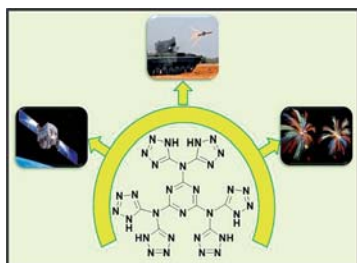


## CONTENTS

### Regular Articles



#### 2,4,6-tris[bis(1H-tetrazol-5-yl)amino]-1,3,5-triazine as a nitrogen-rich material

Muddamarri Hanumantha Rao, Vikas D Ghule and Krishnamurthi Muralidharan. . . . . 657–661

Synthesis, characterization and energetic properties of the molecule, 2,4,6-tris[bis(1H-tetrazol-5-yl)amino]-1,3,5-triazine (**2**) having 79% nitrogen content with high HOF value is discussed. The high nitrogen content associated with high positive heat of formation of the compound **2** underline the structural importance of six tetrazole groups in a molecule.

#### The impact of sugar and fatty acid on the bioactivity of *N*-fatty acyl-*L*-tyrosine aglycone

Srikanth Vudhgiri, R B N Prasad, Y Poornachandra, C Ganesh Kumar, E Anjaneyulu, K Sirisha and Ram Chandra Reddy Jala . . . . . 663–677

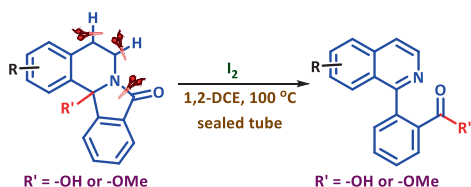
The glycosylated *N*-fatty acyl-*L*-tyrosines with short, medium and long chain unsaturated fatty acids and glycosylated *N*-lipoyl-*L*-tyrosine methyl esters were synthesized and further evaluated for their biological activities to examine the impact of sugar and fatty acid on the bioactivity of *N*-fatty acyl-*L*-tyrosine derivatives.



#### Metal free synthesis of functionalized 1-aryl isoquinolines via iodine mediated oxidative dehydrogenation and ring opening of lactam in isoindoloisoquinolinones

Kamsali Murali Mohan Achari, Muthupandi Karthick and Chinnasamy Ramaraj Ramanathan . . . . . 679–690

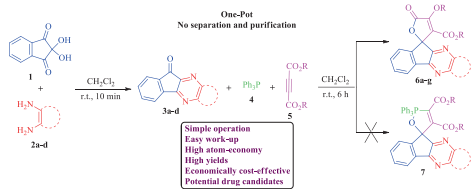
Metal-free synthesis of 1-aryl isoquinolines, which are synthetic precursors for azabenzanthrones or menisporphines, from isoindoloisoquinolinones using iodine under sealed tube conditions is reported. This methodology is successfully utilized to synthesize the 1-azabenzanthrone and analogue of menisporphine, i.e., 5-methoxy-6-hydroxy-1-azabenzanthrone.

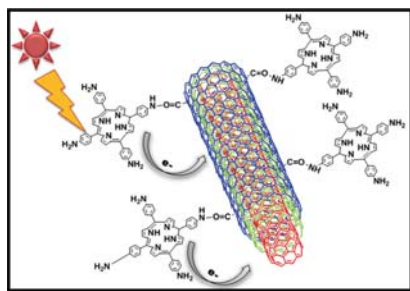


#### An efficient domino one-pot synthesis of novel spirofuran-indenoquinoxalines by vinyltriphenylphosphonium salts

Afshin Yazdani-Elah-Abadi, Malek-Taher Maghsoodlou, Razieh Mohebat and Reza Heydari . . . . . 691–698

A simple and convenient multi-component domino reaction has been described for the synthesis of novel spirofuran-indenoquinoxaline derivatives. Products were obtained by a three-component condensation reaction between ninhydrin, aromatic 1,2-diamines and dialkyl ethylenedicarboxylates in the presence of a catalytic amount of triphenylphosphine in  $\text{CH}_2\text{Cl}_2$  at ambient temperature in excellent yields. This one-pot process produces biologically and pharmacologically significant heterocycles with the formation of five new bonds (one C–C, two C=N and two C–O) and two new rings in a single operation.

