## Journal of Chemical Sciences

## [Formerly: Proceedings of the Indian Academy of Sciences (Chemical Sciences)]

## Volume 117, 2005

## CONTENTS

Perspective Articles
NMR of unfolded proteins
Amarnath Chatterjee, Ashutosh Kumar, Jeetender Chugh, Sudha Srivastava, Neel S Bhavesh and Ramakrishna V Hosur3-21
Underpotential deposition of metals - Progress and prospects in modelling
V Sudha and M V Sangaranarayanan ..... 207-218
Selenium-containing enzymes in mammals: Chemical perspectives
Gouriprasanna Roy, Bani Kanta Sarma, Prasad P Phadnis and G Mugesh ..... 287-303
Full Papers
Self-assembly of a Co(II) dimer through H-bonding of water molecules to a 3D open-framework structure Sujit K Ghosh and Parimal K Bharadwaj ..... 23-26
Studies on NaI/DMSO induced retro-Michael addition (RMA) reactions on some 1,5-dicarbonyl com- pounds
H Surya Prakash Rao and S Jothilingam ..... 27-32
Kinetic, mechanistic and spectral investigation of ruthenium (III)-catalysed oxidation of atenolol by alka- line permanganate (stopped-flow technique)
Rahamatalla M Mulla, Gurubasavaraj C Hiremath and Sharanappa T Nandibewoor ..... 33-42
Superlattice configurations in linear chain hydrocarbon binary mixtures - Case of $n$ - $\mathrm{C}_{28} \mathrm{H}_{58}: n-\mathrm{C}_{x} \mathrm{H}_{2 x+2}$ ( $x=10,12,14,16$ )
P B V Prasad, P B Shashikanth and P Neelima
Synthesis of nanosized silver colloids by microwave dielectric heating
Kirti Patel, Sudhir Kapoor, D P Dave and Tulsi Mukherjee ..... 53-60
Relationship between electrophilicity index, Hammett constant and nucleus-independent chemical shift M Elango, R Parthasarathi, G Karthik Narayanan, A Md Sabeelullah, U Sarkar, N S Venkatasubramaniyan, V Subramanian and P K Chattaraj ..... 61-65
Hydrothermal synthesis and structure of $\left[\left(\mathrm{C}_{4} \mathrm{~N}_{2} \mathrm{H}_{12}\right)_{3}\right]\left[\mathrm{P}_{2} \mathrm{Mo}_{5} \mathrm{O}_{23}\right] \cdot \mathrm{H}_{2} \mathrm{O}$ and $\left[\left(\mathrm{C}_{3} \mathrm{~N}_{2} \mathrm{H}_{12}\right)_{3}\right]\left[\mathrm{P}_{2} \mathrm{Mo}_{5} \mathrm{O}_{23}\right] \cdot 4 \mathrm{H}_{2} \mathrm{O}$ S V Ganesan and Srinivasan Natarajan ..... 219-226
Supramolecular assembly based on a heteropolyanion: Synthesis and crystal structure of $\mathrm{Na}_{3}\left(\mathrm{H}_{2} \mathrm{O}\right)_{6}$ $\left[\mathrm{Al}(\mathrm{OH})_{6} \mathrm{Mo}_{6} \mathrm{O}_{18}\right] \cdot 2 \mathrm{H}_{2} \mathrm{O}$
Vaddypally Shivaiah and Samar K Das ..... 227-233
Ruthenium(II) complexes containing bidentate Schiff bases and triphenylphosphine or triphenylarsine
$P$ Viswanathamurthi, $R$ Karvembu, V Tharaneeswaran and $K$ Natarajan ..... 235-238

Synthesis and characterization of mixed ligand complexes of $\mathrm{Zn}(\mathrm{II})$ and $\mathrm{Co}(\mathrm{II})$ with amino acids: Relevance to zinc binding sites in zinc fingers

P Rabindra Reddy, M Radhika and P Manjula
Syntheses, magnetic and spectral studies on polystyrene supported coordination compounds of bidentate and tetradentate Schiff bases

D Kumar, P K Gupta and A Syamal
247-253
Azomesogens with methoxyethyl tail: Synthesis and characterization
A K Prajapati and H M Pandya
255-261
$\beta$-Sitosterol-3-O- $\beta$-D-xylopyranoside from the flowers of Tridax procumbens Linn.
V K Saxena and Sosanna Albert
Volumetric studies of some amino acids in binary aqueous solutions of $\mathrm{MgCl}_{2} \cdot 6 \mathrm{H}_{2} \mathrm{O}$ at $288 \cdot 15$, and 308.15 K

