**Influence of dielectric constant on chemical speciation of Ca\textsuperscript{II}, Zn\textsuperscript{II} and Mn\textsuperscript{II} with L-valine**

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**Abstract:** The titrations are carried out with sodium hydroxide in varying concentrations (0–60\% v/v) of propylene glycol-water mixtures at ionic strength of 0.16 mol L\textsuperscript{–1} and temperature 303 K. Models containing different number of species were refined by using the computer program MINIQUAD75. The species ML\textsuperscript{+}, ML\textsubscript{2}\textsuperscript{+} and ML\textsubscript{3}\textsuperscript{+} were chosen based on exhaustive modeling studies. The best-fit chemical models were arrived at based on statistical parameters. The linear increase in the stability of the complexes with decreasing dielectric constant of the medium indicates the dominance of electrostatic forces in the equilibrium process under the present experimental conditions. The order of the stabilities of the complexes is Ca\textsuperscript{II} < Mn\textsuperscript{II} < Zn\textsuperscript{II}. The species distribution and the feasible equilibria for the formation of the species are also presented.

Keywords: Chemical speciation, L-valine, propylene glycol, MINIQUAD75.

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**Copper(II) complexes with N-(2-hydroxyethyl)-2-iminodiacetic acid and benzohydrazide ligands: Synthesis, electrochemical, spectroscopic, antimicrobial and SOD activity**

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**Abstract:** Five new copper(II) complexes, viz. [Cu(HIda)(L\textsuperscript{1})] \textsubscript{2}; [Cu(HIda)(L\textsuperscript{2})] \textsubscript{2}; [Cu(HIda)(L\textsuperscript{3})] \textsubscript{3}; [Cu(HIda)(L\textsuperscript{4})] \textsubscript{4}; [Cu(HIda)(L\textsuperscript{5})] \textsubscript{5}; where HIda = N-(2-hydroxyethyl)-2-iminodiacetic acid; L\textsuperscript{1} = benzoylhydrazide; L\textsuperscript{2} = N-[(1)-1-(2-methylphenyl)ethyldene]benzohydrazide; L\textsuperscript{3} = N-[(1)-1-(4-methylphenyl)ethyldene]benzohydrazide; L\textsuperscript{4} = N-[(1)-1-(2-methoxyphenyl)ethyldene]benzohydrazide; L\textsuperscript{5} = N-[(1)-1-(4-methoxyphenyl)ethyldene]benzohydrazide; have been synthesized and characterized by elemental analyses, FAB (fast atomic bombardment), magnetic measurements, electronic absorption, conductivity measurements, cyclic voltammetry (CV) and electron paramagnetic resonance (EPR) spectroscopy. The EPR spectra of these complexes in frozen solutions of DMSO showed a single at \( g \) ca. 2. The trend in \( g \)-value (\( g_{||} > g_{\perp} > 2.00 \)) suggest that the unpaired electron on copper(II) has \( d_{x^2-y^2} \) character. The superoxide dismutase activity reveals that these complexes catalyze the fast disproportionation of superoxide in DMSO solution. The antibacterial and antifungal activities of the complexes have also been investigated.

Keywords: Copper(II) complexes, EPR, CV, SOD activity, antimicrobial activity.
Synthesis, crystal structure of poly-catena-[bis(1,3-dimethyl-imidazolium)penta-iodo-tri-silver(I)

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Abstract: The title complex [(CH₃₂CH(NC₆H₅CHN)C₆H₃)]₂⁺[(Ag₃I₅)₂⁻]ₙ has been synthesized by the reaction of Ag₂O with [CH₃₂CH(NC₆H₅CHN)C₆H₃]⁺I⁻ in a 1:3 molar ratio at 189 ºC in DMSO, and characterized by elemental analysis, ¹H NMR and single-crystal X-ray diffraction analysis. It crystallizes in monoclinic, space group C₂/c with a = 20.7730 (15), b = 9.3968 (5), c = 14.8753 (11) Å, β = 122.906(2)°, V = 2437.8 (3) Å³, Mₑ = 3.140 g/cm³, μ(MoKα) = 8.72 mm⁻¹ and F(000) = 2048. The structure was refined to R = 0.035 and wR = 0.127 for 1921 observed reflections with I > 2σ(I). The asymmetric unit of the title complex [(C₅H₉N₂)⁺]₂⁺[(Ag₃I₅)₂⁻]ₙ, contains two independent Ag⁺ ions, one of which is disordered across a two-fold rotation axis. Both components of disorder are coordinated to the same three I atoms in a flattened trigonal pyramidal geometry. The other Ag⁺ ion is coordinated to four I atoms in a slightly distorted tetrahedral environment and this unit is related across an inversion center to form an Ag₂I₆ unit with two bridging I atoms. All I atoms are bridging to form one-dimensional chains along [001] consisting of alternating AgI₃ and Ag₂I₆ units. The cations lie between the chains.

