

## Electrophoresis, surface charge and surface activity coefficient of ionic adsorbates at interfaces<sup>†</sup>

D. K. Chattoraj

Department of Food Technology & Biochemical Engineering, Jadavpur University, Kolkata-700 032, India

E-mail : dkchattoraj@hotmail.com

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**Abstract :** Historical development of measurements of electrophoretic mobilities of solid particles and proteins using moving boundary techniques have been discussed in brief. Results on micro-electrophoretic methods of mobility measurements of solid particles adsorbed with proteins and other biopolymers have also been elaborated and features of electrophoretic separation of biomolecules using various types of zone electrophoresis techniques have been mentioned. The corrections required in connecting electrophoretic mobilities with electrokinetic or zeta potential using Smoluchowski relation discussed by Henry, Booth, Ghosh and others have been mentioned. The pictures included in the electrical double layers proposed by Helmholtz, Gouy-Chapman and Stern have been discussed. From the adsorption experiments of surfactants at oil-water interfaces, the charge densities ( $\sigma$ ) and diffuse double layer potentials ( $\psi_d$ ) at a given concentration have been evaluated. The data are observed to fit the Stern layer model with counter-ion binding at the charged surface.  $\psi_d$  is found to be significantly higher than zeta potential.

From the boundary tension measurement, the surface tension lowering or surface pressure  $P$  for soluble monobasic and dibasic acids have been calculated at different values of area  $A$  per adsorbed molecule. The electrical pressure  $P_e$  obtained for these acids in the monolayer does not fit the Gouy model of double layer but using Stern model, the extents of counter-ion binding in the monolayer can be calculated. Using the Langmuir surface balance experiments,  $P$ - $A$  curves for insoluble monolayers of different behenate salts have been obtained. At pH 12.0, values of  $P_e$  depends upon extents of counter-ion binding, hydration and other factors.

A new concept of surface activity coefficient based on Raoult's law, and Henry's law have been introduced to explain deviation of  $P$  from their ideal values.  
Keywords : Ionic adsorbates, electrophoresis, surface activity coefficient, surface charge.

## Mixed-ligand complex formation equilibria of Cu<sup>II</sup> with glycylglycinate and guanylyurea

Tannistha Roy Barman and G. N. Mukherjee\*

Department of Chemistry, University College of Science, University of Calcutta, 92, Acharya Prafulla Chandra Road, Kolkata-700 009, India

E-mail : gmchem@rediffmail.com Fax : 91-33-2351-9755/2241-3222

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**Abstract :** Combined spectrophotometric and computer based pH metric investigation on the mixed ligand complex formation equilibria of Cu<sup>II</sup> with glycylglycine ( $\text{H}_3\text{N}^+\text{CH}_2\text{CONHCH}_2\text{COO}^-$ , HGG<sup>±</sup>) and guanylyurea [ $\text{H}_2^1\text{NC}(\text{=O})^2\text{NHC}(=\text{N}^3\text{H})^4\text{NH}_2$ , HGu] in aqueous solution at  $25 \pm 1$  °C, at a fixed ionic strength,  $I = 0.1 \text{ mol dm}^{-3}$  ( $\text{NaNO}_3$ ), indicate variety of binary and ternary complexes :  $[\text{Cu}(\text{GG})^+\text{aq}]$ ,  $[\text{Cu}(\text{GG-H})(\text{H}_2\text{O})]$ ,  $[\text{Cu}(\text{GG-H})(\text{OH})^-]$ ,  $[\text{Cu}(\text{Gu})^+\text{aq}]$ ,  $[\text{Cu}(\text{Gu})(\text{OH})]$ ,  $[\text{Cu}(\text{Gu-H})(\text{OH})^-]$ ,  $[\text{Cu}(\text{GG-H})(\text{Gu})^-]$ ,  $[\text{Cu}(\text{GG-H})(\text{Gu-H})^{2-}]$  and  $[\text{Cu}(\text{GG-H})(\text{Gu-2H})^{3-}]$ . At pH  $\approx 4.5$ , GG<sup>-</sup> ion provides neutral ( $\text{NH}_2$ , C=O) bidentate chelation to Cu<sup>II</sup> and above pH 4.5-5, coordinated GG<sup>-</sup> is transformed to amide deprotonated glycylglycinate dianion, (GG-H)<sup>2-</sup>, which provides terdentate equatorial ( $\text{NH}_2$ , N<sup>-</sup>, COO<sup>-</sup>) chelation to Cu<sup>II</sup>. Consequently in the electronic spectra  $\lambda_{\text{max}}$  of Cu<sup>II</sup> is blue shifted.  $\lambda_{\text{max}}$  of the ternary complex,  $[\text{Cu}(\text{GG-H})(\text{Gu})^-]$ , indicates a square pyramidal geometry existing in a isomeric structural equilibrium, involving bidentate axial ( $=\text{N}^3$ ) and equatorial