Amalendu Pal and Suresh Kumar
Viscometric and thermodynamic studies of interactions in ternary solutions containing sucrose and aqueous alkali metal halides at $293 \cdot 15,303 \cdot 15$ and $313 \cdot 15 \mathrm{~K}$

Reena Gupta and Mukhtar Singh
A trans influence study in propyl (aquo)cobaloxime by imidazoles and amino acids
J V Madhuri and S Satyanarayana
Synthesis of $\mathrm{Pt}, \mathrm{Pd}, \mathrm{Pt} / \mathrm{Ag}$ and $\mathrm{Pd} / \mathrm{Ag}$ nanoparticles by microwave-polyol method
Kirti Patel, Sudhir Kapoor, Devilal Purshottam Dave and Tulsi Mukherjee
Electrochemical determination of hydrogen peroxide using o-dianisidine as substrate and hemoglobin as catalyst

Wei Sun, Hong Jiang and Kui Jiao
Solvent-free microwave-mediated Michael addition reactions
H Surya Prakash Rao and S Jothilingam
Kinetics and mechanism of oxidation of glycine by iron(III)-1,10-phenanthroline complex in perchloric acid medium

TV N Partha Sarathi, A Kalyan Kumar, K Krishna Kishore and P Vani
Kinetics and mechanism of oxidation of chloramphenicol by 1-chlorobenzotriazole in acidic medium
R C Hiremath, R V Jagadeesh, Puttaswamy and S M Mayanna
An investigation into the electro-oxidation of ethanol and 2-propanol for application in direct alcohol fuel cells (DAFCs)

Sagar Sen Gupta and Jayati Datta
Mechanism of protection of adenosine from sulphate radical anion and repair of adenosine radicals by caffeic acid in aqueous solution

M Sudha Swaraga, L Charitha and M Adinarayana
Viscosities of oxalic acid and its salts in water and binary aqueous mixtures of tetrahydrofuran at different temperatures

