

Electroorganic synthesis: A novel route of green synthesis

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Abstract : Electroorganic synthesis of alkanes, alkenes and esters by anodic decarboxylation of potassium salt of palmitic acid, stearic acid, lauric acid and myristic acid, amines by reduction of aromatic nitro compounds, pinacols by reduction of carbonyl compounds, aromatic dimmers by oxidation of aromatic amines, 1,3,4-oxadiazole derivatives by electrocyclization of semicarbazone and acylthiosemicarbazone, aldol condensation of aldehydes, and acetamidation of aromatic compounds were carried out at platinum plate in undivided electrochemical cell at desired potential using simple solvent and supporting electrolyte. All the reactions were carried out at room temperature by using small amount of electricity without involvement of toxic chemicals.

Keywords : Electroorganic synthesis, controlled potential electrolysis, supporting electrolyte, reference electrode, platinum electrodes, green chemistry.

Synthesis, spectral characterization, *in vitro* antimicrobial evaluation and DNA cleavage studies of few macrocyclic complexes

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Abstract : Few macrocyclic complexes of the composition, [ML]X [M = Cu^{II}, Co^{II}, Ni^{II}, Mn^{II}, Zn^{II}, VO^{IV}, Cd^{II} and Hg^{II}; X = Cl₂/SO₄] have been designed and synthesized by the template condensation of malonic acid with 4,4'-diaminodiphenylmethane in ethanol medium. All the synthesized complexes were characterized by microanalytical data, magnetic susceptibility measurements, IR, UV-Vis, ¹H NMR, EPR and mass spectral techniques. They exhibit square-planar geometry except oxovanadium complex, which has square-pyramidal geometry. The electrolytic behaviour and monomeric nature of the complexes were confirmed from their conductance data and magnetic susceptibility. The X-band EPR spectra of Cu^{II}, Mn^{II}, Co^{II} and VO^{IV} complexes in DMSO at 300 and 77 K were recorded and their salient features are reported. The *in vitro* antimicrobial activities of the investigated compounds were evaluated against few microorganisms by well-diffusion technique. It was found that the metal complexes have higher activity than the standard. The cleavage activity of all the complexes was examined on pUC19 DNA using gel electrophoresis experiment in the presence of H₂O₂. From the data, it was found that all the complexes exhibit nuclease activity except vanadyl complex in the presence of H₂O₂.

Keywords : Macrocyclic complexes, DNA cleavage study, square-planar geometry.

Synthesis, characterization and antimicrobial studies of some 3d-metal complexes of chemotherapeutic importance

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Abstract : Complexes of Co^{II}, Ni^{II} and Cu^{II} with the Schiff bases 3-nitrobenzylidene-2,4-dinitroaniline (NDA), 3-nitrobenzylidene-4-aminoacetanilide (NAA) and 2-furfurylidene-2-nitroaniline (FNA) have been synthesized and their characterization have been done by microanalytical data, UV-Vis, IR, ESR spectroscopy, conductance and magnetic susceptibility measurements. Ligand field parameters of some of the complexes have also been calculated. The complexes have also been screened for their antimicrobial potential against selected fungi and bacteria.

Keywords : Schiff base, Co^{II}, Ni^{II}, Cu^{II}, synthesis, antimicrobial studies.

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Densities, viscosities and excess thermodynamic properties of binary liquid mixtures of ethylenediamine with polar and non-polar solvents at 293.15, 303.15 and 313.15 K

