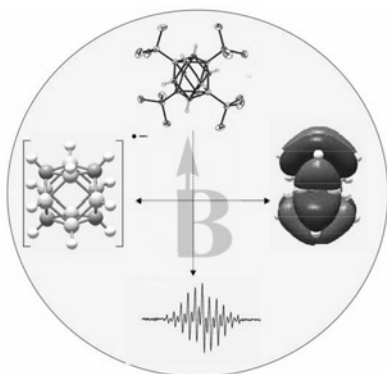


## CONTENTS

### 2nd International Symposium on Materials Chemistry (ISMC-2008)

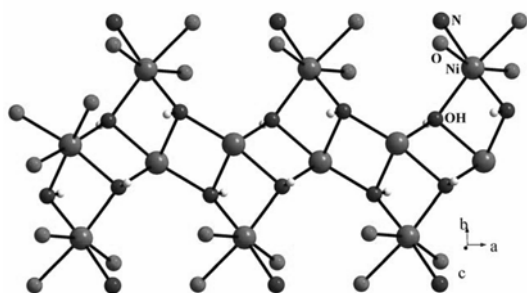
Foreword ..... 5



#### Multidimensional potential of boron-containing molecules in functional materials

Wolfgang Kaim and Narayan S. Hosmane ..... 7–18

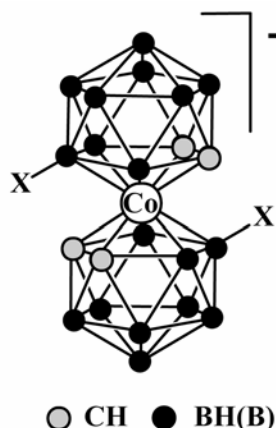
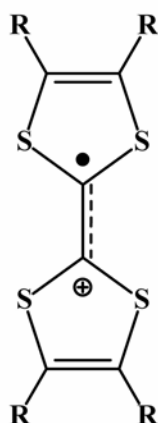
Molecular systems containing boron offer particular mechanisms to accommodate unpaired electrons which may result in stable radicals as spin-bearing materials. Among such materials are organoboron compounds in which the prototypical electron deficient boron vs. carbon centers can accept and help to delocalize added electrons in a two-dimensionally conjugated  $\pi$  system.



#### Magnetic behaviour in metal–organic frameworks—Some recent examples

Partha Mahata, Debajit Sarma and Srinivasan Natarajan ..... 19–35

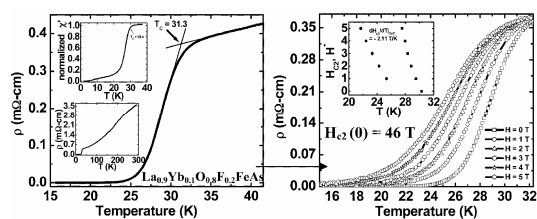
The synthesis, structure and magnetic behaviour of a family of transition metal carboxylates are described. The magnetic behaviour varies from simple paramagnetic to ferromagnetic depending on the structure and interactions.



#### Synthesis, structure and electrical conductivity of fulvalenium salts of cobalt *bis*(dicarbollide) anion and its derivatives

Vladimir Bregadze, Igor Sivaev, Irina Lobanova, Olga Kazheva, Grigorii Alexandrov, Andrey Kravchenko, Vladimir Starodub, Lev Buravov, Lev Titov and Oleg Dyachenko ..... 37–41

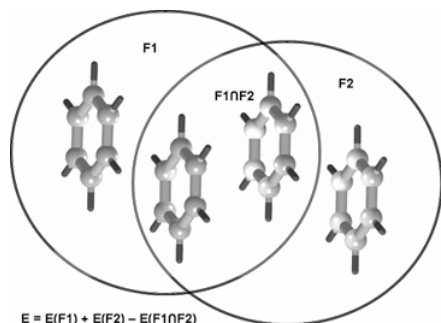
TTF, TTF-BMDT, TTF-BEDT and TMTSF cation radical salts of cobalt *bis*(dicarbollide) anion  $[3,3'\text{-Co}(1,2\text{-C}_2\text{B}_9\text{H}_{11})_2]^-$  or its halogeno derivatives were prepared and their crystal structures and electrical conductivities were determined. Regularities revealed in the crystal packing of the TTF-based radical cation salts are discussed.



### Superconductivity at 31.3 K in Yb-doped La(O/F)FeAs superconductors

J Prakash, S J Singh, S Patnaik and A K Ganguli ..... 43–46

Ytterbium substituted oxypnictides,  $\text{La}_{1-x}\text{Yb}_x\text{O}_{0.8}\text{F}_{0.2}\text{FeAs}$  show enhanced superconducting transition temperature ( $\sim 31.3$  K) as compared to La(O/F)FeAs superconductors ( $\sim 26$  K). The value of upper critical field ( $H_{c2}$ ) at zero temperature is estimated to be about 46 T corresponding to coherence length of  $\sim 27$  Å for the  $x = 0.1$  composition.

