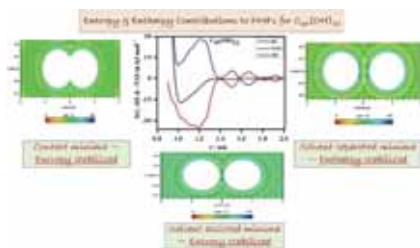


## CONTENTS

### Regular Article

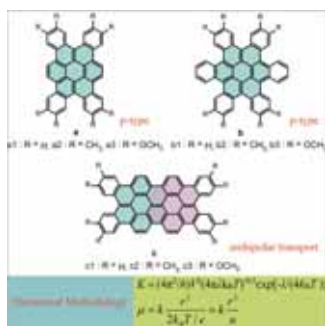


#### Thermodynamics of association of water soluble fullerene derivatives [C<sub>60</sub>(OH)<sub>n</sub>, n = 0, 2, 4, 8 and 12] in aqueous media

Sonanki Keshri and B L Tembe. . . . . 1327–1340

Aqueous solutions of fullerene derivatives have found applications in molecular sensing devices, biochemistry and environmental science. Therefore, it is necessary to have a microscopic understanding of the solvation structure of such macromolecules. Association and dynamics of fullerene and fullerols [C<sub>60</sub>(OH)<sub>n</sub>] in water are addressed by molecular dynamics simulations.

### Regular Article

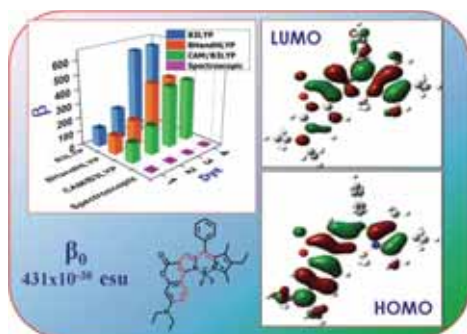


#### Density functional theory calculations of charge transport properties of ‘plate-like’ coronene topological structures

Ziran Chen, Zhanrong He, Youhui Xu and Wenhao Yu . . . . . 1341–1347

Density functional theory was used to compute the charge transport rates of three series of nine coronene topological structures at the M06-2X/6–31+G(d) level. Tetra- and hexabenzocoronene (series a) and hexabenzocoronene (series b) could be candidates for a hole-transporting (p-type) organic semiconductor material, and ‘long plate-like’ coronene topological structures (series c) could be used as an ambipolar transport material.

### Regular Article

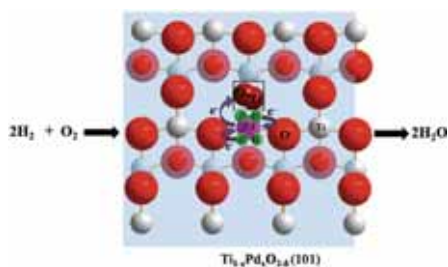


#### Enhanced NLO response in BODIPY-coumarin hybrids: density functional theory approach

Yogesh Erande and Nagaiyan Sekar . . . . . 1349–1361

The NLO properties of coumarin-fused BODIPY hybrid chromophores were studied in detail. Spectroscopic method gave rough estimation of polarizability and hyperpolarizability characteristics of four hybrid chromophores while computational approaches using three different hybrid functionals, B3LYP, CAM-B3LYP and BHandHLYP in combination with 6-311+G(d,p) basis set, gave comparative estimation of these values. BLA/BOA calculations for ground and excited states suggested that the cyanine-type D-π-A framework produces high NLO response. The hybrid molecules are proven to be the better performing NLOphores than the isolated coumarin or BODIPY units.

## Regular Article

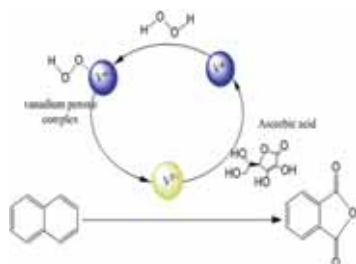


### High rates of catalytic hydrogen combustion with air over $\text{Ti}_{0.97}\text{Pd}_{0.03}\text{O}_{2-\delta}$ coated cordierite monolith

Bhaskar Devu Mukri and M S Hegde . . . . . 1363–1372

$\text{Ti}_{0.97}\text{Pd}_{0.03}\text{O}_{2-\delta}$  catalysts were coated by solution combustion method on  $\gamma\text{-Al}_2\text{O}_3$  coated honeycomb structured cordierite monolith. Among the catalysts,  $\text{Ti}_{0.97}\text{Pd}_{0.03}\text{O}_{2-\delta}$  coated monolith showed high catalytic activity for hydrogen combustion with air. The proposed mechanism of  $\text{H}_2+\text{O}_2$  reaction clarified that  $\text{Pd}^{+2}$  ion state is unaltered in  $\text{TiO}_2$  lattice.