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Abstract : Densities and viscosities of binary liquid mixtures of ethylenediamine with polar and non-polar solvents, viz. methyl alcohol, ethyl alcohol, *n*-propyl alcohol, *n*-butyl alcohol, acetone, methyl ethyl ketone, carbon tetrachloride, benzene and toluene have been measured at 293.15, 303.15 and 313.15 K. From density and viscosity data the values of viscosity deviations (D_h) and the thermodynamic excess properties viz. the excess molar volume (V^E) and the excess Gibbs free energy of activation of viscous flow ($DG^{#E}$) have been determined. The values of D_h , V^E and $DG^{#E}$ have been fitted to Redlich-Kister polynomial equation to estimate the binary coefficients and standard deviation between the experimental and theoretical (calculated) values. From the small magnitude of the values of standard deviation it is concluded that the experimental values of D_h , V^E and $DG^{#E}$ compare fairly well with the theoretical values predicted by Redlich-Kister equation. The effect of increasing temperature on the values of D_h , V^E and $DG^{#E}$ as well as the nature of molecular interactions between the mixing components of the binaries has also been discussed.

Keywords : Densities, viscosities, excess thermodynamic properties, binary mixtures.

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Extraction chromatographic method of preconcentration and separation of fluoride with high molecular mass liquid anion exchanger, Aliquat-336

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Abstract : A selective method has been developed for the extraction chromatographic separation of fluoride with Aliquat- 336 (liquid cation exchanger) coated on silanised silica gel. Its quantitative

extraction has been achieved in HCl medium at 0.1–0.3 M range. The effects of acid with different concentrations, flow-rate, stripping agents on extraction and elution have been investigated. Exchange capacity and break-through capacity of the prepared exchanger at different temperatures with respect to fluoride have been determined. The extraction equilibrium constant (K_{ex}) and different standard thermodynamic parameters have also been calculated by temperature variation method. Effect of influent concentration and influent volume on preconcentration factor (PF) has been investigated. Fluoride has been separated from synthetic binary and multi-component mixtures containing various anions associated with it in environmental samples. The method effectively permits sequential separation of fluoride from synthetic mixture containing its congeners, chloride, bromide and iodide of analytical group. The method was found effective for removal and recovery of fluoride from industrial waste and environmental samples following its preconcentration on the column. A plausible mechanism for the extraction of fluoride has been suggested.

Keywords : Aliquat-336, extraction chromatography, preconcentration, separation of fluoride, selective separation.

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Oxidation of some aromatic secondary alcohols by Cr^{VI} supported on Amberlyst A-26 (Cl⁻) : A kinetic and mechanistic investigation

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Abstract : A kinetic study of the controlled oxidation of some aromatic secondary alcohols by Cr^{VI} supported on Amberlyst A-26 (Cl⁻) were found to proceed through ester formation. The ester thus formed decomposes in a slow step and produces chromium(IV). Chromium(IV) is formed as an intermediate which will further oxidize another molecule of aromatic secondary alcohol because our oxidant was supported on polymeric material and generates a free radical in a fast step. The free radical reacts with another oxidant site in the polymeric reagent in a fast step leading to the formation of chromium(V). In the final step the intermediate chromium(V) reacts with secondary alcohol to produce ketone. Various thermodynamic activation parameters were also calculated at different temperatures.

Keywords : Kinetic, oxidation, Cr^{VI} supported, mechanism, Amberlyst A-26 (Cl⁻).

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Solvent effects and ion-solvent interactions from the studies of the solubility and dissociation constants of oxalic acid in aquo + 2-propanol mixtures and determination of single-ion Gibbs energies of transfer from water to 2-propanol + H₂O mixtures

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Abstract : The solvent effects on the dissociation of the simplest dibasic organic acid were examined from the determination of the first and second dissociation constants of oxalic acid conductometrically and pH-metrically in water + 2-propanol mixtures (0–87 wt% of 2-propanol). The solubility values of oxalic acid and potassium hydrogen oxalate were also determined. The dissociation constants and the solubility values were used to calculate the Gibbs energies of transfer DG^0_t of oxalic acid (H_2OX), bioxalate (HOX^-), oxalate (OX^{2-}) and potassium (K^+) ions from water to aquo-propanolic mixtures. These represent the ‘medium effects’ or quantitative measures of solute or ion-solvent interactions of the respective species in going from water to 2-propanol + water mixtures. pK_1 , pK_2 and the solubility values of oxalic acid increase continuously with increase in organic co-solvent. DG^0_t (H_2OX) and DG^0_t (H^+) are negative i.e. favourable but DG^0_t (H_2OX), DG^0_t (OX^{2-}) and DG^0_t (K^+) are in general positive and hence unfavourable for the dissociation processes. The increase in basicity facilitated the dissociation processes but decrease in dielectric constant and H-bonding capability enhances the association processes as the organic co-solvent increases.