(O=C)/(H<sub>2</sub><sup>1</sup>N)/(H<sup>1</sup>N=C) chelation by Gu<sup>-</sup> ion. Above pH 7, [Cu(GG-H)(Gu)<sup>-</sup>] undergoes deprotonation of the (H<sup>1</sup>N=) and HO-(enolic) moieties of coordinated Gu<sup>-</sup> in successive steps.  
Keywords : Glycylglycine, guanylurea, copper(II), mixed ligand complexes, formation constants.

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## Synthesis, reactions and physico-chemical (IR, UV-Visible, FAB-MS and thermogravimetric) studies of new complexes of nickel(II) containing {2-(*o*-hydroxyphenyl)}-benzimidazole moiety<sup>†</sup>

Raj Kumar Dubey<sup>a\*</sup>, Chandrakant M. Mishra<sup>b</sup>, Pragma Baranwal<sup>a</sup> and Shiva Shankar Dubey<sup>c</sup>

<sup>a</sup>Synthetic Inorganic & Metallo-Organic Research Laboratory, Department of Chemistry, University of Allahabad, Allahabad-211 002, Uttar Pradesh, India

E-mail : rajalkoxy@yahoo.com

<sup>b</sup>Department of Chemistry, R. J. College, Ghatkopar, Mumbai-400 086, India

<sup>c</sup>Department of Chemistry, S. M. D. College, Poonpoo, Patna, Bihar, India

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**Abstract :** Mono-{2-(*o*-hydroxyphenyl)}-benzimidazole nickel(II) chloride, [(m-Cl)<sub>2</sub>Ni<sub>2</sub>{h<sup>2</sup>-(pbz)}<sub>2</sub>] (1) and bis-{2-(*o*-hydroxyphenyl)}-benzimidazole nickel(II), [Ni{h<sup>2</sup>-(pbz)}<sub>2</sub>] (2) have been prepared by the reactions of nickel(II) chloride with {2-(*o*-hydroxyphenyl)}-benzimidazole (pbzH) in 1 : 1 and 1 : 2 molar ratio(s), respectively. Complex 1 was treated with sodium salts of Schiff bases (sb) [sb = smabH, sapH], isopropoxide, aluminiumtetraisopropoxide, aryloxo- and alkoxo-salts in the presence of THF-C<sub>6</sub>H<sub>6</sub> to synthesise mixed ligand complexes of the types : [(smab)Ni{h<sup>2</sup>-(pbz)}] (1a), [(sap)Ni{h<sup>2</sup>-(pbz)}] (1b), [(m-OPri)<sub>2</sub>Ni<sub>2</sub>{h<sup>2</sup>-(pbz)}<sub>2</sub>] (1c), [(m-OAr)<sub>2</sub>Ni<sub>2</sub>{h<sup>2</sup>-(pbz)}<sub>2</sub>] (1d) and [(m-OPri)<sub>2</sub>Al(OPri)<sub>2</sub>Ni{h<sup>2</sup>-(pbz)}] (1e). All these new products have been characterised by spectroscopic [IR, Electronic (UV-Visible), FAB-MS], thermogravimetric and magnetic studies.  
Keywords : Nickel(II) complexes of {2-(*o*-hydroxyphenyl)}-benzimidazole, synthesis and spectroscopic studies.