M L Parmar and M K Guleria
Thiol peroxidase-like activity of some intramolecularly coordinated diorganyl diselenides
Sangit Kumar and Harkesh B Singh

```
Synthesis and anion exchange reactions of a layered copper-zinc hydroxy double salt, \(\mathrm{Cu}_{1.6} \mathrm{Zn}_{0.4}(\mathrm{OH})_{3}\) (OAc). \(\mathrm{H}_{2} \mathrm{O}\)
Jacqueline Therese Rajamathi, Sylvia Britto and Michael Rajamathi

Highly active and reusable catalyst from \(\mathrm{Fe}-\mathrm{Mg}\)-hydrotalcite anionic clay for Friedel-Crafts type benzylation reactions

Vasant R Choudhary, Rani Jha and Pankaj A Choudhari
Fluorescence spectroscopic studies on binding of a flavonoid antioxidant quercetin to serum albumins
Beena Mishra, Atanu Barik, K Indira Priyadarsini and Hari Mohan
Mechanism of interaction of vincristine sulphate and rifampicin with bovine serum albumin: A spectro-
scopic study
Bhalchandra P Kamat and Jaldappa Seetharamappa
Influence of charged microenvironment on redox potential and diffusion coefficient of \(\left[\mathrm{Fe}_{4} \mathrm{~S}_{4}(\mathrm{SPh})_{4}\right]\left(\mathrm{NBu}_{4}\right)_{2}\) in DMF and inside CTAB film on electrode surface

Raben Ch Roy and Diganta Kumar Das
Adsorption studies of iron(III) on chitin
G Karthikeyan, \(N\) Muthulakshmi Andal and K Anbalagan
663-672

Dielectric studies of binary mixtures of \(n\)-propyl alcohol and ethylenediamine
B S Narwade, P G Gawali, Rekha Pande and G M Kalamse
Modified Pippard relationship describing the Raman frequency shifts of the rotatory lattice mode of ammonia solid II in the vicinity of its melting point
H Karacali and H Yurtseven

Erratum

\section*{Special Issue on Recent Advances in Bio-inorganic Chemistry}

Foreword
T K Chandrashekar

Meso-functionalized octamethoxyporphyrins: A new class of nonasubstituted porphyrins
Pradeepta K Panda and V Krishnan

Metal ion coordination in ' \(R\) ' and ' \(T\) ' state hybrid hemoglobins as revealed by optical, EPR and sulphhydryl reactivity studies

S Ramasamy, Swarnalatha Venkateshrao, J M Rifkind and P T Manoharan
Core-modified octaphyrins: Syntheses and anion-binding properties
Rajneesh Misra, Venkataramanarao G Anand, Harapriya Rath and Tavarekere K Chandrashekar
Synthesis, photophysical and metal ion signalling behaviour of mono- and di-azacrown derivatives of 4-aminophthalimide
NB Sankaran, M Sarkar and A Samanta

Fixation of \(\mathrm{CO}_{2}\) in air: Synthesis and crystal structure of a \(\mu_{3}-\mathrm{CO}_{3}\)-bridged tricopper(II) compound Jhumpa Mukherjee, V Balamurugan, Maninder Singh Hundal and Rabindranath Mukherjee

Synthesis, characterisation of few N -substituted 1,8-naphthalimide derivatives and their copper(II) complexes

Nilotpal Barooah, Chandan Tamuly and Jubaraj B Baruah

Effect of copper-sulphur bond on the DNA photo-cleavage activity of 2-(methylthio)ethylpyridine-2
carbaldimine copper(II) complexes

Tarkeshwar Gupta, Ashis K Patra, Shanta Dhar, Munirathinam Nethaji and Akhil R Chakravarty
Synthesis and characterization of a chiral dimeric copper(II) complex: Crystal structure of \(\left[\mathrm{Cu}_{2}(\mu-\right.\) \(\left.\mathrm{Cl})_{2}(\mathrm{HL})_{2}\right] \cdot \mathrm{H}_{2} \mathrm{O}\left(\mathrm{H}_{2} \mathrm{~L}=S\right.\)-(-)-2-[(2-hydroxy-1-phenyl-ethylimino)-methyl]-phenol)
Chullikkattil P Pradeep, Panthapally S Zacharias and Samar K Das
Synthesis and crystal structure of 5-(4'-carboxyphenyl)-10,15,20-tri(4'-t-butylphenyl)porphinato zinc(II) complex
P Bhyrappa, C Arunkumar and J J Vittal
Fluorescence-enhancement with different ionic inputs in a cryptand-based multi-receptor signalling system Bamaprasad Bag and Parimal K Bharadwaj
Mixed-ligand complexes of ruthenium(II) incorporating a diazo ligand: Synthesis, characterization and DNA binding
Megha S Deshpande and Avinash S Kumbhar
Fluorescence properties of meso-tetrafurylporphyrins
\(\quad\) Iti Gupta and M Ravikanth

Rhodium and iridium complexes of N-(2'-hydroxyphenyl)pyrrole-2-aldimine: Synthesis, structure, and
spectral and electrochemical properties
Semanti Basu, Indrani Pal, Ray J Butcher, Georgina Rosair and Samaresh Bhattacharya
Biocatalysis by metallated cyclotriphosphazenes: \(\mathrm{L}_{2} \mathrm{Zn}\left(\mathrm{NO}_{3}\right)_{2}\left\{\mathrm{~L}=\right.\) spiro \(\left.-\mathrm{N}_{3} \mathrm{P}_{3}\left[\mathrm{O}_{2} \mathrm{C}_{12} \mathrm{H}_{8}\right]\left[\mathrm{N}\left(\mathrm{CH}_{3}\right) \mathrm{NH}_{2}\right]\right\}\) as a synthetic phosphoesterase and nuclease

