# Journal of Chemical Sciences

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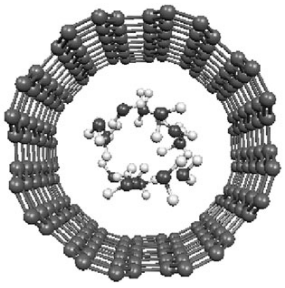
CONTENTS

## Special issue on Theoretical Chemistry Symposium 2006





Molecular dynamics simulations of water containing a narrow carbon nanotube as a solute are carried out to investigate the hydration characteristics of the nanotube for different solute- water interaction, system size and also for different diameter and wall thickness of the nanotube.

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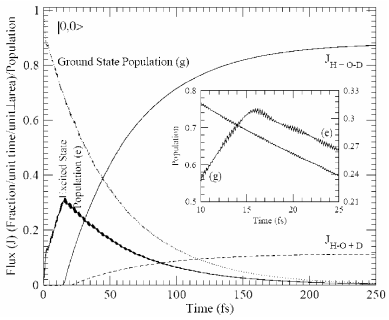




Selective control of HOD photo-dissociation (H–O + D ← HOD → H + O–D) has been theoretically investigated using CW lasers with appropriate carrier frequency and single vibrational initial state. Results indicate both selectivity and large flux yield (J) in the chosen H + O – D or H – O + D channel may be achieved using simple CW lasers. Further improvements result from the use of Field Optimized Initial State (FOIST) based combination of initial states.

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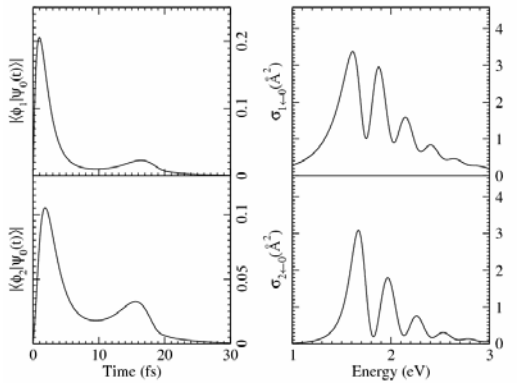




A newly developed time dependent wave packet (TDWP) approach to the calculation of vibrational excitation cross-sections has been applied to formation and decay of the $^2\Pi$ $CO^-$ shape resonance in e-CO scattering. The results show that the SCF level local complex potential (LCP) in conjunction with the TDWP approach can reproduce experimental features quite satisfactorily.

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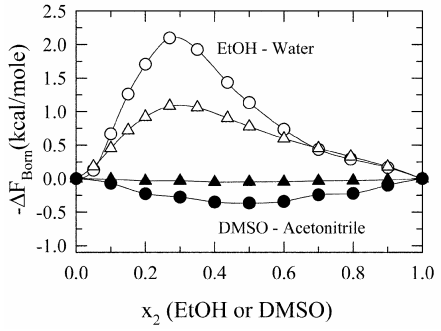




Mean Spherical Approximation (MSA) predicts that non-ideality in Born free energy of solvation of a uni-positive ion in ethanol-water mixture is more pronounced than in dimethylsulfoxide-acetonotrile mixture.

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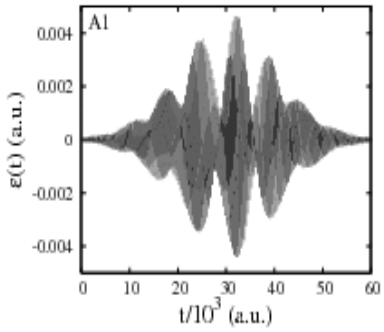
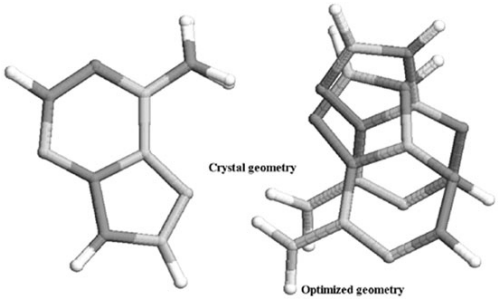
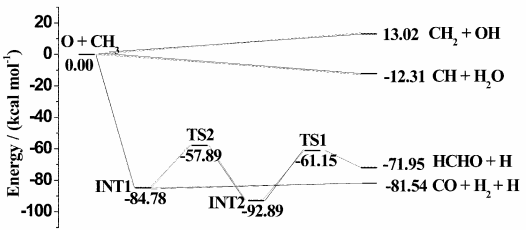


