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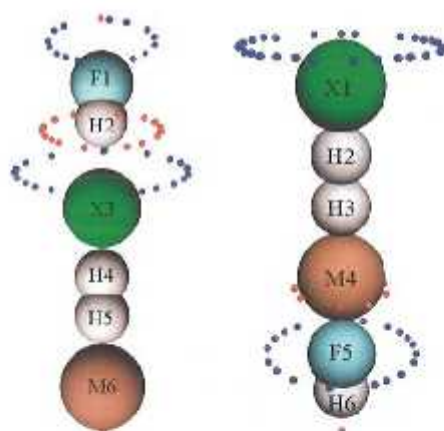
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## CONTENTS

769 Does HF prefer to be attached to X or M of XHHM (X = F, Cl, Br; M=Li, Na, K) system? A B3LYP and MP2 theoretical investigation into cooperativity effect

Stronger cooperativity effect in F-H...X-H...H-M than in X-H...H-M...F-H leads to F-H preferring to be attached to X.

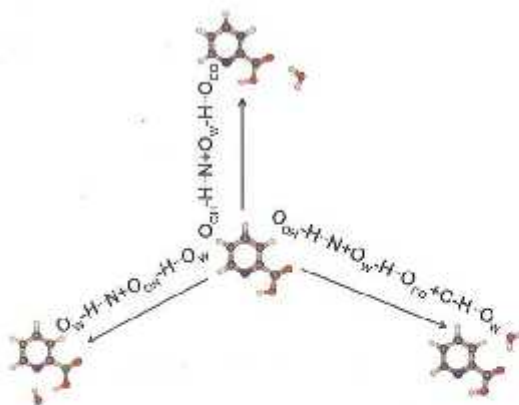


•: surface maxima, •: surface minima

Hai-bin Wang, Wen-jing Shi\*, Fu-de Ren & Ying-xin Tan

782 Theoretical study of hydrogen bonded picolinic acid-water complexes

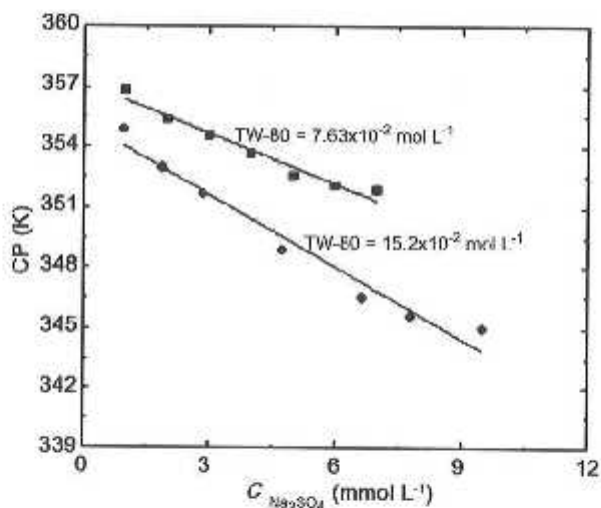
Quantum chemical calculations performed on the hydrogen bonded picolinic acid-water complexes by Hartree-Fock, second-order Moller-Plesset perturbation theory, density functional theory, and density functional theory with dispersion correction using 6-311++G(d,p) basis set have identified three monohydrated complexes, all of which are minima on the potential energy surface at all levels of computations. Among the three hydrated picolinic acid complexes, the structures PA-W1 and PA-W3 retain intramolecular O-H...N interactions upon hydration. Of these, the complex PA-W1, containing three different types of hydrogen bonding, is the most stable structure.



Mridula Guin\*, Ananth N Nayak & Netsal M Made Gowda

- 793 Physicochemical studies on effect of additives on clouding behavior and thermodynamics of polyoxyethylene (20) sorbitan monooleate

Cloud point of Tween 80, is determined in aqueous medium and in presence of aqueous solutions of salts, viz., sodium chloride, sodium sulfate, sodium nitrate, and, water soluble polymers, viz., polyvinylpyrrolidone, polyvinyl alcohol, polyethylene glycol. The addition of salts lowers the cloud point of Tween 80 with  $\text{SO}_4^{2-}$  the most efficient cloud point depresser as compared to the other monovalent ions,  $\text{Cl}^-$  and  $\text{NO}_3^-$ . The values of change in standard free energy, enthalpy and entropy decrease with increase of concentration of Tween-80.