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## Molecular structure of an oxorhenium(V) '3+1' mixed ligand complex

Jnan Prakash Naskar<sup>a</sup> and Shubhamoy Chowdhury<sup>b\*</sup>

<sup>a</sup>Department of Chemistry, Jadavpur University, Kolkata-700 032, India

E-mail : jpnaskar@rediffmail.com Fax : 91-33-24146223

<sup>b</sup>Shree Ramakrishna B. T. College, Bugmari House, Darjeeling-734 101, West Bengal, India

E-mail : s.chowdhury08@gmail.com

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**Abstract :** Reaction of [Re(O)(Cl){h<sup>3</sup>-(SCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>S}] with 3-amino-5-mercapto-1,2,4-triazole in 1 : 2 molar proportion in acetonitrile gives rise to a red compound, [ReO{h<sup>3</sup>-(SCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub>S}(C<sub>2</sub>H<sub>3</sub>N<sub>4</sub>S)] (1). Subsequent crystallisation of it from a 1 : 1 mixture of acetonitrile and *N,N*-dimethylformamide (DMF) affords red crystals of 1.DMF. The X-ray structure shows that each molecule of the Re<sup>V</sup> complex is connected to another nearest neighbouring Re<sup>V</sup> complex via a DMF molecule with extensive hydrogen bonding. The complex displays a rare example of a 3D network involving all of the possible intermolecular hydrogen bonding and weak C-H...p interaction.  
Keywords : Oxorhenium complex, supramolecular, crystal structure, '3+1' mixed ligands.

## Synthesis, magnetic and spectral studies of copper(II) complexes of 2-substituted benzaldehyde semicarbazones and thiosemicarbazones

Brajesh Kumar, S. K. Sangal\* and Arun Kumar

Department of Chemistry, Meerut College, Meerut-250 001, Uttar Pradesh, India

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**Abstract :** Some complexes of divalent copper have been synthesized by refluxing the metal salts with the ligands 2-chlorobenzaldehyde semicarbazone/thiosemicarbazone (cbse, cbtsc) and 2-ethoxybenzaldehyde semicarbazone/thiosemicarbazone (ebse, ebtsc). All these complexes are characterized on the basis of elemental analysis, magnetic susceptibility measurements, IR and electronic spectral studies. IR spectral data of the complexes reveals bidentate complexing nature of the ligands coordinating through oxygen atom of carbonyl group/sulphur atom of thioketo form and azomethine nitrogen atom. High spin configuration has been indicated by magnetic moment of the complexes. For all the metal complexes the probable structures are also reported here.

**Keywords :** Thiosemicarbazone, copper(II), synthesis, benzaldehyde thiosemicarbazone.

## Volumetric and ultrasonic studies of molecular interactions in binary liquid mixtures of styrene with toluene at different temperature s

Anwar Ali<sup>a\*</sup>, Firdosa Nabi<sup>a</sup>, Mohammad Tariq<sup>b</sup>, Rajan Patel<sup>a</sup>, Shahjahan<sup>a</sup> and Shadma Tasneem<sup>a</sup>

<sup>a</sup>Department of Chemistry, Jamia Millia Islamia (Central University), New Delhi-110 025, India

*E-mail :* anwar\_jmi@yahoo.co.in, anwarali.chem@gmail.com

<sup>b</sup>Laoboratory of Molecular Thermodynamics, Instituto de Tecnologia Quimica e Biologia, Universidade de Nova De Lisboa, Oeiras, Portugal

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**Abstract :** This paper presents experimental data for densities ( $\rho$ ) and ultrasonic speeds ( $u$ ) of pure styrene and toluene and of their binary liquid mixtures over the entire composition range at 298.15, 303.15, 308.15 and 313.15 K. From the experimental data the excess molar volumes ( $V^E$ ), deviations in isentropic compressibilities ( $\Delta k_s$ ), and in acoustic impedances ( $\Delta Z$ ), were calculated for the binary mixtures over the entire composition range at all the temperatures. Moreover, partial molar volumes,  $V_{f,1}^0$  and  $V_{f,2}^0$  and partial molar isentropic compressibilities,  $K_{f,1}^0$  and  $K_{f,2}^0$  at infinite dilution of styrene in toluene and toluene in styrene were examined. The variations of these parameters with composition of mixture suggest the strength of interactions between the component molecules under study.

