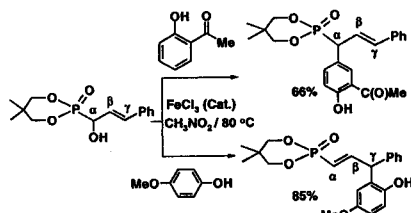


### Synthesis and characterization of mononuclear copper(II) complexes of pyridine 2-carboxamide: Their application as catalyst in peroxidative oxidation and antimicrobial agents

Suvendu Samanta, Shounak Ray, Sutapa Joardar and Supriya Dutta ..... 1451–1463

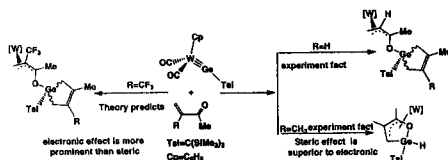
X-ray structural characterization, pH-induced co-ordination mode switching phenomenon, peroxidative oxidation catalysis and antimicrobial activity of water soluble, discrete mononuclear complexes of copper(II) using the simplest pyridine 2-carboxamide ligand (HL) and its deprotonated form have been investigated thoroughly.



### FeCl<sub>3</sub> catalysed regioselective allylation of phenolic substrates with (α-hydroxy)allylphosphonates

Mandala Anitha, Ramesh Kotikalapudi and K C Kumara Swamy ..... 1465–1475

Regioselective allylation of phenolic substrates using phosphono-allyl alcohols was achieved by using even catalytic amounts of FeCl<sub>3</sub>. Both vinylphosphonates and allylphosphonates are obtained, the ratio depending upon the substrate.



### Mechanism for the Reaction of a Tungsten-Germolyne Complex with α, β-Unsaturated Ketones: A DFT Study

Meng Li, Qiaoqiao Yang and Ran Fang ..... 1477–1483

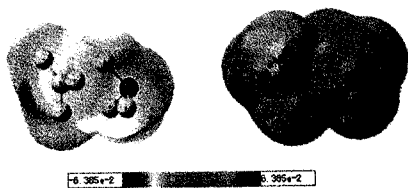
Results of theoretical analysis for the reaction mechanism involving a tungsten-germylyne complex with α, β-unsaturated ketones have been reported. The effect of substituents at the α position (H, Me and CF<sub>3</sub>) of the unsaturated ketones has been demonstrated.



### Silica functionalized Cu(II) catalysed selective oxidation of benzyl alcohols using TEMPO and molecular oxygen as an oxidant

Manjulla Gupta, Pankaj Sharma, Monika Gupta and Rajive Gupta ..... 1485–1489

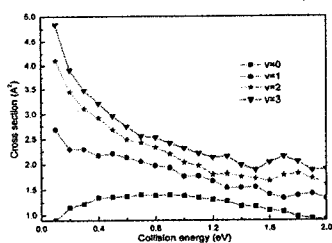
This work deals with the oxidation of benzyl alcohols catalyzed by silica functionalized copper (II) and co-catalyzed by TEMPO using molecular oxygen as an oxidant. The catalytic system works very selectively and exclusively forming only aldehydes.



### Theoretical study on the molecular and crystal structures of nitrogen trifluoride and its adduct with BF<sub>3</sub>

Hongchen Du ..... 1491–1496

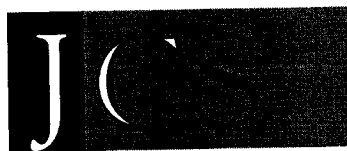
The adduct NF<sub>3</sub>·BF<sub>3</sub> exists as a complex but is not ionic. The heat of formation of the gas (–1266.09 kJ·mol<sup>–1</sup>) is slightly higher than the condensed phase (–1276.37 kJ·mol<sup>–1</sup>). Its crystal form belongs to P21/c space group. The calculated large band gap (6.06 eV) proves that the crystal is stable.



### Influence of collision energy and vibrational excitation on the dynamics for the H+HBr→H<sub>2</sub>+Br reaction

Yanhua Wang, Min Peng, Jianying Tong and Yuliang Wang . 1497–1504

A detailed dynamical study of reaction, H+HBr (v=0-3, j=0) → H<sub>2</sub>+Br, with QCT method has been performed. Both present QCT and available QM results for the HBr (v=0, j=0) have been found to be fairly consistent with each other. The reaction switches from activated to capture-type with increase of the quantum number v.



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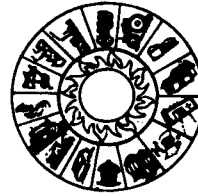
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PHOTO: LUCA LOCATELLI

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