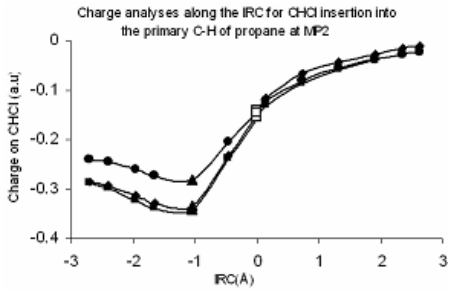


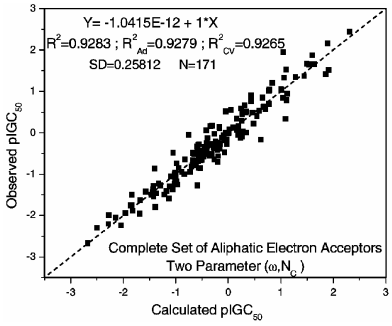


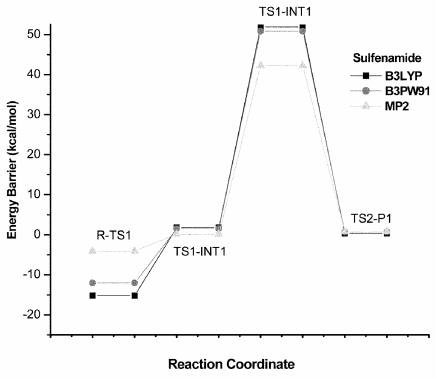







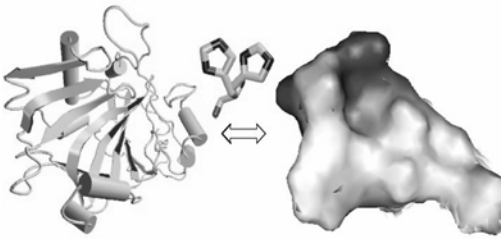






**Reaction mechanism of *O*-acylhydroxamate with cysteine proteases**



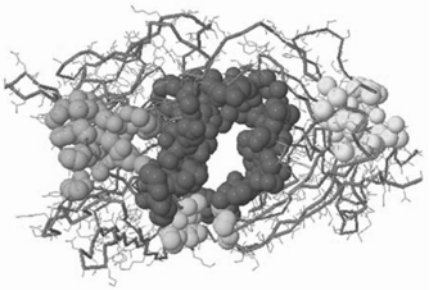
The gas-phase reaction mechanism of O-acylhydroxamate with cysteine proteases has been investigated using ab initio and density functional theory. On the irreversible process, after breakdown tetrahedral intermediate (INT1), small 1–2 anionotropic has been formed and rearranged to give stable byproducts sulfenamide (P1) and thiocarbamate (P2) with considerable energy loss. While, on the reversible part of this reaction mechanism, intermediate (INT2) breaks down on oxidation, to form a stable product (P3).