Keywords: Polymeric, silver, crystal structure, imidazolium.


CeO₂-Cs₂O-CuO highly efficient catalyst for the synthesis of 5,6,7,8-tetrahydro-4-aryl-2-(phenylamino)quinoline-3-carbonitrile derivatives

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Abstract: Mesoporous CeO₂-Cs₂O-CuO catalyst was prepared by co-precipitation method. Prepared catalytic material was analysed by means of powder X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive spectroscopy (EDS), BET surface area and Py-adsorption FT-IR study to identify the morphology, elemental compositions, surface area and acidic sites. Prepared catalyst was used for the synthesis of 5,6,7,8-tetrahydro-4-aryl-2-(phenylamino)quinoline-3-carbonitrile derivatives. The synthesis of these derivatives was carried out in one-pot four-component, reaction of aromatic aldehydes, cyclohexanone, malononitrile and aromatic amine. This protocol has several advantages such as non-toxic, non corrosive, clean, easy separation of catalyst.

Keywords: Heterogeneous catalyst, XRD, SEM, EDS, multicomponent reaction, medicinal uses.


Thermodynamic studies of adduct formation reactions between organotin(IV)dichlorides and NiII macrocycles

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Abstract: This article presents σ-acceptor strength for the diorganotin(IV) dichlorides: dimethylindichloride, diphenylindichloride and dibutylindichloride as Lewis acids toward some macrocyclic nickel(II) complexes. Thermodynamic of the adducts formation of the tin(IV) dichlorides with Ni(II)tetraaza Schiff base complexes such as: [Ni(Me₂-Bzo₂[14]-tetraeneN₄)], [Ni(Me₄-4-CH₃Bzo₂[14]tetraeneN₄)], [Ni(Me₄-4-ClBzo₂[14]tetraeneN₄)] and [Ni(Me₂Ph₂-Bzo₂[14]tetraeneN₄)], [Ni(Me₂Ph₂-4-CH₃Bzo₂[14]tetraeneN₄)], [Ni(Me₂Ph₂-4-ClBzo₂[14]tetraeneN₄)] that Me₄-Bzo₂[14]tetraeneN₄ denotes: (5,7,12,14-tetramethyl dibenz[b,i][1,4,8,11]tetraazacycloc-tetradecine), was studied in acetonitrile by means of UV-Vis spectrophotometric analysis. The thermodynamic parameters and the formation constant values show the acidity trend for diorganotin(IV) dichlorides as follow: Ph₂SnCl₂ > Me₂SnCl₂ > Bu₂SnCl₂. Adducts have been synthesized and fully characterized by ¹H NMR, ¹¹⁹Sn NMR, IR, UV-Vis spectra and elemental microanalysis (C.H.N) methods. The trend of the adduct formation of the nickel complexes with a given tin acceptor decrease as follow: [Ni(Me₄-4-CH₃Bzo₂[14]tetraeneN₄)] > [Ni(Me₄-Bzo₂[14]tetraeneN₄)] > [Ni(Me₂Ph₂-4-CH₃Bzo₂[14]tetraeneN₄)] > [Ni(Me₂Ph₂-Bzo₂[14]tetraeneN₄)] > [Ni(Me₂Ph₂-4-ClBzo₂[14]tetraeneN₄)].

Keywords: Diorganotin(IV) dichlorides, thermodynamic, tetraaza Schiff base, nickel(II) complex.