## Regular Article

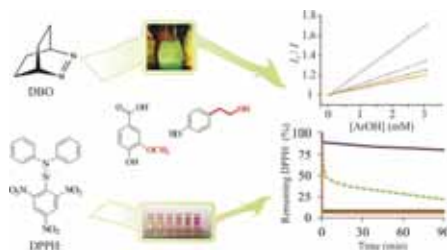


### Liquid-phase oxidation of naphthalene with $\text{H}_2\text{O}_2$ in the presence of ordered mesoporous $\text{V-}m\text{-Al}_2\text{O}_3$ catalysts

Zhiwei Zhou, Yang Yu, Juan Qin, Jiaqi Zhang, Fulin Cheng and Wenliang Wu . . . . . 1373–1380

In the presence of hydrogen peroxide as oxidant and ascorbic acid as reductant, ordered mesoporous  $\text{V-}m\text{-Al}_2\text{O}_3$  catalysts were synthesized via a facile one-pot evaporation-induced self-assembly method and successfully applied to the liquid-phase oxidation of naphthalene

## Regular Article

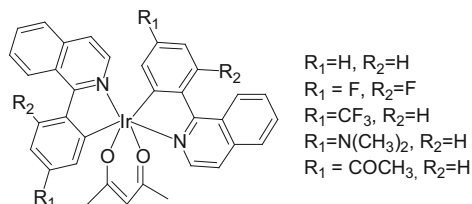


### Exploring antioxidant reactivity and molecular structure of phenols by means of two coupled assays using fluorescence probe (2,3-diazabicyclo[2.2.2]oct-2-ene, DBO) and free radical (2,2-diphenyl-1-picrylhydrazyl, DPPH)

Mercedes Becerra-Herrera, Ana Sayago and Rafael Beltrán . . . . . 1381–1390

Interactions between DBO (fluorescence quenching) and DPPH (radical scavenging) with fifteen phenolic compounds, which are present in olive oil and wine, served as a measure of antioxidant activity of the phenols and correlated to the molecular structure.

## Regular Article

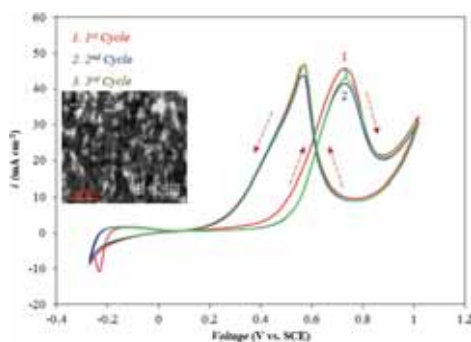


### Synthesis, photophysical, electrochemical and electroluminescence studies of red emitting phosphorescent Ir(III) heteroleptic complexes

Farman Ali, Pabitra K Nayak, N Periasamy and Neeraj Agarwal . . . . . 1391–1398

Heteroleptic, cyclometalated ( $\text{C}^*\text{N}$ ) Iridium(III) complexes of acetylacetonate (acac) and 1-phenylisoquinoline were synthesized and their photophysical, electrochemical and electroluminescence properties were studied. The OLED of Ir complex as emitting material showed turn-on voltage at  $\sim 4.5$  V, maximum brightness of  $7600 \text{ cd/m}^2$  and current efficiency of  $\sim 7.0 \text{ cd/A}$  at a brightness of  $\sim 100 \text{ cd/m}^2$ .

## Regular Article

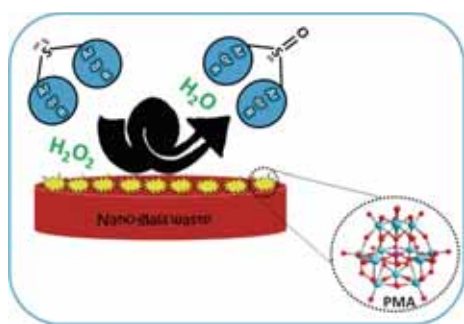


### Electrochemical investigation of electrodeposited platinum nanoparticles on multi walled carbon nanotubes for methanol electro-oxidation

Hajar Mokarami Ghartavol, Roozbeh Siavash Moakhar and Abolghasem Dolati . . . . .1399–1410

Electrodeposition of platinum nanoparticles (PtNPs) on multiwall carbon nanotubes (MWCNTs)/flourine-doped tin oxide glass (FTO) was conducted successfully. The electrodeposition mechanism of PtNPs nucleation and growth on MWCNTs was studied. It was found that fine and well-distributed PtNPs/MWCNTs electrode shows a high electrochemical activity for methanol electro-oxidation.