The pK -values can be suitably utilised to prepare buffer solutions in 2-propanol + water mixtures. The solvent effect and solvation phenomena can be better understood from the collection of single-ion values of transfer. These may be utilised to calculate the solubilities of electrolytes in 2-propanol + water mixtures.

Attempts have been made to understand the solvation processes in terms of the structure of the aquo-organic mixtures and Walden products.

Keywords : Gibbs energies of transfer of single-ions, ion-solvent interactions, medium effect, oxalic acid, solubility, thermodynamic dissociation constants, 2-propanol + water mixtures, Walden product.

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Thermodynamic properties of binary liquid mixtures containing 1, 2-ethanediol and primary alcohols at different temperature

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Abstract : Densities and viscosities of the binary mixtures of 1,2-ethanediol with primary alcohols such as methanol, ethanol, 1-propanol and 1-butanol were measured at 293.15, 303.15 and 313.15 K and refractive index for same systems were measured at 303.15 K over the entire composition range. This experimental data were used to calculate excess molar volumes (V^E), viscosity deviations ($\Delta\eta$) and refractive index deviations (Δn_D). These results were fitted to Redlich-Kister polynomial equation and results have been discussed in terms of molecular interaction and structural effects. The excess properties were found to be either positive or negative depending on the molecular interaction and the nature of liquid mixtures.

Keywords : Binary mixtures, primary alcohols, 1,2-ethanediol.

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Modeling of *Clostridium histolyticum* collagenase inhibitory activity of some sulfonyl-1-amine hydroxamates : A molecular connectivity approach

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Abstract : Topological modeling of protease inhibitory activity of some sulfonyl-1-amine hydroxamates which are known to be *Clostridium histolyticum* collagenase inhibitors has been presented in this paper. Out of the pool of topological indices used Randic and Kier-Hall connectivity indices are found most suitable for the modeling of inhibitory activity.

Keywords : ChC inhibitors, protease inhibitors, QSAR, connectivity indices, topological modeling.

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Facile synthesis and biological evaluation of some ethoxyphthalimide derivatives of pyrazolythiazoloisoxazoles and pyrazolythiadiazoles