Spectrophotometric determination of mercury(II) in environmental, soil, medicinal and biological samples using 2-benzoylpyridine-4-methyl-3-thiosemicarbazone (BPMT)

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Abstract: Analytical and biological applications of 2-benzoylpyridine-4-methyl-3-thiosemicarbazone (BPMT) are reported for the first time. The reagent (BPMT) has been synthesized and characterized by IR, NMR, and mass spectral data. BPMT reacts with mercury(II) in slightly acidic medium (pH 6.0 sodium acetate-acetic acid buffer) to form deep yellow coloured complex. The complex shows maximum absorbance at 410 nm. The molar absorptivity and Sandell’s sensitivity of the method are found to be 4.7 × 10⁴ L mol⁻¹ cm⁻¹ and 0.0103 µg cm⁻² of mercury(II). The composition of the complex is found to be 1 : 1 (M : L). The method is successfully applied to a number of environmental, biological, medicinal and soil samples. The results are comparable with those obtained by dithizone method. The proposed system has high sensitivity, accuracy and precision (s = 0.078 for 4 µg/ml in BPMT method).

Keywords: Spectrophotometry, mercury determination, 2-benzoylpyridine-4-methyl-3-thiosemicarbazone, water, medicinal, biological and soil samples.

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Synthesis, characterization and ion exchange behavior of a new four components cation exchanger based on SnIV

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Abstract: Present paper describes a new method for synthesis of tin(IV) iodotungstosilicate (TITTS) exchanger. Ion exchange capacity (IEC) of the exchanger is found to be 0.86 meq/g for Na+, possesses good stability against high temperature up to 600 °C and chemicals of different strengths. IEC is determined for different metal ions, distribution studies are done and $K_d$ values are calculated. The exchanger is selective for lead ions as shown by $K_d$ value (176.78). IR of the compound indicates all the four expected components. XRD and SEM show that exchanger is in amorphous form. The synthesized material is useful in separation, water softening and water decontamination.

Keywords: Inorganic exchanger, exchange capacity, stability, $K_d$ value.


32- and 28-Macro cyclic poly ammonium cations assisted pseudo two-dimensional assembly of citrate stabilized gold nanoparticles

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Abstract: Macro cyclic poly ammonium cations (MCPAC), [32]ane-(NH$_2^+$)$_8$Cl$^-$ (32-MCPAC), and [28]ane-(NH$_2^+$)$_6$O$_2$Cl$^-$ (28-MCPAC), which are highly water soluble, are well reputed for their anion recognition and metal nanoparticles (MNs) stabilization properties. First time, we have employed them as cross-linkers for organizing negatively charged citrate-stabilized gold nanoparticles (Au-NPs) into a pseudo two-dimensional (2-D) array. Assembled Au-NPs were characterized by UV-Vis spectroscopy and Transmission Electronic Microscopy (TEM). The UV-Vis spectrum of citrate-stabilized Au-NPs so prepared of diameter ~12 nm shows Surface Plasmon Resonance (SRP) at ca. 520 nm, indicating discrete nature of Au-NPs. The UV-Vis spectra of Au-NPs in the presence of 32-/28-MCPAC show red-shifted and broadened SRP maxima centered at ca. 580 nm for 32-MCPAC and at ca. 605 nm for 28-MCPAC which are attributed to the inter-particle plasmon absorbance, indicating large compact isotropic assembly of Au-NPs. The concrete evidence was obtained from the TEM images which reveal that the particles are arranged pseudo 2-D without any severe agglomeration. Photographs of all the solutions were taken and indicate how the color of almost discrete Au-NPs (wine-red color) changes to get assembled Au-NPs (bluish). The study of pH effect on assembling Au-NPs reveals that the electrostatic attraction followed by hydrogen bonding interaction between MCPAC and citrate ions leads to the formation of 2-D array of Au-NPs. In addition, at pH 12.30 when the cross-linking property of MCPACs was nullified, Au-NPs were formed rod-like aggregation. Assembled Au-NPs would be futuristic promising materials, especially for optoelectronic devices.

Keywords: Gold nanoparticles, macrocyclic polyammonium cations, assembly, 2-D array, water.