## Regular Article

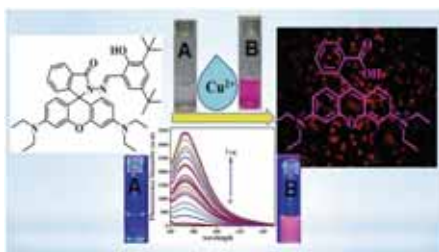


### Nano-sized glass as an economically viable and eco-benign support to anchor heteropolyacids for green and sustainable chemoselective oxidation of sulfides to sulfoxides

Somayeh Zolfagharinia, Eskandar Kolvari, Nadiya Koukabi and Maliheh M Hosseini. . . . .1411–1421

Nano-glass waste-supported phosphomolybdic acid (n-GW/PMA) was synthesized as a novel, highly efficient and retrievable nanocatalyst for the chemoselective, green and rapid oxidation of sulfides to sulfoxides through an experimental design (CCD) approach. The prepared catalyst was characterized by FT-IR, TGA, XRD, FE-SEM and EDX techniques.

## Regular Article

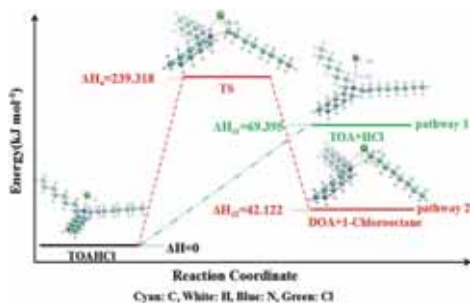


### A new rhodamine based 'turn-on' Cu<sup>2+</sup> ion selective chemosensor in aqueous system applicable in bioimaging

Abhishek Maji, Somenath Lohar, Siddhartha Pal and Pabitra Chattopadhyay. . . . .1423–1430

A new 'turn-on' non-cytotoxic rhodamine hydrazone derivative (**L**) senses Cu<sup>2+</sup> ion in nano molar region selectively in 20 mM HEPES buffer [pH 7.4; water/acetonitrile (9:1 v/v)] and is an efficient biomarker to detect Cu<sup>2+</sup> ions in living cells.

## Regular Article



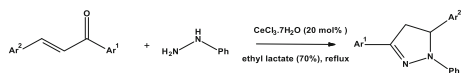
### Mechanism studies on thermal dissociation of tri-n-octylamine hydrochloride with FTIR, TG, DSC and quantum chemical methods

Chunhua Dong, Xingfu Song, Evert Jan Meijer, Guilan Chen, Yanxia Xu and Jianguo Yu . . . . .1431–1440

The thermal dissociation of tri-n-octylamine hydrochloride was investigated with both the quantum chemical simulation and experimental methods. Intrinsic reaction coordinate (IRC) calculations suggest that the products are tri-n-octylamine and HCl rather than di-n-octylamine and 1-chlorooctane. Furthermore, the dissociation is a two-stage process as determined by experimental analysis.

## Regular Article

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### An eco-friendly synthesis of 2-pyrazoline derivatives catalysed by $\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$

Prabhat Bhat, Gomathi Shridhar, Savita Ladage and  
Lakshmy Ravishankar . . . . . 1441–1448

A facile protocol for the synthesis of 1,3,5-triaryl-2-pyrazolines is described. The solvent ethyl lactate, obtained from renewable sources, is biodegradable. The catalyst  $\text{CeCl}_3 \cdot 7\text{H}_2\text{O}$  is a water-tolerant Lewis acid with low toxicity. Easy and clean work up, recyclable solvent and catalyst are the merits of the protocol. The reaction works well for all systems giving good yields of the desired products.

## Regular Article

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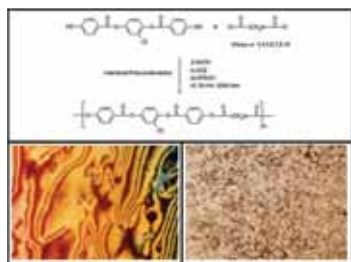
### A novel tandem Betti/Ullmann oxidation reaction as an efficient route for synthesis of new oxazepine derivatives

Reza Teimuri-Mofrad, Mahdi Gholamhosseini-Nazari,  
Somayeh Esmati and Aziz Shahrissa. . . . . 1449–1459

A novel tandem Betti/Ullmann/oxidation reaction was introduced for synthesis of new oxazepine derivatives. This method provides a new and useful strategy for the construction of heterocycles. In this regard,  $\text{Fe}_3\text{O}_4@\text{SiO}_2$ -boric acid nanoparticles have been synthesized and used for the synthesis of desired novel Betti bases based on kojic acid derivatives.