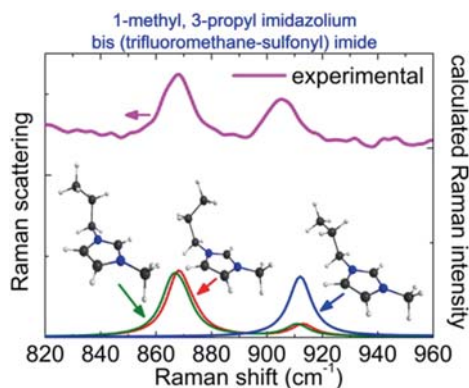




### Synthesis, characterization and photoluminescence properties of tetra(aminophenyl) porphyrin covalently linked to multi-walled carbon nanotubes

G Prabhavathi, M Arjun and R Yamuna . . . . . 699–706

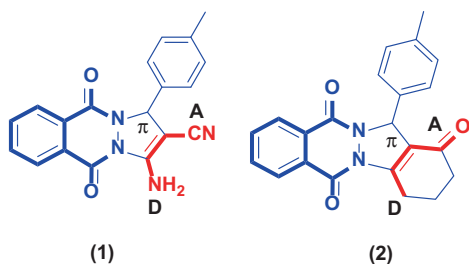
5,10,15,20-meso-tetra(4-aminophenyl) porphyrin (TAP) was covalently functionalized with MWCNTs through an amide linkage. Fluorescence quenching of TAP by MWCNTs were observed in different solvents. The absorption and emission spectra of this nano-hybrid exhibits strong positive solvatochromism, increasing with the solvent polarity.



### Synthesis, experimental and theoretical vibrational studies of 1-methyl and 1,2-dimethyl, 3-propyl imidazolium bis(trifluoromethanesulfonyl) imide

M Drai, A Mostefai, A Paolone, B Haddad, E Belarbi, D Villemin, S Bresson, O Abbas, Y Chaker and M Rahmouni . . . . . 707–719

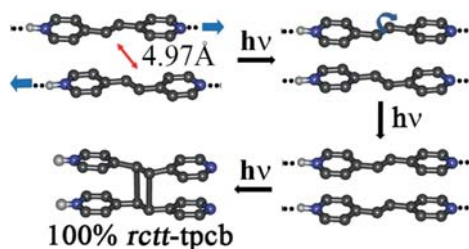
We synthesized and investigated the vibrational properties of two ionic liquids, namely, 1-methyl,3-propyl imidazolium bis(trifluoromethane-sulfonyl) imide ([1-MPrIM<sup>+</sup>][CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>N<sup>-</sup>]) and 1,2-dimethyl,3-propyl imidazolium bis(trifluoromethane-sulfonyl) imide ([1-MPrIM<sup>+</sup>][CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>N<sup>-</sup>]). Methylation in the C2 position gives rise to specific marker bands in the Raman and IR spectra. The comparison of the experimental data and the computed spectra at DFT level shows that three conformers of the imidazolium ions are present in both ionic liquids.



### Synthesis, characterization, X-ray structure, optical properties and theoretical calculations of condensed phthalazines

Esmalamera, Lyamine Messaadia, Sofiane Bouacida, Aissa Chibani, Karim Bouchouit, Bouchta Sahraoui and Abdelmalek Bouraiou . . . . . 721–731

Two condensed phthalazine compounds were synthesized and characterized by IR, UV-Vis, NMR spectroscopy and Single Crystal XRD. The geometrical parameters of both the compounds obtained from XRD studies are in accordance with the calculated values. Their electronic contributions  $\chi_{THG}^{(3)}$  have been measured using the third harmonic generation technique on thin films at 1064 nm.



### Solid state photodimerization in an organic salt of 1,2-bis(4-pyridyl) ethylene and trifluoromethane sulphonic acid via pedal-like motion

Abdul Malik P Peedikakkal . . . . . 733–739

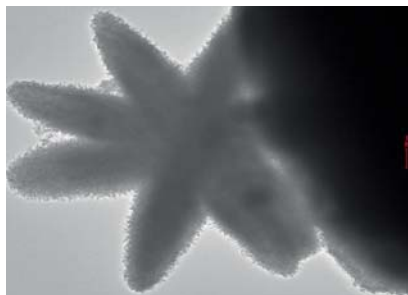
A novel organic salt of *trans*-1,2-bis(4-pyridyl)ethylene and trifluoromethane sulphonic acid was characterized by X-ray crystallography. The salt shows unusual photoreactivity *via* pedal-like motion of C=C double bonds which change from criss-cross to parallel orientation. The photodimerized product undergoes acid-catalyzed isomerization in solution and produces all the isomers of tetrakis(4-pyridyl)cyclobutane.