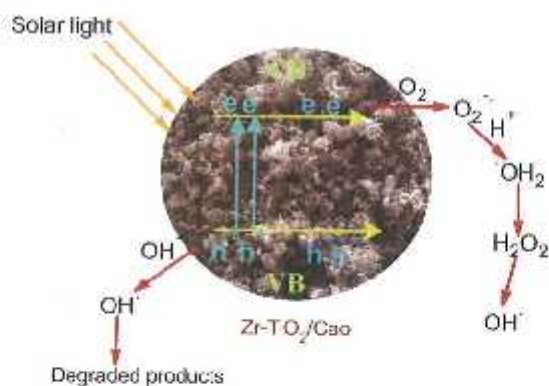


Md. Anamul Hoque\*, Attikunahar Mitu,  
Mohammad-Omar-Faruk Patoary &  
D M Shafiqul Islam

### Notes

- 803 Solar light induced photodegradation of oxytetracycline using Zr doped  $\text{TiO}_2/\text{CaO}$  based nanocomposite

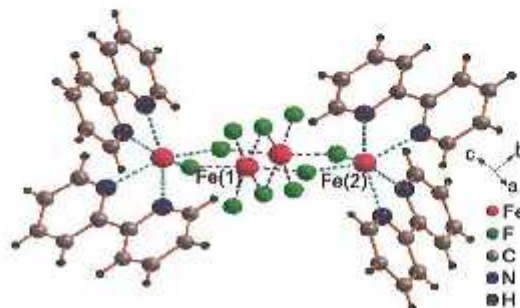
Zr- $\text{TiO}_2/\text{CaO}$  exhibits significant photocatalytic activity under solar light for OTC degradation. The monohydrate fluorosulfate of bipyridine is built up from  $\text{Fe}_4\text{F}_{10}\text{N}_8$  tetrahedron connected by eight nitrogen atoms of four 2,2'-bipyridine molecules and separated by  $\text{H}_2\text{O}$  molecules. The main feature of this atomic arrangement is the coexistence of two oxidation states of iron cations and hybrid class II with 0-D dimensionality.



Pankaj Raizada\*, Bhanu Priya, Pankaj Thakur &  
Pardeep Singh

- 810 A new hybrid iron fluoride bipyridine with mixed valence:  $\text{Fe}_2\text{F}_3(2,2'\text{-bipyridine})_2\cdot\text{H}_2\text{O}$

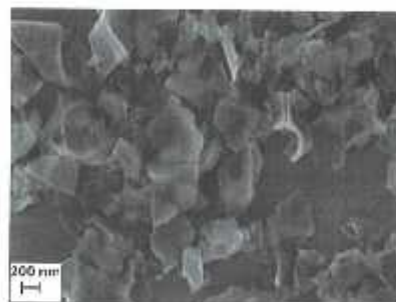
The new mixed compound  $\text{Fe}_2\text{F}_3(2,2'\text{-bipyridine})_2\cdot\text{H}_2\text{O}$  crystallizes in the triclinic system with space group  $P\bar{1}$ .



Mouma Smida\*, Mohamed Damak & Santiago Garcia-Granda

- 816 Synthesis and characterization of [Ni-Al-Fe] nanocomposite and its application for the removal of cadmium(II) and zinc(II) ions

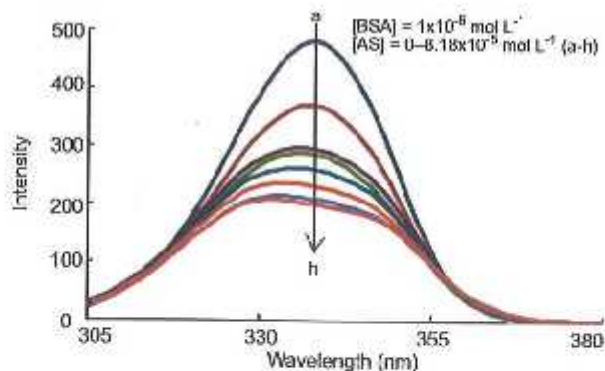
[Ni-Al-Fe] nanocomposite of 10 nm size has been synthesized via solution combustion route using aqueous solutions containing aluminum nitrate, iron nitrate and nickel nitrate as oxidizers and glycine as fuel. The synthesized composite has been used as a potential adsorbent for the removal of Cd(II) and Zn(II) from aqueous solution. The process reaches equilibrium within 35 min and is highly pH dependant; the removal of Cd(II) is significant at a pH 6.5 while the removal of Zn(II) is significant at pH 9.0.



Y V S Sai Krishna, R Ravichandra Babu\* & P V Satyam

- 820 Investigations on interaction between atazanvir sulphate and bovine serum albumin by fluorescence spectroscopy

The interaction between bovine serum albumin and atazanvir sulphate has been investigated at the physiological pH 7.4 using fluorescence spectroscopy. Synchronous fluorescence spectra and three dimensional spectra show that the conformation of BSA undergoes a change upon interaction with AS.



Umesh S Mote\* & G B Kolekar