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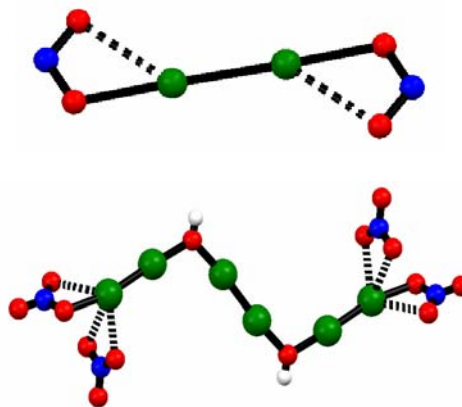
February 2011

## CONTENTS

### Rapid Communication

**137 On mercurous nitrite and a basic mercurous nitrate derivative**

Mercurous nitrite, when left in air with adhering mother liquor, is slowly converted to a basic mercurous nitrate ( $n = 2$ ) belonging to the homologous family of general formula,  $\text{Hg}_2\{(\text{OH})\text{Hg}_2\}_n(\text{NO}_3)_{n+2}$ .

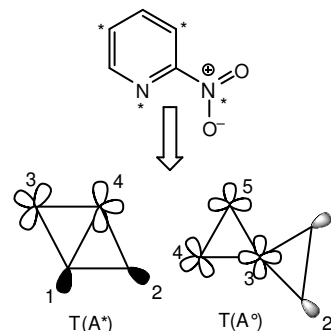


Subhas Samanta, Sreebrata Goswami &  
Animesh Chakravorty\*

### Papers

**141 A novel molecular descriptor, TG index, for calculating the detonation properties of explosives**

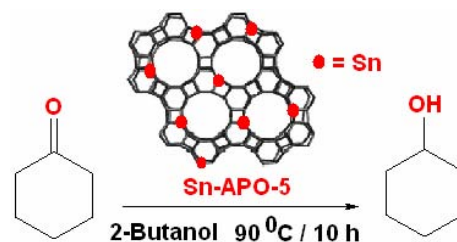
A novel molecular descriptor index (TG) has been defined for modeling and estimation of detonation parameters of explosives. The index is simple to calculate, unique for each molecule and is applicable to heteroatom containing species.



Lemi Türker\* & Selçuk Gümüş

**149 Synthesis, characterization and catalytic activity of SnAPO-5 in hydrogenation reaction**

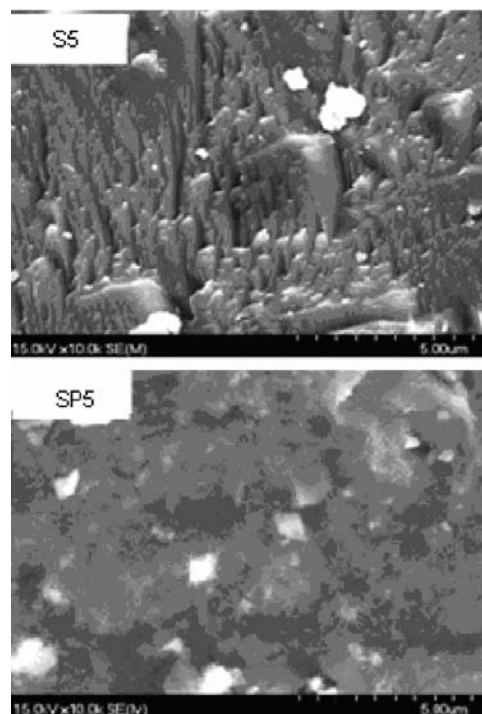
Tin containing aluminophosphate molecular sieve, SnAPO-5, has been synthesized hydrothermally with Sn(II) and Sn(IV) salts as precursors. The material exhibits good hydrogenation activity for reduction of cyclohexanone to cyclohexanol under liquid-phase reaction conditions.



Manickam Sasidharan & Asim Bhaumik\*

**156 Influence of promoter and  $\text{Fe}^{2+}/\text{Fe}^{3+}$  ratio on microstructure of fused iron catalysts for ammonia synthesis**

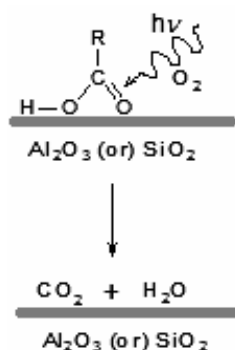
Addition of promoters and the  $\text{Fe}^{2+}/\text{Fe}^{3+}$  ratio significantly influence the microstructure of fused iron catalyst. Catalysts with high  $\text{Fe}^{2+}/\text{Fe}^{3+}$  ratio are superior in terms of promoter effects as well as pore distribution, leading to higher catalytic activity.