Spectrophotometric determination of palladium(II) with N-decylpyridine-4-amine from malonate media

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Abstract: Spectrophotometric determination of palladium(II) with N-decylpyridine-4-amine in xylene from malonate medium was carried out. Palladium(II) was extracted quantitatively with 10 ml of 1 x
Spectrophotometric determination of nickel at microgram level in environmental matrices using 4-hydroxybenzaldehyde thiosemicarbazone

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Abstract: The reagent 4-hydroxybenzaldehyde thiosemicarbazone (4-HBTS) has been synthesized, characterised and its analytical applications were investigated. The reagent 4-HBTS reacts with Ni\textsuperscript{II} in aqueous solution in the pH range 5–6 at room temperature and forms a green coloured 1:2 [Ni\textsuperscript{II}:4-HBTS] complex with stability constant $2.76 \times 10^{11}$. The complex has maximum absorption at 362 nm. The molar absorptivity and Sandell's sensitivity for the coloured solution are found to be $2.13 \times 10^{4}$ M\textsuperscript{–1} cm\textsuperscript{–1} and 0.0027 µg/cm\textsuperscript{2} respectively. Beer's law is obeyed in the range of 0.117–1.117 µg/mL.

The interference of various diverse ions has been studied. The procedure was successfully applied for the determination of nickel in water, waste water samples and in different alloy samples.

Keywords: Nickel determination, spectrophotometry, 4-hydroxybenzaldehyde thiosemicarbazone, waste water, alloy samples.

Investigation of the conductance, micellization and dissociation behaviour of uranyl caprylate and laurate in mixed organic solvents

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Abstract: Conductance measurements were employed to determine the critical micellar concentration (CMC), molar conductance at infinite dilution, degree of dissociation, dissociation constant and thermodynamic parameters for dissociation and association processes of uranyl caprylate and laurate in 50/50 benzene-dimethylsulphoxide (v/v) mixture. These soaps behave as a weak electrolytes in dilute solutions below the CMC and Debye-Huckel-Onsager's equation is not applicable to these solutions. The thermodynamic parameters indicate that the micellization process is favoured over the dissociation process.

Keywords: Uranyl soaps, critical micellar concentration, micellization heat of dissociation, free energy.
Triflumizole encapsulation by 2-hydroxypropyl and sulphated derivatives of β-cyclodextrin

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Abstract : Spectroscopic studies were done on the inclusion of triflumizole (TF) into the cavities of two derivatives of β-cyclodextrin namely hydroxypropyl-β-cyclodextrin (HP-β-CD) and sulphated-β-cyclodextrin (S-β-CD). The affinity of TF for the cavities of cyclodextrin derivatives was found to be dependent on the interaction forces responsible for complexation. Solubility enhancement of TF by HP-β-CD and S-β-CD has been explained using a thermodynamic approach. Calculations of the thermodynamic parameters showed that the inclusion reaction was favored by entropy-enthalpy compensation phenomenon. Phase solubility studies showed that both the inclusion complexes were of A type indicating enhancement of the solubility of TF molecule upon encapsulation.

Keywords : Hydroxypropyl-β-cyclodextrin, inclusion complexes, solubility, sulphated-β-cyclodextrin, triflumizole.

Characterization of tobacco leaves in different brands of cigarettes (Indian and Foreign) and their impacts from the social and forensic point of view

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Abstract : Smoking of cigarettes containing tobacco, a widely used delicacy for common masses, has been regarded to be the causes of cancer, heart and a host of other diseases. In spite of extensive researches on tobacco and its different products like nicotine, polycyclic aromatic hydrocarbons, there appears to be a void in the findings. Efforts have been made to make a comparative study on the tobacco and its constituents in different brands of cigarettes ultimately to be related to have some idea on the effectiveness of the filter beds (of cigarettes) in removing nicotine and other hazardous chemicals. Efforts have been made to find out the origin of cigarettes by isotope-ratio monitoring and determining the relative abundances of total isotopes of nicotine (present in tobacco of different brands) using GC-MS and SIM mode of measurements. The observations are also of importance to identify counterfeit cigarettes as well as criminals (a new aspect).

Keywords : Cancer, cigarette brands, criminology, counterfeit cigarettes, gas chromatography-mass spectrometry (GC-MS), isotope ratio, nicotine, polycyclic aromatic hydrocarbons, SIM.
Photo oxidative degradation of metanil yellow by photo-Fenton reagent

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Abstract : At normal laboratory temperature and atmospheric pressure, experiment on waste water containing metanil yellow by photo-Fenton process were conducted to examine the effect of operating variables like the concentration of ferric ion, concentration of metanil yellow, pH, hydrogen peroxide and light intensity on the reaction rate. Metanil yellow was completely oxidized and degraded into CO\textsubscript{2} and H\textsubscript{2}O in this experiment. A mechanism for photochemical bleaching of metanil yellow by photo-Fenton's reaction has been processed.