**Effect of electrostatic interactions on the formation of proton transfer pathways in human carbonic anhydrase II**



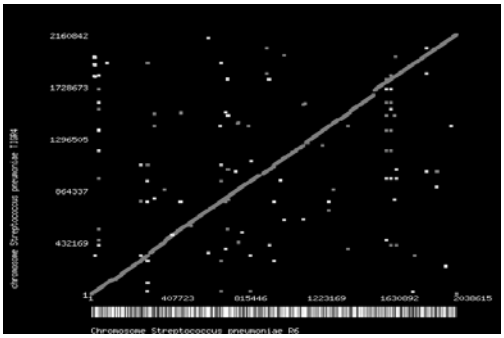
We investigate the role of electrostatic interactions on the formation of dynamical proton pathways through the sidechain conformational fluctuation of His-64 in the enzyme HCA II. The mechanistic implication of our results in the context of shuttling of protons in and out of the active site is also discussed.



**Docking of B-cell epitope antigen to specific hepatitis B antibody**



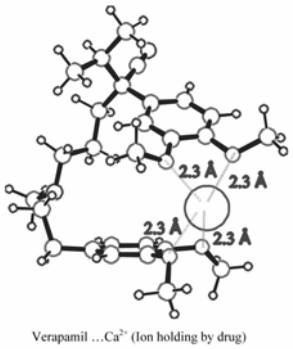
The interaction of pres1 region of hepatitis B virus B-cell epitope antigen with specific hepatitis B neutralizing monoclonal antibody was examined by docking study. The stability of the docked antigen–antibody complex is due to hydrogen bonding and van der Waals interactions.



**On the analysis of the virulence nature of TIGR4 and R6 strains of *Streptococcus pneumoniae* using genome comparison tools**



Comparative results of genome features, whole genome alignment and gene role category particularly virulence factors between TIGR4 and R6 of *Streptococcus pneumoniae* show the important proteins associated with the strain uniqueness and pathogenesis variations. Low identity between the virulence factors including capsular polysaccharides of R6 with TIGR4 shows the avirulence nature of R6.

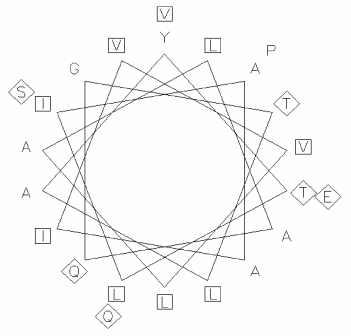


Verapamil …$Ca^{2+}$ (Ion holding by drug)

**Phenylalkylamines as calcium channel blockers**



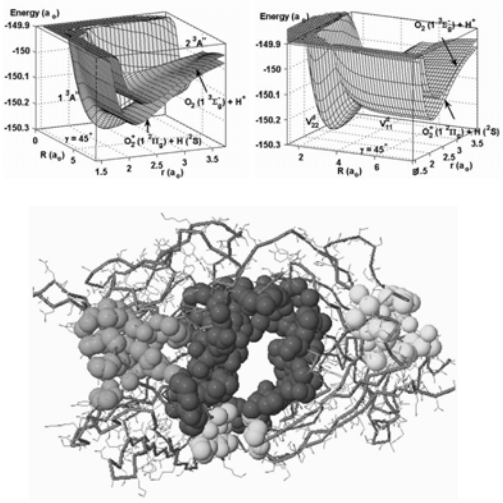
In this study *ab initio* HF coupled with intermolecular interaction calculations have been performed to study mechanistic aspects of benzothiazepines.It is predicted that ternary complex i.e. drug $Ca^{2+}$ channel stability may determine potency regulation in these drugs.



***In silico* characterization of antifreeze proteins using computational tools and servers**



Sequence analysis and characterization of seventeen fish antifreeze proteins retrieved from Swiss-Prot database have been done using various computational tools and servers. Identification, visualization and analysis of transmembrane regions and disulphide bonds have also been carried out.



*Cover picture:* Potential energy surfaces for the $H^+ + O_2$ system; active binding sites in hepatitis B antibody. For details see the article A Saieswari and Sanjay Kumar (pp 423–431) and R Rajkannan and E J Padma Malar (pp 553–558), respectively.

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