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Abstract : Reaction of acetylacetone with hydrazine hydrate gave 3,5-dimethyl-1*H*-pyrazole (1) which when reacted with ethylchloroacetate in acetone and thiosemicarbazide yielded ethyl-3,5-dimethyl-1*H*-pyrazol-1-yl-acetate (2) and 2-[(3,5-dimethyl-1*H*-pyrazol-1-yl)acetyl]hydrazine carbothioamide (3) respectively. Compound 3 acted as a key intermediate for both the series of final compounds. In one pathway, it was converted to corresponding thiadiazole (11) by treatment with conc. H₂SO₄ and NH₃ which on condensation with *w*-bromoethoxyphthalimide (10) gave 5-[(3,5-dimethyl-1*H*-pyrazol-1-yl)methyl]-*N*-ethoxyphthalimido-1,3,4-thiadiazol-2-amine (12). In another pathway, 3 reacted with chloroacetic acid to furnish 2-[(3,5-dimethyl-1*H*-pyrazol-1-yl)-4-oxo-1,3-thiazolidin-2-ylidene]acetohydrazide (4). Reaction of 4 with various araldehydes (5a-d) gave 5-[(4-substituted phenyl)methylidene]-4-oxo-1,3-thiazolidin-2-ylidene]-2-[(3,5-dimethyl-1*H*-pyrazol-1-yl)acetohydrazide (6a-d) which were further treated in two alternate routes. Firstly, with 10 to yield 5-[[4-substituted phenyl)methylidene]-3-*N*-ethoxyphthalimido-4-oxo-1,3-thiazolidin-2-ylidene]-2-(3,5-dimethyl-1*H*-pyrazol-1-yl)acetohydrazide (8a-d). Cyclisation of these derivatives using hydroxylamine hydrochloride produced the target compounds 3-(4-substituted phenyl)-6-*N*-ethoxyphthalimido-3,3a-dihydro[1,3]thiazolo[4,5-*c*]isoxazol-5(6*H*)-ylidene-2-(3,5-dimethyl-1*H*-pyrazol-1-yl)acetohydrazide (9a-d). In parallel, 6a-d were first cyclised with hydroxylamine hydrochloride to give 3-[(4-substituted phenyl)-3,3a-dihydro[1,3]thiazolo[4,5-*c*]isoxazol-5(6*H*)-ylidene-2-(3,5-dimethyl-1*H*-pyrazol-1-yl)acetohydrazide (7a-d) and then condensed with 10 to yield the final compounds 9a-d. Structural elucidation of synthesized compounds was accomplished by IR, ¹H NMR, ¹³C NMR and mass spectral data. Final compounds were screened for their antimicrobial activity.

Keywords : Pyrazole, thiazole, isoxazole, thiadiazole, carbothioamide, *w*-bromoethoxyphthalimide, thiazolidinone, thiosemicarbazide.

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Composition and antimicrobial activity study on essential oil from the aerial parts of Chinese licorice (*Glycyrrhiza uralensis* Fisch.)

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Abstract : *Glycyrrhiza uralensis* Fisch. has been used in Traditional Chinese Medicine (TCM) as one of the most important crude drug for thousands of years. By steam distillation, the essential oil from the aerial parts of licorice (*Glycyrrhiza uralensis* Fisch.) was obtained and analyzed by GC-MS. 28 components representing 74.39% of the total oil content were identified for the first time in this species. The main compounds in the oil were b-cadinene (12.28%), b-caryophyllene (10.04%), g-cadinene (9.49%), phytol (8.43%), a-cadinene (4.43%), caryophyllene oxide (3.65%) and a-gurjunene (3.48%). The antimicrobial activity of the oil was evaluated by investigation of MIC and MBC.

Keywords : *Glycyrrhiza uralensis* Fisch., essential oil, GC/MS, steam distillation, antimicrobial activity.

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Solvent-free microwave-expedited synthesis of ferrocenylenones and ferrocenyl-1,5-diketones using hydrotalcite

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Abstract : An efficient, facile microwave-assisted synthesis of ferrocenylenones and ferrocenyl-1,5-diketones is described using hydrotalcite as base under solvent-free condition. This protocol is extremely fast and is applicable to a wide variety of substrates.

Keywords : Acetophenone, acetylferrocene, aromatic aldehydes, ferrocenylchalcones, ferrocenylenones, 1,5-diketones, hydrotalcite. J. Indian Chem. Soc.,

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Fatty acids and sterols in the seeds of *Cassia auriculata* and *Cassia siamea*

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Abstract : The comparative study on the composition of fatty acids and sterols in the seed oil of *Cassia auriculata* Linn. and *Cassia siamea* Lam. was carried out. The total oil content in the seeds was found 3.25% in *Cassia auriculata* and 2.99% in *Cassia siamea*. Sterols and fatty acids have been isolated and characterized on the basis of chemical and GC analysis. Three sterols (cholesterol, stigmasterol and b-sitosterol) and four fatty acids (palmitic acid, stearic acid, oleic acid and linoleic acid) were found from the seed oil of both the plants. All compounds were identified by comparison with authentic samples. Linoleic acid, stigmasterol, b-sitosterol were identified as major constituents of the oil.