### Synthesis and evaluation of aromaticity and tautomerization of pyrazolopyridazin(on)es

Nurettin Menges and İshak Bildirici . . . . . 741–752

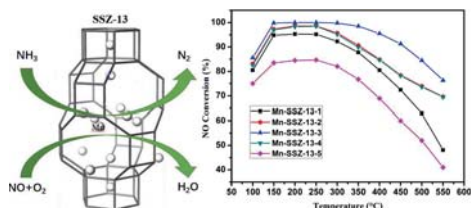
Aromaticity of Pyrazolopyridazine was calculated and the effect of bicyclic system on aromaticity was revealed. Furthermore, tautomerization of the same skeleton was investigated and the dominant tautomer was identified by means of aromaticity, bond order, and LOL map.



### Surfactant-assisted sacrificial template-mediated synthesis, characterization and photoluminescent properties of LaPO<sub>4</sub>:Eu<sup>3+</sup> phosphor

Heena Khajuria, Jigmet Ladol, Rajinder Singh,  
Haq Nawaz Sheikh and Vinay Kumar . . . . .753–764

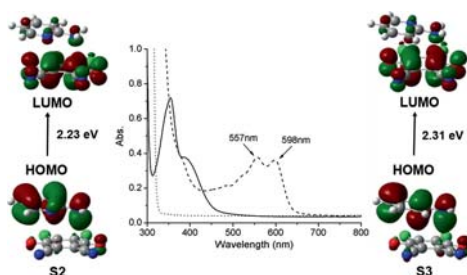
Synthesis of Eu<sup>3+</sup> doped LaPO<sub>4</sub> nanostructures via surfactant-assisted self-sacrificing route under hydrothermal conditions using the La(OH)CO<sub>3</sub>:Eu<sup>3+</sup> precursor as a template is reported. This route resulted in the formation of uniform and well dispersed morphology with efficient photoluminescent intensity.



### SSZ-13-supported manganese oxide catalysts for low temperature selective catalytic reduction of NO<sub>x</sub> by NH<sub>3</sub>

Yongzhou Ye, Fei Shen, Hongning Wang and Ruoyu Chen . . .765–774

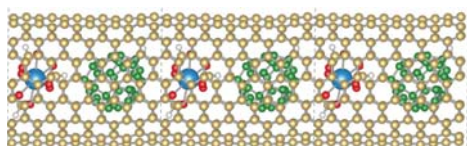
Synthesis and characterization of Mn/SSZ-13 catalysts with varying Mn content by a hydrothermal and co-precipitation method are reported. Among the synthesized catalysts, Mn-SSZ-13-3 shows the best NH<sub>3</sub>-SCR, particularly at low temperature. Besides, the catalytic mechanism of Mn/SSZ-13 catalyst is reported.



### Theoretical study on the molecular structure, intermolecular interaction and spectral features of 2-aminopyridine/ 2,3-dichloro-5,6-dicyano-1,4-benzoquinone complex

Hailong Wang . . . . .775–782

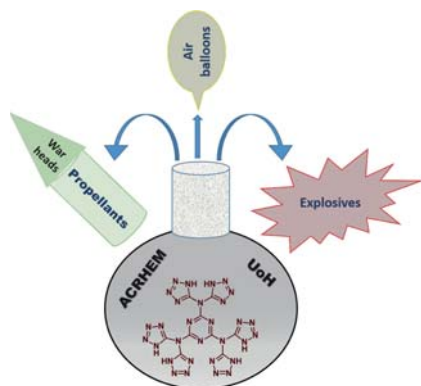
Four probable structures of the 2-AP/DDQ complex were located by DFT calculation. The bonding characteristics between the two molecules of the complex were investigated by NBO and AIM analysis. Two new absorption bands observed in the UV-Vis absorption spectrum of the complex were attributed in accordance with the TDDFT results.



### Can uranyl complexes encapsulate to carbon nanotubes? A periodic DFT study

K Srinivasu and Mahesh Sundararajan . . . . .783–790

The use of functionalized fullerene as removable corks which can seal single walled carbon nanotubes has the ability to bind uranyl complexes very efficiently is revealed through density functional theory based calculations.



Cover picture: High energy density materials. For details, see the paper by Muddamarri Hanumantha Rao *et al.* (pp. 657–661)