**Keywords :** Densities, ultrasonic speeds, thermodynamic properties, intermolecular interactions, binary mixtures.

## Voltammetric behaviour of pyrantel pamoate at a composite polymer membrane electrode

D. C. Tiwari<sup>a</sup>, Rajeev Jain<sup>b\*</sup> and Gaurav Sahu<sup>b</sup>

<sup>a</sup>School of Studies in Physics, <sup>b</sup>School of Studies in Chemistry, Jiwaji University, Gwalior-474 011, Madhya Pradesh, India

E-mail : rajeevjain54@yahoo.co.in

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**Abstract** : Voltammetric behaviour of pyrantel pamoate was studied in Britton-Robinson buffer system at composite polymer membrane working electrode. Cyclic voltammetric method has been developed for the determination of drug in pharmaceutical formulation. A well-defined cathodic peak was observed for the pyrantel pamoate in the entire pH range. The current increases steadily with diffusion scan rate and concentration. The results indicate that the process is irreversible and diffusion controlled. This composite film showed good current response.

**Keywords** : Pyrantel pamoate, composite polymer electrode, cyclic voltammetry.

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## Mathematical standardisation on random chain model : Gaussian to computational approach

Jaydip Datta<sup>a</sup>, Chiranjib Bhattacharjee<sup>b\*</sup>, Durgadas Mukherjee<sup>c</sup>, B. R. De<sup>e</sup> and T. K. Bhattacharya<sup>d</sup>

<sup>a</sup>Department of Chemistry and Chemical Technology, Vidyasagar University, Midnapur -721 102,  
West Bengal, India

<sup>b</sup>Department of Chemical Engineering, Jadavpur University, Kolkata-700 032, India

E-mail : cbhattacharyya@chemical.jdvu.ac.in

<sup>c</sup>Mahadevananda Mahavidyalaya, Monirampur, Barrackpore, North 24 -Parganas, West Bengal, India

<sup>d</sup>Department of Chemical Technology, University of Calcutta, 92, Acharya Prafulla Chandra Road,  
Kolkata-700 009, India

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**Abstract** : Random Chain model is mathematically standardised using Taylor's expansion series, second order partial differential equation and Laplace transformation in details to establish the most important physical properties like probability distribution function and mean square separation of end to end of a biopolymer chain. A multivariable function correlating mean end to end separation, number of monomer unit and length of each monomer unit is established. Finally the output equations are standardised by an object oriented programming language like C++ for biopolymers like Catalase, Myosin and Bushy shunt virus.

**Keywords** : Mean square separation of end to end, Random Chain, Taylor's expansion series, second order partial differential equation, Laplace transformation, Catalase, Myosin, Bushy shunt virus, rotational isomer model.

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## Apparent molar volumes and viscosities of solutions of mono - and disaccharides in water and in (DMSO + water) mixed solvent systems at 293.15, 303.15 and 313.15 K