Keywords : Photochemical degradation, photo-Fenton, metanil yellow, advance oxidation processes.

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Bioremediation of Cd\textsuperscript{II} from aquatic systems by Bermuda grass matrix

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Abstract : This work was undertaken to explore low cost and efficient sorbents for the removal of cadmium(II) from aqueous solution. For this purpose dried Bermuda grass was taken. The optimum experimental conditions were established for maximum removal of Cd\textsuperscript{II} from the aqueous solution. Besides studying the effect of temperature, pH, contact time, concentration of metal ion and adsorbent doses the adsorption kinetics and equilibrium were also investigated. Kinetic studies suggested that the adsorption follows second order reaction. Equilibrium data were analyzed using Langmuir and Freundlich isotherms.

Keywords : Adsorbent, cadmium, dried Bermuda grass, Langmuir and Freundlich isotherms, intra-particle diffusion, thermodynamics.

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Inclusion complexation of hydroxybenzenes with natural and modified \(\alpha\)- and \(\beta\)-cyclodextrins

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Abstract : Host-guest association between four hydroxybenzenes such as 1,2-dihydroxybenzene (2DHB), 1,3-dihydroxybenzene (3DHB), 1,4-dihydroxybenzene (4DHB) and 1,2,3-trihydroxybenzene (3HB) with \(\alpha\)-CD, \(\beta\)-CD, HP-\(\alpha\)-CD and HP-\(\beta\)-CD were carried out using UV-Visible, steady-state and time-resolved fluorescence, FT-IR, \(^1\text{H}\) NMR and semi-empirical methods (PM3). Stoichiometry ratios, binding constants and stability of the inclusion complexes were studied, showing that 1 : 1/host :
guest complexes was formed. From the computational study, we found that (i) the stability of the four inclusion complexes are the same, (ii) the four HBs are fully encapsulated into the CDs, (iii) the negative Gibbs energy and enthalpy changes for the inclusion complexes indicated that the formation of these complexes is spontaneous and exothermic, (iv) hydrogen bonding interactions play a major role in the inclusion process and (v) the computational results indicate that the formation of all the inclusion complexes are enthalpy driven process.

Keywords: Dihydroxybenzenes, cyclodextrins, inclusion complex, supramolecular chemistry, semi-empirical calculation.

Determination of trace metal contents of tobacco in different brands of cigarettes – a valuable tool in forensic investigation and criminology

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Abstract: Tobacco leaves used in cigarettes for smoking contain various toxic trace elements. These are expected to be absorbed in human body relatively in excess and may exceed toxic limits due to repeated uses of cigarettes through years. Trace metal contents like cobalt, nickel, copper, zinc, lead, cadmium, arsenic and mercury were determined quantitatively for tobacco in different brands of Indian cigarettes. They may not be health hazards at low concentrations but the cumulative effects for years of frequent cigarette smoking may prove to be fatal.

Metal contents in cigarettes may be used to differentiate and establish the smuggled or counterfeit origin of cigarettes but it is a relatively less used tool of potential interest from the point of view of forensic investigation and criminology.

Keywords: Counterfeit cigarettes, criminology, health hazards, metal contents, tobacco leaves, toxic elements.

Defluoridation performances of tailor-made thin film polyamide composite membranes

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Abstract: To set the ball rolling on enhancing life expectancy, it is worthwhile to ensure the access to a life of good quality. Of the factors that make a quality life, fresh water as the ingredients basic to human advancement. A significant step toward the efficient applications of thin film composite membrane is fluoride removal from water. The efficiency of filtration is controlled by base polymer polysulfone (PS) concentration and follows the increasing trend with the PS concentration though sacrifices its water fluxes. The fluoride feed concentrations also influence the membrane performances. Thin film composite membrane (Memb-III) (having PS 18% w/w in dimethyl formamide) shows maximum 92.8% separation of 20 mg/L fluoride, sacrifices 65% volume flux ($J_V$) compared to Memb-I (having 13% w/w PS). Modifications of thin film composite membrane by polystyrene sulfonate show maximum 2% improvement in separation for all the membranes. The polystyrene sulfonate modified membrane, Memb-III-PSSA (i.e. TFC membrane based on PS18% with PSSA) shows the maximum rejection.

