

Indian Journal of Chemistry

Sect. A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical

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CODEN: ICACEC; ISSN: 0376-4710 (Print), 0975-0975 (online)

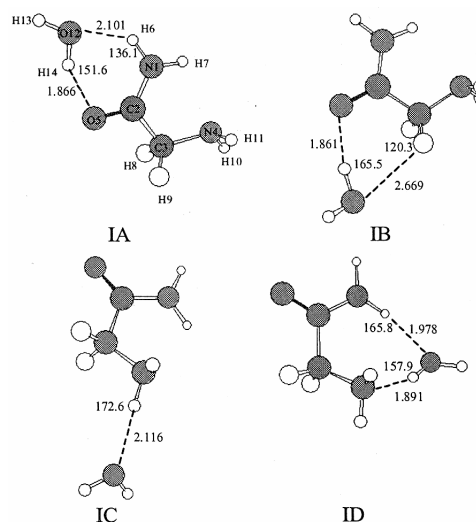
VOLUME 50A

NUMBER 7

JULY 2011

CONTENTS

- 959 Study of the glycine amide and water dimer using density functional theory**
- The hydrogen bonding in complexes formed between glycine amide and water molecule have been investigated by DFT at 6-311++g(d,p) basis set. There are four reasonable geometries of the conformer I-water system, with the global minimum being a cyclic double-hydrogen bonded structure.



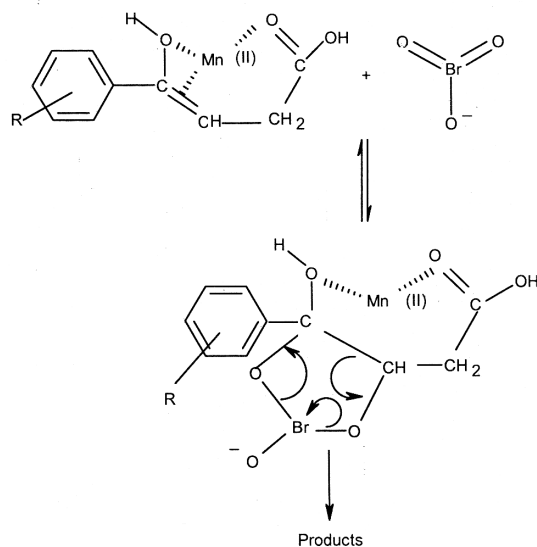
Yongfeng Guo

- 970 Performance of phosphoric acid doped polyaniline as electrode material for aqueous redox supercapacitor**
- Chemical and electrochemical syntheses of phosphoric acid doped polyaniline have been carried out in the presence and absence of surfactant for aqueous redox supercapacitor application of energy storage devices. The electrochemically grown samples exhibit higher capacitance values (244-305 F/g) than the chemically grown samples.

S Radhakrishnan, R Muthukannan, U Kamatchi,
Chepuri R K Rao* & M Vijayan

- 979** Mechanistic investigations on manganese(II) catalyzed oxidation of substituted 4-oxo-4-arylbutanoic acids by bromate in acid medium

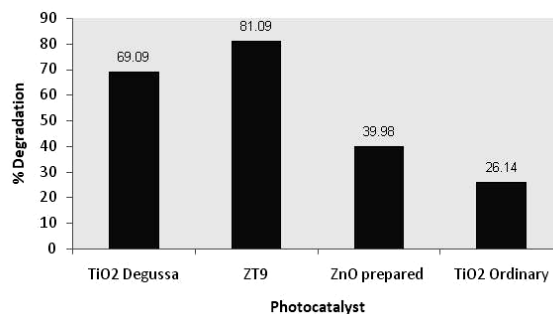
Participation of the neighboring group of 4-oxo acid and intramolecular catalysis of Mn(II) is proposed in Mn(II)-catalyzed acid bromate oxidation of 4-oxo acids, wherein both the C-C bond-breaking and C-O bond-making are involved. However, these two processes are influenced in different ways by the electron withdrawing and electron releasing substituents, leading to a non-linear Hammett's plot.



Cherkupally Sanjeeva Reddy* &
Padma Sunitha Manjari

- 991** Environmental remediation of wastewater containing azo dyes with a heterostructured nanophotocatalyst

The heterostructured ZnO/TiO₂ nanophotocatalyst with a molar ratio of 1:9 (ZnO:TiO₂) shows promising photocatalytic activity with a higher rate of decolourisation of the azo dye than TiO₂-P25 Degussa. The efficiency of the photocatalyst is maximum at pH 7, an important aspect in its commercial application in wastewater treatment.

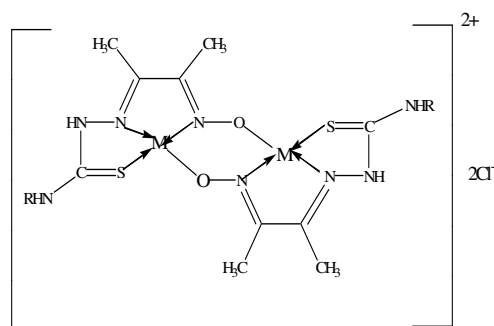


Priti Bansal, Amit Dhir, N Tejo Parksh &
Dhiraj Sud*

Notes

- 996** DNA binding and cleavage activities of cationic dinuclear copper(II) and nickel(II) complexes with novel oxime-thiosemicarbazones

Dinuclear copper(II) and nickel(II) complexes with novel oxime-thiosemicarbazones are synthesized and characterized based on spectral data. The complexes show significant oxidative cleavage of double strand pBR 322 plasmid DNA. The complexes bind CT-DNA very strongly ($10^5 - 10^6 M^{-1}$) due to supramolecular (non-covalent) interaction between cationic complexes and negatively charged phosphate diester backbone of DNA.



P Haribabu & K Hussain Reddy*

- 1002** Oxidation of alcohols with hydrogen peroxide catalyzed by supported Fe(III) porphyrins

Mild and efficient oxidation of alcohols into carbonyl compounds with hydrogen peroxide catalyzed by iron(III) tetrakis(*p*-sulfonato-phenyl)porphyrinato) acetate, supported on polyvinylpyridine and Amberlite IRA-400, at room temperature is reported. The catalysts show high activity, not only in the oxidation of benzyl and linear alcohols, but also in the oxidation of secondary alcohols at room temperature.

Shahla Masoudian* & Hooriye Yahyaei

- 1006** L-cysteine-nano-gold modified glassy carbon electrode and its application for determination of dopamine hydrochloride

Electrochemical behaviour of dopamine hydrochloride at L-cysteine-gold-nanoparticle modified glassy carbon electrode is investigated. The CGN-modified electrode promotes the electrochemical oxidation/reduction of dopamine hydrochloride by considerably accelerating the rate of electron transfer. The modified electrode shows a detection limit of 0.3 mg L^{-1} .

Yang Song, Yuan-Zhi Song*, An-Feng Zhu & Hui Zhong