Vineeta and Mukhtar Singh\*

Department of Chemistry, Agra College, Agra-282 002, Uttar Pradesh, India

E-mail : mukhtarsingh2003@rediffmail.com

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**Abstract :** Apparent molar volumes ( $V_f$ ) and viscosities ( $h$ ) of solutions of mono- and disaccharides viz. glucose, fructose, sucrose and maltose have been determined in water and in dimethyl sulphoxide (DMSO) + water solvent systems of varying composition (10, 20 and 30%, w/w) at 293.15, 303.15 and 313.15 K as a function of molal concentration of saccharides. The  $V_f$  and  $h$  data have been analysed in the light of equations,  $V_f = V_f^0 + S_v m$  and  $(\eta_{rel} - 1)/c = A + Bc$  respectively. The activation thermodynamic quantities  $\Delta m_2^{0\#}$ ,  $\Delta H_2^{0\#}$  and  $\Delta S_2^{0\#}$  of viscous flow for mono- and disaccharides in water and in (DMSO + water) mixed solvent systems have been determined at 293.15, 303.15 and 313.15 K. The results in regard to solute-solvent and solute-solute interactions in water and in (DMSO + water) mixed solvent systems have been discussed in terms of the values of  $V_f^0$ ,  $S_v$  and those of  $A$  and  $B$ . The values of limiting apparent molar expansibilities ( $f_E^0$ ) and that of  $(\partial^2 V_f^0 / \partial T^2)_p$  have been determined from temperature dependence of  $V_f^0$ . The results of the study reveal that mono- and disaccharides behave as structure-makers in water and also in (DMSO + water) mixed solvent systems of varying composition.

**Keywords :** Apparent molar volumes, viscosities, mono- and disaccharides, mixed solvents.

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## 1,3-Dipolar cycloadditions. Part-XVI : Frontier molecular orbitals of *C*-aryl-*N*-methyl nitrones<sup>1,2</sup> – A DFT study

Avijit Banerji\* and Nivedita Acharjee

Centre of Advanced Studies on Natural Products including Organic Synthesis, Department of Chemistry, University College of Science, University of Calcutta, 92, Acharya Prafulla Chandra Road,  
Kolkata-700 009, India

*E-mail* : ablabcu@yahoo.co.uk

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**Abstract :** Molecular orbital calculations have been performed by DFT calculations using B3LYP theory and 6-31 G (d) level of approximation for *C*-(4-chlorophenyl)-*N*-methyl nitron on the basis of its optimised geometry. The effect of substitutions on orbital energies have been deduced by comparison to other nitrones and 1,3-dipoles.

**Keywords :** *C*-(4-Chlorophenyl)-*N*-methyl nitron, frontier molecular orbital energies.

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## Synthesis and pharmacological studies on some phthalimidoxy substituted quinoline derivatives

Dinesh Bhambi, Devendra K. Sain, Vijay K. Salvi, Chirag Sharma and G. L. Talesara\*

Synthetic Organic Chemistry Research Laboratory, Department of Chemistry, M. L. Sukhadia University, Udaipur-313 001, Rajasthan, India

*E-mail* : gtalesara@yahoo.com

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**Abstract :** Synthesis of novel *Nc*-[2-(4-substitutedphenyl)-3-*N*-ethoxyphthalimido-5-oxoimidazolidene-1-yl]-2-(quinoline-8-yloxy)acetamide derivatives (6a-e) with potential biological activities were carried out by adopting the reaction scheme given below. Compound ethyl-(quinoline-8-yloxy)acetate (2) was synthesized by refluxing 8-hydroxyquinoline with ethylchloroacetate in presence of  $K_2CO_3$ .

Ethyl-(quinoline-8-yloxy)acetate (2) was converted to corresponding hydrazide (3) on treatment with hydrazine hydrate which on further condensation with various araldehydes gave respective Schiff's bases (4a-e). These on cyclisation with glycine yielded corresponding oxoimidazolidenes (5a-e). Active H of imidazolidionones (5a-e) was replaced by ethoxy phthalimide to yield final products (6a-e).