## Regular Article

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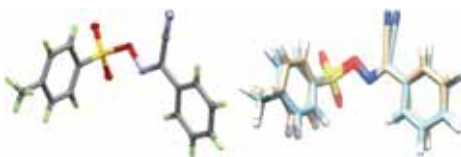
### Thermotropic liquid crystalline polyesters derived from 2-chloro hydroquinone

Nagesh Manurkar, Sayaji More, Khudbudin Mulani, Nitin Ganjave and  
Nayaku Chavan . . . . . 1461–1468

The present study deals with the synthesis of thermotropic liquid crystalline polyesters derived from bis[4-hydroxy benzoyloxy]-2-chloro-1,4-benzene (BHBOCB) and aliphatic dicarboxylic acid chlorides by interfacial polycondensation methodology.

## Regular Article

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### Synthesis, crystallographic characterization, DFT and TD-DFT studies of Oxyma-sulfonate esters

Saied M Soliman, Hazem A Ghabbour, Sherine N Khattab,  
Mohammed R H Siddiqui and Ayman El-Faham . . . . . 1469–1481

An eco-friendly method was used to synthesise three oxyma-sulfonate esters using two-phase (dichloromethane-water) method in presence of sodium carbonate for scavenging HCl. The oxyma sulfonate esters were characterized using different spectroscopic techniques (FT-IR, NMR, UV-Vis) as well as X-ray single crystal diffraction analysis. The electronic and spectroscopic properties of these esters were computed using DFT/B3LYP method.

## Regular Article

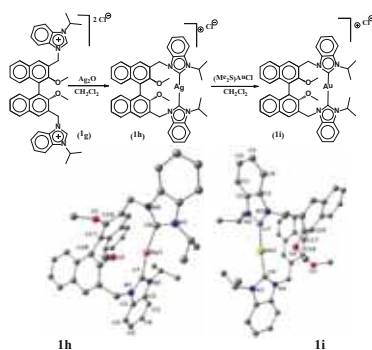


### Schiff base transition metal complexes for Suzuki–Miyaura cross-coupling reaction

Rasheeda M Ansari and Badekai Ramachandra Bhat . . . . . 1483–1490

The transition metal Schiff base complexes synthesized and characterized by SCXRD, Mass spectrometry, TGA, UV–Vis and FTIR analysis. Magnetic susceptibility measurements were also examined to know the plausible geometry of the complex. The synthesized complexes were systematically investigated for Suzuki–Miyaura cross-coupling reactions and optimized to enhance the yield of the Suzuki reaction.

## Regular Article

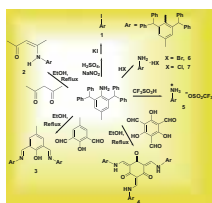


### Axially chiral benzimidazolium based silver(I) and gold(I) bis-NHC complexes of R-BINOL scaffold: synthesis, characterization and DFT studies

Sonali Ramgopal Mahule. . . . . 1491–1498

Synthesis and characterization of  $\{[L(L'-NHC)_2]M\}Cl$  ( $M = Ag$  and  $Au$ ) (**1h**) and (**1i**) silver(I) and gold(I) complexes are reported. Molecular structures of these benzimidazole based, axially chiral complexes of R-BINOL scaffolds were determined by the computational studies. The results of spectroscopic and analytical data as well as the computational study show that the ligand (**1g**) prefers to form mononuclear bis-NHC silver(I) and gold(I) complexes in the given conditions.

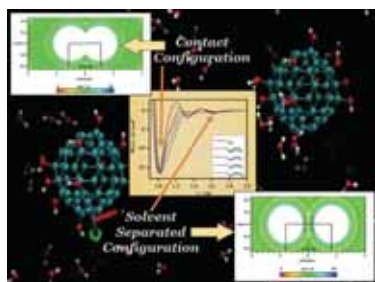
## Regular Article



### Sterically encumbered 2,6-dibenzhydryl-4-methylphenyl derived ligand systems: synthesis and structures

Priya Saxena and Ramaswamy Murugavel . . . . . 1499–1512

A bulky amine was employed to synthesise various compounds containing 2,6-dibenzhydrylphenyl group. These compounds include a bulky iodo-derivative, one mono-, one bis- and one tris-Schiff base, one triflate salt of the bulky amine and two co-crystals of the bulky amine with HBr or HCl.



Cover picture: Potentials of mean force between the COMs of  $C_{60}$ ,  $C_{60}(OH)_2$ ,  $C_{60}(OH)_4$ ,  $C_{60}(OH)_8$ , and  $C_{60}(OH)_{12}$  in water.

For details, see the paper by Sonanki Keshri and B L Tembe (pp. 1327–1340)