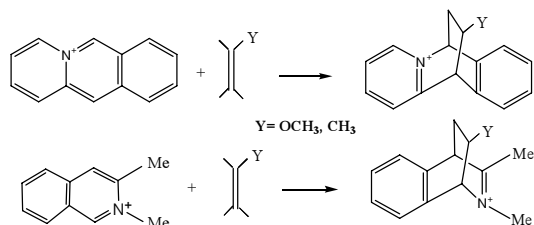


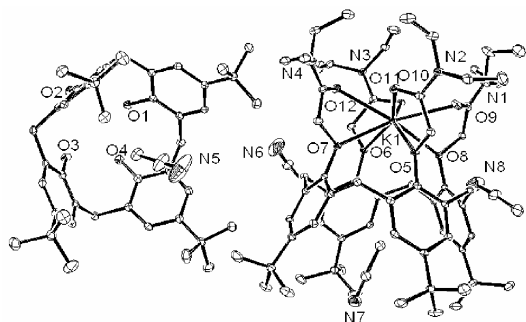
CONTENTS



Regio and stereoselectivity in ionic cycloadditions

Venkatachalam Tamilmani, Durairajan Senthilnathan and Ponnambalam Venuvanalingam 225–236

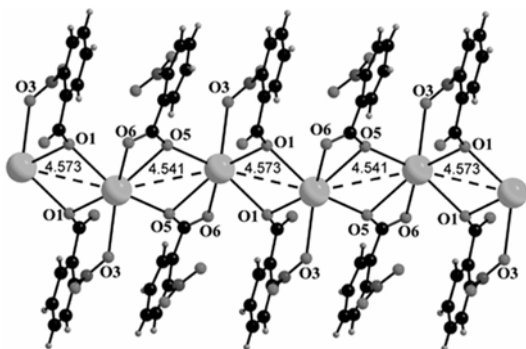
DFT calculations performed at B3LYP/6-31G(d) level show that these ionic cycloadditions are LUMO_{diene} controlled and pass through highly asynchronous concerted TSs and the *syn* 2 adduct is favoured in agreement with experiment. Though electrostatic and frontier orbital control play a significant role in these additions, electrostatic control dominates in the initial phase.



Influence of alkali and alkaline earth ions on the *O*-alkylation of the lower rim phenolic-OH groups of *p*-*tert*-butyl-calix[4]arene to result in amide-pendants: Template action of K⁺ and the structure of K⁺ bound tetra-amide derivative crystallized with a *p*-*tert*-butyl-calix[4]arene anion

Amjad Ali, Chebrolu P Rao and Philippe Guionneau 237–247

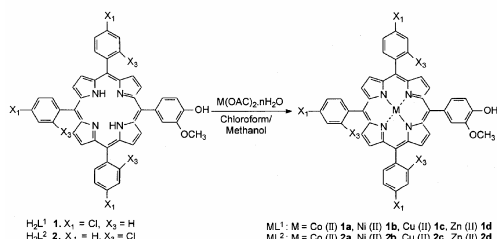
Role of alkali metal ions on the formation of amide derivatives of *p*-*tert*-butyl-calix[4]arene has been addressed and template action of K⁺ has been demonstrated. The crystal structure of the *p*-*tert*-butyl-calix[4]arene-monoanion along with K⁺ bound tetra-amide derivative has been shown for the first time.



A one-dimensional barium(II) coordination polymer with a coordinated nitro group of 2-nitrobenzoate

Bikshandarkoil R Srinivasan, Santosh Y Shetgaonkar and Pallepogu Raghavaiah 249–257

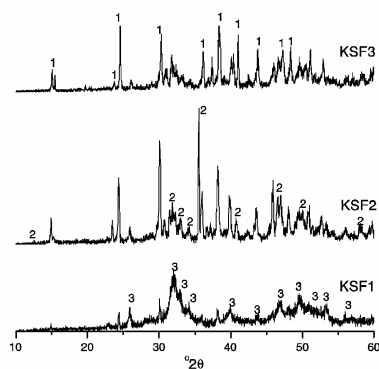
In one-dimensional coordination polymer $[[\text{Ba}(\text{H}_2\text{O})_3]_2(\mu_2\text{-}2\text{-nba-O,O,O-NO}_2)_2(\mu_2\text{-}2\text{-nba-O,O,O}')_2]_n$, alternating pairs of $\{\text{Ba}(\text{H}_2\text{O})_3\}$ units are bridged by a pair of $(\mu_2\text{-}2\text{-nba-O,O,O-NO}_2)$ and $(\mu_2\text{-}2\text{-nba-O,O,O}')$ ligands resulting in alternating Ba...Ba distances of 4.5406(15) and 4.5726(14) Å across the chain.