Zhi-ying Pu, Yi-fan Zheng\*, Hua-zhang Liu & Xiao-nian Li

**163 Photodegradation of carboxylic acids on  $\text{Al}_2\text{O}_3$  and  $\text{SiO}_2$  nanoparticles**

Photonic efficiencies of  $\text{Al}_2\text{O}_3$  and  $\text{SiO}_2$  nanoparticles are comparable to those of widely used nanosemiconductors, viz.,  $\text{TiO}_2$  P25 Degussa,  $\text{TiO}_2$  Hombikat,  $\text{TiO}_2$  anatase,  $\text{TiO}_2$  rutile,  $\text{ZnO}$ ,  $\text{SnO}_2$ , and  $\text{ZrO}_2$ . Photodegradation of carboxylic acids on  $\text{Al}_2\text{O}_3$  and  $\text{SiO}_2$  nanoparticles increases linearly with acid concentration and photon flux.

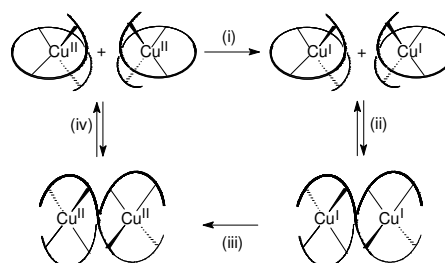


C Karunakaran\*, R Dhanalakshmi, G Manikandan & P Gomathisankar

**Notes**

**171 Effect of an ancillary ligand on single helix-double helix interconversion in copper complexes. Copper(I)-water bond**

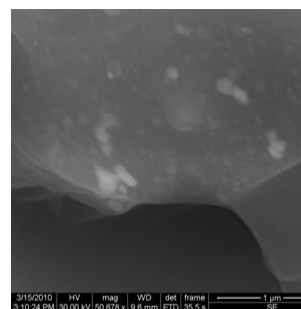
A copper-water bond at the fifth position in a single helical copper(II) complex, which persists in the corresponding copper(I) species, blocks the pathways (ii)-(iv) usually observed in copper helicates.



Senjuti De, Shubhamoy Chowdhury, Michael G B Drew & Dipankar Datta\*

**176 Synthesis of nickel nanoparticles with fcc and hcp crystal structures**

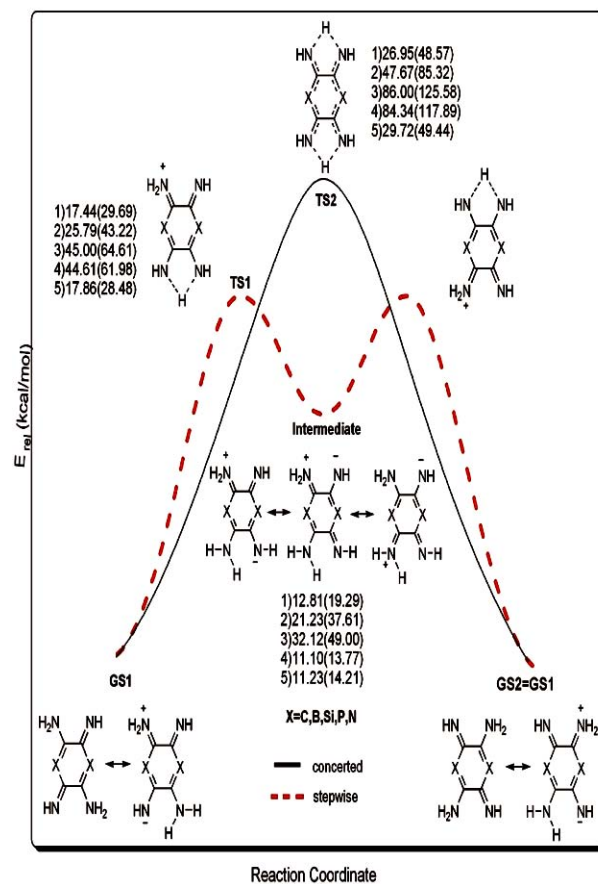
Calcination of nickel nanoparticles at 450 °C results in the sintering of nickel nanoparticles, thereby increasing the crystallite size. SEM image reveals that the particle size is in the range of 5–58 nm for fcc-Ni nanoparticles calcined at 450 °C for 10 min.



K Joseph Antony Raj & B Viswanathan\*

**180 Heteroatom effect on intramolecular double proton transfer of 3,6-diiminocyclohexa-1,4-diene-1,4-diamine: A theoretical study**

Intramolecular proton transfer in 3,6-diiminocyclohexa-1,4-diene-1,4-diamine and some hetero derivatives has been investigated at HF and DFT (B3LYP) levels of theory in both, concerted and stepwise, mechanisms.



Hasan Tahermansouri\*, Shahram Moradi & Robabeh Sayyadi

Authors for correspondence are indicated by (\*)