**Keywords :** 8-Hydroxyquinoline, oxoimidazolidene, ethoxy phthalimide.

## Synthesis of 2(S),4(S),5(R)-1-acyl-5-arylproline-2,4-dicarboxylic esters

Sharad Kumar Panday<sup>a\*</sup>, Jagdish Prasad<sup>a</sup> and Dinesh Kumar Dikshit<sup>b</sup>

<sup>a</sup>Department of Chemistry, Faculty of Engineering and Technology, M. J. P. Rohilkhand University,

Bareilly-243 006, Uttar Pradesh, India

E-mail : drsharadpandey@yahoo.com

<sup>b</sup>Medicinal Chemistry Division, Central Drug Research Institute, Lucknow-226 001, Uttar Pradesh, India

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**Abstract** : *N*-Arylidineglycine methyl ester 2 (Ar = 4-ClC<sub>6</sub>H<sub>4</sub>) undergoes base catalyzed [3+2] cycloaddition with (-)-menthyl acrylate to give the proline 4 that has been acylated with acetic anhydride and *L*-*N*-benzyloxycarbonylglutamic anhydride to the corresponding 1-acylproline.  
**Keywords** : Ester, synthesis, proline, acylation.

## Effect of 1-butyl-3-methylimidazolium-based ionic liquid on the resolution of three components in Herba Artemisiae Scopariae by RP-HPLC

Ye Wang and Kyung Ho Row\*

Center for Advanced Bioseparation Technology, Department of Chemical Engineering, Inha University,

253 Yonghyun-Dong, Nam-Ku, Incheon 402-751, Korea

E-mail : rowkho@inha.ac.kr Fax : 82-32-872-4046

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**Abstract** : The chromatographic behavior of three components of Herba Artemisiae Scopariae, chlorogenic acid, caffeic acid and rutin on C<sub>18</sub> column was examined using different concentrations of a 1-butyl-3-methylimidazolium tetrafluoroborate ionic liquid as an additive in acetonitrile/water (20/80, v/v) mobile phase. The results showed that 1-butyl-3-methylimidazolium tetrafluoroborate, optimal concentration 0.5 mM, was quite effective in retaining the three components. The mechanism of retention of three components on C<sub>18</sub> column in the presence of ionic liquid additive has been discussed.  
**Keywords** : [Bmim][BF<sub>4</sub>], chlorogenic acid, caffeic acid, rutin, additive.

## Nucleophiles, nucleophilicity and relationship between nucleophilicity and basicity

Tridib Tripathy<sup>a</sup> and B. R. De<sup>b\*</sup>

<sup>a</sup>Department of Chemistry, Midnapur College, Paschim Medinipur-721 101, West Bengal, India

<sup>b</sup>Department of Chemistry, Vidyasagar University, Paschim Medinipur-721 102, West Bengal, India

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**Abstract :** The concept of nucleophilicity and electrophilicity are most useful in understanding polar reactions. Polar reactions proceed by the movement of pairs of electrons from areas of high electron density, called nucleophiles to areas of low electron density called electrophiles or from filled orbitals to empty orbitals. Nucleophiles also control the rate of bimolecular substitution reaction. Certain aspects of this concept, however; not been treated with sufficient clarity. The aim of this write up is to clarify these aspects and to report a comparative study about nucleophilicity and basicity.  
**Keywords :** Nucleophilicity, basicity, solvent.

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## Mass, IR, UV and EPR spectral characterization of the complexes of $(\text{NPH}_2)_3$ with $\text{Cu}^{\text{II}}$ compound

Yogendra Pal Singh and S. P. S. Jadon\*

Department of Chemistry, S. V. College, Aligarh-202 001, Uttar Pradesh, India

E-mail : sps\_jadon@yahoo.co.in

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**Abstract :** Hexahydrocyclotriposphazene (HHCTP) was refluxed with  $\text{Cu}^{\text{II}}$  acetate in chlorobenzene when two products,  $\text{Cu}^{\text{II}}\text{A}$  and  $\text{Cu}^{\text{II}}\text{B}$  were obtained. On the basis of their Mass, IR, UV and EPR spectral investigations,  $\text{Cu}^{\text{II}}\text{A}$  and  $\text{Cu}^{\text{II}}\text{B}$  complexes have been formulated as  $(\text{P}_9\text{N}_9\text{H}_{16}-\text{Cu})$  and  $(\text{P}_3\text{N}_3\text{H}_2-\text{Cu})_2$  respectively.