V Chandrasekhar, V Krishnan, R Azhakar, C Madhavaiah and S Verma
Mixed-ligand copper(II) complexes of dipicolylamine and 1,10-phenanthrolines: The role of diimines in the interaction of the complexes with DNA
\(S\) Ramakrishnan and M Palaniandavar

Iron(III) porphyrin-catalysed oxidation reactions by \(m\)-chloroperbenzoic acid: Nature of reactive intermediates

A Agarwala, V Bagchi and D Bandyopadhyay
Porphyrin-anthraquinone dyads: Synthesis, spectroscopy and photochemistry
P Prashanth Kumar, G Premaladha and Bhaskar G Maiya

\section*{Special Issue on Chemical Reactivity}

Foreword
P K Chattaraj
Chemical hardness and density functional theory
Ralph G Pearson
DFT reactivity indices in confined many-electron atoms
Jorge Garza, Rubicelia Vargas, Norberto Aquino and K D Sen
The electron-propagator approach to conceptual density-functional theory
Junia Melin, Paul W Ayers and J V Ortiz
\begin{tabular}{l|} 
A density functional theory-based chemical potential equalisation approach to molecular polarizability \\
Amita Wadehra and Swapan K Ghosh \\
Relation between the Fukui function and the Coulomb hole \\
P Senet and M Yang \\
Condensation of the highest occupied molecular orbital within the electron localization function domains \\
E Chamorro, M Duque, C Cárdenas, J Santos, W Tiznado and P Fuentealba \\
Molecular quantum similarity using conceptual DFT descriptors \\
\(\quad\) Patrick Bultinck and Ramon Carbó-Dorca \\
Hardness and excitation energy \\
A Nagy \\
Electron localization functions and local measures of the covariance \\
Paul W Ayers \\
Geometric interpretation of density displacements and charge sensitivities \\
Roman F Nalewajski \\
The reaction force: Three key points along an intrinsic reaction coordinate \\
P Politzer, A Toro-Labbé, S Gutiérrez-Oliva, B Herrera, P Jaque, M C Concha and J S Murray \\
On the significance of ELF basins \\
Andreas Savin \\
Dynamic behavior of chemical reactivity indices in density functional theory: A Bohn-Oppenheimer \\
quantum molecular dynamics study \\
Shubin Liu \\
Third-order energy derivative corrections to the Kohn-Sham orbital hardness tensor \\
Pzonka Mineva \\
Equalization equations in reactant resolution \\
Jacek Korchowiec \\
Separability of local reactivity descriptors \\
Akhilesh Tanwar and Sourav Pal \\
Generalized density-functional theory: Conquering the N-representability problem with exact functionals \\
for the electron Levy \\
\hline
\end{tabular}

The coordination chemistry of boron porphyrin complexes \(\mathrm{B}_{2} \mathrm{OX}_{2}(\mathrm{~T} p \mathrm{YPP})\left(\mathrm{X}=\mathrm{OH}, \mathrm{F} ; \mathrm{Y}=\mathrm{Cl}, \mathrm{CH}_{3}\right)\) and their chemical reactivities

G I Cárdenas-Jirón, F Espinoza-Leyton and T L Sordo
Chemical reactivity of hypervalent silicon compounds: The local hard and soft acids and bases principle viewpoint

Francisco Méndez, María de L Romero and José L Gazquez
Application of localized reactivity index in combination with periodic DFT calculation to rationalize the swelling mechanism of clay type inorganic material

Abhijit Chatterjee
A philicity based analysis of adsorption of small molecules in zeolites Angeles Cuán, Marcelo Galván and Pratim Kumar Chattaraj ..... 541-548
Basis set effects on energy and hardness profiles of the hydrogen fluoride dimer Miquel Torrent-Sucarrat, Miquel Duran, Josep M Luis and Miquel Solà ..... 549-554
Performance of density functional theory methods to describe intramolecular hydrogen shifts Nelly González-Rivas and Andrés Cedillo ..... 555-560
Regioselectivity in the \([2+2]\) cyclo-addition reaction of triplet carbonyl compounds to substituted alkenes (Paterno-Büchi reaction): A spin-polarized conceptual DFT approach B Pintér, F De Proft, T Veszprémi and P Geerlings ..... 561-571
Bottlenecks in the prediction of regioselectivity of [4+2] cycloaddition reactions: An assessment of reactivity descriptors G Gayatri and G Narahari Sastry ..... 573-582
Investigation of the role of the \(\mathrm{C}-\mathrm{PCM}\) solvent effect in reactivity indices
Piotr Ordon and Akitomo Tachibana ..... 583-589
Study of atomic and condensed atomic indices for reactive sites of molecules P Kolandaivel, G Praveena and P Selvarengan ..... 591-598
A conceptual DFT approach towards analyzing toxicity
U Sarkar, D R Roy, P K Chattaraj, R Parthasarathi, J Padmanabhan and V Subramanian ..... 599-612
Some late-term thoughts of a density-functional theorist
Robert G Parr ..... 613-615
Subject Index ..... 687-697
Author Index ..... 698-702```