Keywords: Water, fluoride, thin film composite membranes, separation.
Photovoltaic properties of 2-(coumarinyl-6-azo)imidazoles and their derivatives

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Abstract: Photovoltaic property of 2-(coumarinyl-6-azo)imidazoles and their derivatives, 1-alkyl-2-(coumarinyl-6-azo)imidazoles have been studied. Light-energy conversion efficiency (\(\eta\)) is dependent on charge anisotropy in the molecule. Substitution of methyl group (1-Me) at imidazolyl ring increases the photovoltaic power conversion efficiency (\(\eta\)), fluorescence quantum yield (\(\phi\)) and excited state life time (\(\tau\)). DFT calculation has been carried out from the optimized structures and data are used to interpret the photovoltaic property of the compounds.

Keywords: 2-(Coumarinyl-6-azo)imidazoles, photovoltaic property, DFT computation.

Photophysical investigations on interaction of \(p\)-bromoacetanilide with eosin in solution

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Abstract: The photophysical properties of \(p\)-bromoacetanilide were studied in neat methanol solution. The characteristic excitation and emission spectra were recorded and compared with the behavior in the solid state. Interaction of \(p\)-bromoacetanilide with an anionic fluorophore, eosin, was studied by steady state measurements and the behavior was gauged by using Stern-Volmer kinetics. A significant decrease in fluorescence intensity was observed and this was attributed to a combined phenomenon of static and dynamic quenching. The ground state interaction between the halide ions were found to be predominant than the dynamic quenching. The rate constants of the quenching phenomena were obtained from modified Stern-Volmer equation.

Keywords: \(p\)-Bromoacetanilide, eosin, methanol, luminescence, quencher.

Effects of ultrasonic assist on the solution properties of hydrophobically associating polyacrylamide

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Abstract: In order to study the effects of ultrasonic assist during the synthesis process on the solution properties of hydrophobically associating polyacrylamide (U-HAPAM), U-HAPAM was prepared by acrylamide, 2-acrylamido-2-methyl propane sulfonic acid, acrylic acid and octadecyl acrylate (ODA). The solution properties of U-HAPAM and control sample (HAPAM, without ultrasonic assist) were investigated through rheometer, laser particle size analyzer and AFM. The molecular structure of U-HAPAM was investigated by FT-IR. The results showed that the critical association concentrations (C*) changed from 0.35 wt% (HAPAM) to 0.28 wt% (U-HAPAM), which was attributed to the well dispersion of ultrasound for ODA. Learned from laser particle size analyzer and AFM, U-HAPAM had stronger hydrophobic association than HAPAM. The novel method of preparation of HAPAM should be adequately attracted attention.

Keywords: Hydrophobic association, polyacrylamide, ultrasonic assisted polymerization, octadecyl acrylate, solution properties.

Synthesis, characterization and evaluation of in vitro antimicrobial activity of carbonyl derivatives of sulphonamide compounds

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Abstract: Sulphonamide compounds (1-4) were synthesized by simple condensation of sulphanilamide with carbonyl derivatives. The compounds were characterized by elemental analysis, IR, 1H and 13C NMR spectroscopy. All the carbonyl derivatives form Schiff base compounds (2-4) with sulphanilamide while with acetylacetone; the Schiff base compound formed undergoes keto-enol tautomer and then crystallized as 4-(4-oxopent-2-ylamino)benzene sulphonamide compound (1) in which azomethine nitrogen atom is protonated. The 1H and 13C NMR spectroscopy data indicates the formation of the compounds and reveals the protonation of azomethine nitrogen atom in compound 1 which has also been confirmed by X-ray crystal structure. All the compounds were screened for antibacterial and antifungal activities against different microbes. Compound 1 and 2 were found to be effective antifungal agents against C. albicans while 3 and 4 shown antibacterial activities against Escherichia coli and Salmonella paratyphi. The minimum inhibition concentration of all the compounds were also determined and compared with standard drugs.

Keywords: Sulphonamides, X-ray crystallography, antibacterial and antifungal activity.

Sterol composition of Ajuga bracteosa Wall Benth., Ajuga macrosperma Wall ex Benth. and Ajuga parviflora Benth.