**Keywords :** Hexahydrocyclotriposphazene (HHCTP),  $(\text{NPH}_2)_3$ ,  $\text{Cu}^{\text{II}}$  acetate.

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## Computational study of structure and vibration of Schiff base of furfural and glycine

M. Sivasankaran Nair\* and C. Ravi Samuel Raj

Department of Chemistry, Manonmaniam Sundaranar University, Tirunelveli-627 012, Tamilnadu, India

E-mail : msnairchem@rediffmail.com

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**Abstract :** Eight conformers of Schiff base between furfural and glycine suitable for complex formation were studied using AM1, *ab initio* HF and DFT (B3LYP) methods. It was found that conformer 1 is more stable and used for further studies. DFT, HF, MP2 and AM1 calculations were carried out to study its structure. The geometry was optimized using the Eigenvector method and 6-31G\* basis set was employed. Vibrational spectrum was calculated using HF, MP2 and AM1 methods. The bond lengths, bond angles, dihedrals and vibrational frequencies calculated by different methods compare each other. The Schiff base is potentially tridentate capable of binding through furan oxygen, imino nitrogen and carboxylato oxygen atoms.

**Keywords :** Schiff base, amino acid, computation, furfural, vibration, *ab initio*, DFT.

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## Effect of temperature on the partial molar volumes of some high valency electrolytes in water-rich region of binary aqueo-organic mixtures

M. L. Parmar\* and D. S. Banyal

Department of Chemistry, Himachal Pradesh University, Summer Hill, Shimla-171 005, Himachal Pradesh, India

**Abstract :** Partial molar volumes of some high valency electrolytes viz. potassium ferrocyanide and potassium ferricyanide have been determined in aqueous and binary aqueo-organic mixtures of acetonitrile (ACN) and methanol (MeOH) in water-rich region [5, 10, 15, 20 and 25% by weight of ACN and MeOH] from solution density measurements at 303.15 K, and in water and 5% (w/w) ACN + H<sub>2</sub>O and MeOH + H<sub>2</sub>O at five equidistant temperatures [298.15, 303.15, 308.15, 313.15 and 318.15 K]. The density data have been analysed by means of Masson's equation. The partial molar volumes ( $V^0_\nu$ ) and slopes ( $S^*_\nu$ ) have been interpreted in terms of ion-solvent and ion-ion interactions, respectively. The partial molar volumes vary with temperature as a power series of temperature. Structure making/breaking capacities of the high valency electrolytes have been inferred from the sign of  $[\partial^2 V^0_\nu / \partial T^2]_p$  i.e. the second derivative of partial molar volumes w.r.t. temperature at constant pressure. The high valency electrolytes behave like common electrolytes in water and like symmetrical tetra-alkyl ammonium salts in binary aqueo-organic mixtures. The high valency electrolytes act as structure breakers in water and structure makers in binary aqueo-organic mixtures. The behaviour of high valency electrolytes changes on the addition of organic solvent.

**Keywords :** High valency electrolytes, partial molar volumes, binary aqueo-organic mixtures.

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## Kinetics and mechanistic investigation of *N*-bromonicotinamide oxidation of aromatic aldehydes

M. Kavitha, K. Shenbagam, M. Balasubramanian, R. Sridharan and N. Mathiyalagan\*

P.G. and Research Department of Chemistry, St. Joseph's College (Autonomous),  
Thiruchirappalli-620 002, Tamilnadu, India

*E-mail* : sjcmathi@yahoo.co.uk, kavi\_19475@yahoo.co.in

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**Abstract :** *N*-Bromonicotinamide (NBN) oxidation of aromatic aldehydes is investigated in aqueous acetic acid and perchloric acid medium over the temperature range of 313–328 K. The reaction exhibits first order dependence on [NBN] and the zero order dependence on [substrate]. The fractional order dependence of rate on [H<sup>+</sup>] suggests complex formation between NBN and H<sup>+</sup>. The reaction fails to induce polymerization of acrylonitrile under the experimental conditions employed. Arrhenius and activation parameters are evaluated. Effects of dielectric constant and ionic strength of the medium on the reaction rate have been studied. Oxidation products are identified. A most probable reaction mechanism is proposed and an appropriate rate law is deduced to account for the observed kinetic data.