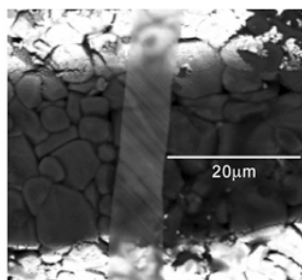


### Molecular tailoring approach for exploring structures, energetics and properties of clusters

Shridhar R Gadre, K V Jovan Jose and Anuja P Rahalkar

..... 47–56

Illustrations of building and optimizing large atomic/molecular clusters at *ab initio* level of theory are presented. Molecular electrostatic potential and molecular tailoring approach are employed for this purpose.

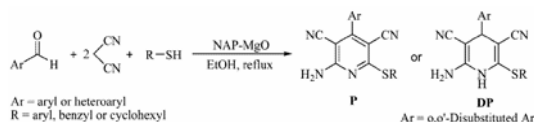


### Development of gas sensors using ZnO nanostructures

S K Gupta, Aditee Joshi and Manmeet Kaur ..... 57–62

Gas sensors have been fabricated using ZnO nanostructures. The response of the ZnO sensors to  $\text{H}_2\text{S}$  arises from grain boundaries only whereas both grain boundaries and intragrain resistances contribute towards response to NO. Highly selective NO sensors were made using isolated ZnO nanobelts.

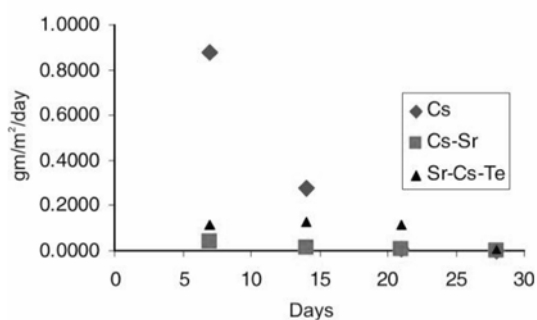
### One-pot, three-component synthesis of highly substituted pyridines and 1,4-dihydropyridines by using nanocrystalline magnesium oxide



M Lakshmi Kantam, Koosam Mahendar and

Suresh Bhargava ..... 63–69

Nanocrystalline MgO is an effective catalyst for multi-component reactions (MCRs) of structurally diverse aldehydes with various thiols and malononitrile to give 2-amino-4-aryl-3,5-dicyano-6-sulfanylpiperidines dihydropyridines in moderate to high yields. The catalyst can be recovered and re-used with consistent activity.

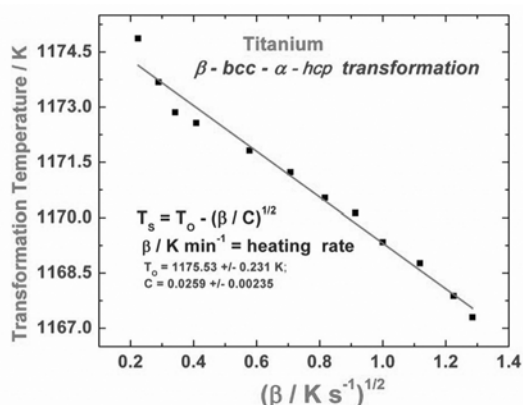


### Microwave-assisted low temperature synthesis of sodium zirconium phosphate (NZZP) and the leachability of some selected fission products incorporated in its structure – A case study of leachability of cesium

A H Naik, S B Deb, A B Chalke, M K Saxena, K L Ramakumar,

V Venugopal and S R Dharwadkar ..... 71–82

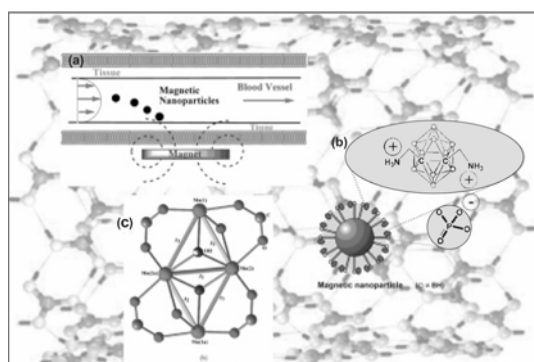
Leaching of selected fission products (Cs, Sr, Ru, Te) introduced in sintered sodium zirconium phosphate (NZZP) pellets was studied in water and 80% saturated brine solution at 30 and 90°C respectively. About 85 to 90% of the fission products immobilized in NZZP matrix were retained on prolonged leaching. The maximum leaching was observed for cesium.



**Kinetics of solid state phase transformations: Measurement and modelling of some basic issues**

S Raju and E Mohandas ..... 83–89

The effect of thermal history, in particular the interrelationship between the isothermal isochronal reference frame descriptions of solid transformation kinetics is described. A simple scaling of the effect of heating and cooling rates on the polymorphic transformation kinetics in metallic systems is attempted.



Cover picture: (a) Magnetic drug delivery mechanism and (b) Magnetic nanoparticles as BNCT carriers. For details see the paper by W Kaim and N S Hosmane (pp. 7–18). (c) The various possible magnetic exchange pathways in a Mn<sub>4</sub> cluster. For details see the paper by Partha Mahata *et al* (pp 19–35). At the background is MTA optimized (H<sub>3</sub>BO<sub>3</sub>)<sub>64</sub> cluster at HF/6-31++G(*d*, *p*) level of theory. For details see the paper by S R Gadre *et al* (pp. 47–56).