium(VI) from aqueous solution.

Keywords : Biosorption, algae, chromium(VI), total chlorophyll content, metal removal.