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Abstract: The sterol composition of Ajuga bracteosa Wall Benth., Ajuga macrosperma Wall ex Benth. and Ajuga parviflora Benth. was studied. The sterols were isolated from the leaves and subjected to GC-MS analysis. The sterol composition of Ajuga bracteosa Wall Benth. was found to be 3α-hydroxy-5α-cholest-7-en-24-oic acid, 24-methylcholesterol and 24-oxocholesterol. The sterol composition of Ajuga macrosperma Wall ex Benth. was found to be 3β-hydroxy-5α-cholestane-17β-ol, 3β-hydroxy-5α-cholest-7-en-24-oic acid and 24-methylcholesterol. The sterol composition of Ajuga parviflora Benth. was found to be 3α-hydroxy-5α-cholestane-17β-ol, 3β-hydroxy-5α-cholestane-17β-ol and 24-oxocholesterol.
Abstract: Sterols isolated from Ajuga bracteosa Wall Benth., Ajuga macrosperma Wall ex Benth. and Ajuga parviflora Benth. of family Lamiaceae were studied by GC-MS analysis of their trimethylsilyl ether derivatives. Individual sterols and conjugated authentic samples were used for identification of components present in the sterol mixtures isolated from the plants. A. bracteosa Wall Benth. was found to contain the highest amount of dehydrocleyosterol (51.14%) followed by cleyosterol (36.18%) of the total sterol content. Campesterol (2.30%), sitostanol (1.27%) was present in lower quantities. A. macrosperma Wall ex Benth. contained dehydrocleyosterol (58.89%), cleyosterol (35.58%), sitosterol (1.89%) and campesterol (1.73%). A. parviflora Benth. contained cleyosterol (58.71%), sitosterol (0.93%) and campesterol (0.76%). Stigmasterol could not be detected in any samples.

Keywords: Lamiaceae, Ajuga bracteosa, Ajuga macrosperma, Ajuga parviflora, sterols.

Multicomponent analysis of a ternary mixture of paracetamol, ibuprofen and caffeine in Novafen capsules with the aid of chemometrics

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Abstract: Net analyte signal standard addition method (NASSAM) has been presented for the simultaneous determination of paracetamol, ibuprofen and caffeine by spectrophotometry. The method combines the advantages of the standard addition method with the net analyte signal concept which enables the extraction of information concerning a certain analyte from spectra of multi-component mixtures. This method has some advantages such as the use of a full spectrum realization in determination step, therefore, it does not require calibration and prediction steps and only a few measurements are required for the determination. The simultaneous determination of paracetamol, ibuprofen and caffeine was performed in Britton-Robinson buffer (pH 10.0). Three pharmaceutical compounds were determined in concentration ranges of 0.4–320 µmol L⁻¹, 0.4–240 µmol L⁻¹ and 0.4–260 µmol L⁻¹ respectively. For study the accuracy of the proposed method, NASSAM has been successfully applied to the simultaneous determination of pharmaceutical compounds in some synthetic and pharmaceutical formulations (Novafen capsules) with the recoveries in the range of 84.3–108.7% with the RSD (%) of 0.43–3.9%.

Keywords: Paracetamol, ibuprofen, caffeine, NASSAM, Novafen.

Successive ratio spectra derivative method for simultaneous determination of aspirin, ascorbic acid and paracetamol in some pharmaceutical formulations

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Abstract: Successive ratio derivative method based on the spectrophotometric data has been developed for the simultaneous determination of a ternary mixture containing aspirin, ascorbic acid and paracetamol, without prior separation. The method is based on the successive derivative of ratio

spectra in two steps. The mathematical explanation of the procedure is illustrated. The concentrations of three compounds in their mixture are determined by using their respective standard addition plots at either the maximum/minimum selected wavelengths. The selected wavelengths for determination of aspirin, ascorbic acid and paracetamol are 296.0, 257 and 261.0 nm respectively. The mean recoveries for determination of aspirin, ascorbic acid and paracetamol were 100.8, 99.4 and 100.0 respectively in some ternary mixtures with the limit of detections \( (3S_b) \) as 0.29, 0.76 and 0.48 \( \mu \text{mol L}^{-1} \) in Britton-Robinson buffer solution (pH 11.0). The method was applied successfully for the analysis of Afebryl tablet and effervescent powders containing aspirin, ascorbic acid and paracetamol.

Keywords: Aspirin, ascorbic acid, paracetamol, successive ratio derivative method, analysis.