Synthesis and characterization of new *meso*-substituted unsymmetrical metalloporphyrins

Babasaheb P Bandgar and Pradip B Gujarathi 259–266

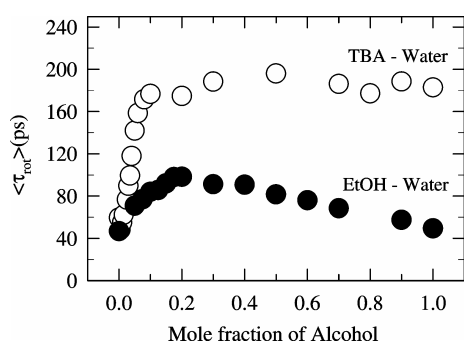
The synthesis and characterization of new *meso*-substituted unsymmetrical metalloporphyrins (A₃B) has been described.



Analysis of urinary stone constituents using powder X-ray diffraction and FT-IR

Pragnya A Bhatt and Parimal Paul 267–273

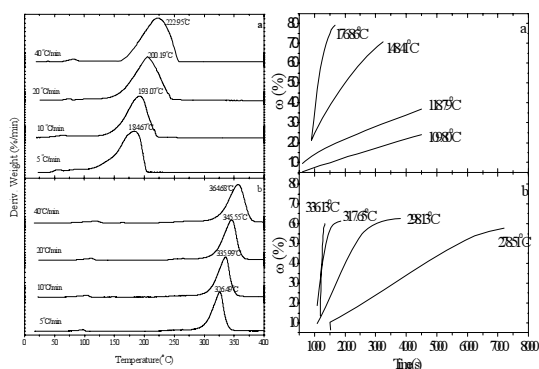
Constituents of urinary stones of patients from western India have been analysed on the basis of powder XRD, IR, TGA and SEM image. The analysis revealed that calcium oxalate monohydrate is the common constituent of all of the stones; however, hydroxyl and carbonate apatite phases are also detected in the patients with relatively older case history.



Structural transition in alcohol–water binary mixtures: A spectroscopic study

Tuhin Pradhan, Piue Ghoshal and Ranjit Biswas 275–287

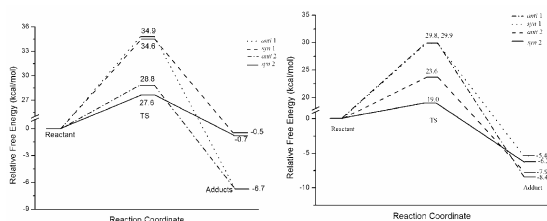
Effects of alcohol induced strengthening of hydrogen-bonding (H-bonding) network and structural transition in aqueous alcohol mixtures on equilibrium solvation and rotational properties of a dipolar probe molecule (C153) have been studied at different ethanol and tertiary butanol (TBA) mole fractions by using the steady state and time resolved spectroscopy.



Studies on the thermal decomposition kinetics of LiPF₆ and LiBC₄O₈

Li Shi-You, Ma Pei-Hua, Cui Xiao-Ling, Ren Qi-Du and Li Fa-Qiang 289–292

Thermal decomposition of LiPF₆ and LiBOB were studied using TG–DTG method with different heating rate or at different constant temperature. *n* and *E* for both LiPF₆ and LiBOB were calculated from the non-isothermal kinetics or the isothermal kinetics. The results obtained from the two ways can validate each other.



Cover picture: Free energy profile for the [2 + 4⁺] reaction of acridinium cation and methyl vinyl ether. For details see the paper by Venkatachalam Tamilmanni *et al* (pp 225–236).