**Keywords :** *N*-Bromonicotinamide, aldehydes, oxidation, kinetics, mechanism.

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## Synthetic modification of b-sitosterol with 2-amino-1,3,4,6-tetra-*O*-hydroxy-2-deoxy-b-D-glucofuranose hydrochloride

Parul Grover<sup>a\*</sup>, Jitender Singh<sup>a</sup>, K. L. Dhar<sup>b</sup> and Lovekesh Mehta<sup>c</sup>

<sup>a</sup>Lord Shiva College of Pharmacy, Sirsa-125 055, Haryana, India

*E-mail* : parul.grvr@gmail.com

<sup>b</sup>I. S. F. College of Pharmacy, Moga, Punjab, India

<sup>c</sup>Ind-Swift Labs Ltd., Mohali, Punjab, India

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**Abstract :** Coupling of b-sitosterol with glucosamine yields glucoside which has enhanced bioavailability due to number of polar groups present in the glucoside and is expected to possess enhanced anti-arthritic activity due to synergistic effects of both anti-arthritic drugs.

Keywords : b-Sitosterol, glucosamine, anti-arthritis.

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## Novel graphical method for the simultaneous determination of stability constant and molar absorptivity of some metal – Chrome Azurol S complexes

Laljee Yadav<sup>a</sup>, Preyas Ankit<sup>a</sup>, V. S. Tripathi<sup>a</sup>, M. C. Chattopadhyaya<sup>a\*</sup> and Sharda Sundaram Sanjay<sup>b</sup>

<sup>a</sup>Chemistry Department, University of Allahabad, Allahabad-211 002, Uttar Pradesh, India

*E-mail* : mcc46rediffmail.com

<sup>b</sup>Chemistry Department, Ewing Christian College, Allahabad-211 002, Uttar Pradesh, India

*E-mail* : sharda100@rediffmail.com

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**Abstract** : Stability constants and molar absorptivities of complexes formed by Chrome Azurol S (tri sodium salt of 3 $\alpha$ -sulpho-2 $\alpha$ :6 $\alpha$ -dichloro-3 $\beta$ :3 $\zeta$ -dimethyl-4-hydroxy-fuschsone-5:5-dicarboxy acid) with metal ions like Al<sup>III</sup>, Sc<sup>III</sup>, Cu<sup>II</sup>, Th<sup>IV</sup> and U<sup>VI</sup> ions have been determined by a novel graphical method in which neither the concentration of ligand has to be kept high in comparison to the concentration of metal ion nor any term has to be omitted to get the linear equation.

**Keywords** : Metal complexes, CAS, stability constant, molar absorptivity.

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## Studies on synthesis of 2-methyl-3,1-benzoxazine-4(4H)-one dyes and their application on nylon and polyester fibres

H. D. Navadiya<sup>a</sup>, N. K. Undavia<sup>a\*</sup> and B. S. Patwa<sup>b</sup>

<sup>a</sup>Department of Chemistry, <sup>b</sup>Department of Industrial Chemistry, Sir P. P. Institute of Science, Bhavnagar University, Bhavnagar-364 002, Gujarat, India

*E-mail* : dr.navadiya@yahoo.com

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**Abstract** : A series of 3-{4-[4-(4-aryloxy)-benzenesulfonyl]phenyl}-2-methyl-3H-quinazolin-4-one derivatives (3) have been obtained by a reaction of a various coupling agent (a-g) with diazonium salt containing 4-oxo-quinazolin moiety (2). The diazonium salt 2 is obtained by the reaction of 4(2-methyl-4-oxo-3-quinazolinyl)-4 $\alpha$ -aminodiphenylsulfone with NaNO<sub>2</sub> and HCl. The product is characterized by spectral and analytical data. Most of the tested compounds show promising dyeing properties.

**Keywords** : 4-Oxo-quinazolin, diazotization, dyeing.