Keywords : *Cassia siamea*, *Cassia auriculata*, GLC, b-sitosterol, stigmasterol, palmitic acid, cholesterol, oleic acid, linoleic acid, stearic acid.

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Microwave assisted novel synthesis of isoxazole and their antibacterial activity

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Abstract : 3-[3-(2-Hydroxyphenyl)-isoxazol-5-yl]-chromen-4-one (4a-d) have been synthesized by the action of 1-(2-hydroxy-phenyl)-3-(4-oxo-4H-chromen-3-yl)-propane-1,3-diones and hydroxylamine hydrochloride in ethanolic medium under microwave irradiation. All the products have been evaluated for their antimicrobial activity against some Gram-positive and Gram-negative bacterial strains.

Keywords : Isoxazole, microwave, antimicrobial activity.

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Synthesis and biological activity of some new 1,3-thiazolyl-6-bromoquinazolin-4(3H)ones

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Abstract : The title compound 1,3-thiazolyl-6-bromoquinazolin-4(3H)ones 5_{i-xv} have been synthesized from the molecule 2-[(2,6-dichlorophenyl)amino]phenyl acetic acid **1** through multi-step reaction sequence. The structures of new compounds have been confirmed by elemental analyses, IR, ^1H and ^{13}C NMR spectral data. All the compounds were evaluated for their *in vitro* antibacterial and antifungal activities.

Keywords : Quinazolin-4(3H)one, 1,3-thiazole, antibacterial, antifungal.

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Benzophenone and methyl orange sensitized photooxidation of flavone and 4-methoxy flavone : A comparative study

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Abstract : Benzophenone and methyl orange sensitized photooxidation of flavone and 4-methoxy flavone (1a and b) by UV light in presence of air gave different products. With benzophenone where substrate is in the excited state, it gave 2a and b and with methyl orange and where oxygen is in the excited state, it gave 3a and b. The structures of the products have been confirmed by spectral and elemental analyses.

Keywords : UV, photooxidation, flavone, 4-methoxy flavone.

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Benzophenone and methyl orange sensitized photooxidation of flavone and 4-methoxy flavone : A comparative study

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Abstract : Benzophenone and methyl orange sensitized photooxidation of flavone and 4-methoxy flavone (1a and b) by UV light in presence of air gave different products. With benzophenone where substrate is in the excited state, it gave 2a and b and with methyl orange and where oxygen is in the excited state, it gave 3a and b. The structures of the products have been confirmed by spectral and elemental analyses.

Keywords : UV, photooxidation, flavone, 4-methoxy flavone.

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A novel one flask synthesis of 1,2-substituted 5-imidazolones

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Abstract : One flask synthesis of 4-arylmethylene-1-phenyl-2-styryl-2-imidazolin-5-ones was achieved by the phenyl isothiocyanate-mediated condensation of *N*-acetyl glycine with aromatic aldehydes.

Keywords : 5-Imidazolones, synthesis, aromatic aldehydes.

Naturally occurring odd number fatty acids in the rhizome oil of *Alpinia speciosa* K. Schum.

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Abstract : Contrary to usual observations, the rhizome oil of *Alpinia speciosa* K. Schum. is found to contain not only one but as much as five odd number carbon atoms containing natural fatty acids, apart from eight even carbon fatty acids. Among the fatty acids containing odd number of carbon atoms, the useful pentadecanoic acid (C-15) is main (21.9%) and others are C-23 (5.7%), C-13 (1.9%), C-11 (3.1%) and C-9 (0.1%). Among the fatty acids containing even number of carbon atoms, the highly unsaturated linolenic acid (C-18:3) is main (27.4%) and the next is the very useful arachidic acid (C-20), 22.4%. The total saturated fatty acids constitute 65.7% and unsaturated 34.3%.

Keywords : *Alpinia speciosa*, *Alpinia zerumbet*, *Alpinia nutans*, Zingiberaceae, fatty oil, natural fatty acids.