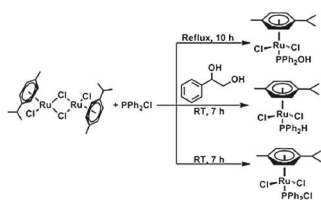


## CONTENTS

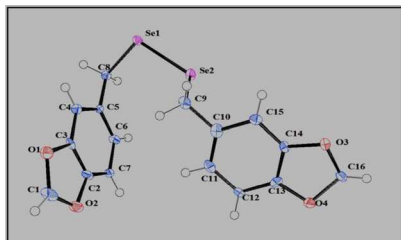
### Regular Articles



#### Synthesis and unexpected reactivity of $[\text{Ru}(\eta^6\text{-cymene})\text{Cl}_2(\text{PPh}_2\text{Cl})]$ , leading to $[\text{Ru}(\eta^6\text{-cymene})\text{Cl}_2(\text{PPh}_2\text{H})]$ and $[\text{Ru}(\eta^6\text{-cymene})\text{Cl}(\text{PPh}_2\text{OH})]$ complexes

Arun Kumar Pandiakumar and Ashoka G Samuelson . . . . . 1329–1338

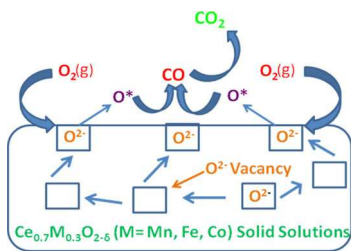
Synthesis and unusual reactivity of some ruthenium half-sandwich complexes including an unusual organocatalysed conversion of  $\text{PPh}_2\text{Cl}$  to  $\text{PPh}_2\text{H}$  are reported.



#### Synthesis and characterization of novel benzo[*d*][1,3]dioxole substituted organo selenium compounds: X-ray structure of 1-((benzo[*d*][1,3]dioxol-5-yl)methyl)-2-((benzo[*d*][1,3]dioxol-6-yl)methyl)diselane

Yogesh Nagpal, Rajeev Kumar and K K Bhasin . . . . . 1339–1346

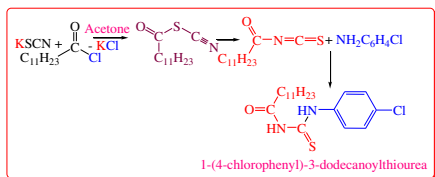
A direct and concise method is reported to furnish novel benzo[*d*][1,3]dioxole incorporated diselenide using stable and readily available starting material. 1-((benzo[*d*][1,3]dioxol-5-yl)methyl)-2-((benzo[*d*][1,3]dioxol-6-yl)methyl)diselane, thus synthesized was transformed into various synthetically important unsymmetrical monoselenides by cleavage of Se–Se bond with sodium borohydride or rongalite.



#### Investigation of physicochemical properties and catalytic activity of nanostructured $\text{Ce}_{0.7}\text{M}_{0.3}\text{O}_{2-\delta}$ ( $\text{M} = \text{Mn}, \text{Fe}, \text{Co}$ ) solid solutions for CO oxidation

P Venkataswamy, D Jampaiah, C U Aniz and Benjaram M Reddy . . . . . 1347–1360

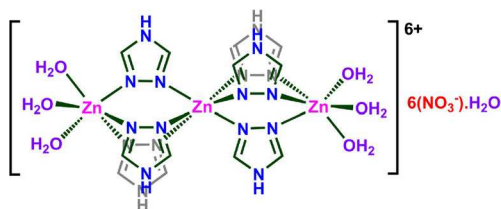
The presence of structural oxygen vacancies, low temperature reducibility and synergetic interaction between Ce–O and Mn–O oxides were responsible for superior CO oxidation performance of Ce–Mn–O nano oxide compared to pure  $\text{CeO}_2$ , Ce–Fe–O and Ce–Co–O samples.



#### Aggregation and electrochemical properties of 1-(4-chlorophenyl)-3-dodecanoylthiourea: A novel thiourea-based non-ionic surfactant

Imdad Ullah, Afzal Shah, Musharaf Khan, Khalida Akhter and Amin Badshah . . . . . 1361–1367

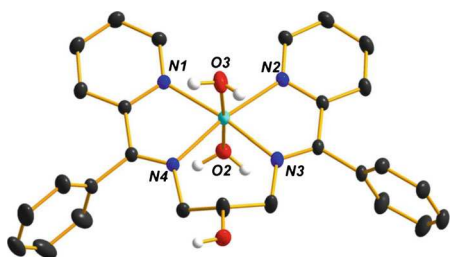
A novel thiourea-based non-ionic surfactant 1-(4-chlorophenyl)-3-dodecanoylthiourea (4CPDT) was synthesized from decanoyl chloride, potassium thiocyanate and 4-chloroaniline in high yield. The structural chemistry of the compound was done by multiple nuclear NMR ( $^1\text{H}$ ,  $^{13}\text{C}$ ) and FT-IR. UV-Visible spectrophotometry and pendant drop methods were used to evaluate the CMC in ethanol and hexane.



### Crystal structure and solid-state properties of discrete hexa cationic trinuclear Zinc Triazole cluster

Chatla Naga Babu, Paladugu Suresh, Arruri Sathyanarayana, Prasenjit Das and Ganesan Prabusankar . . . . . 1369–1373

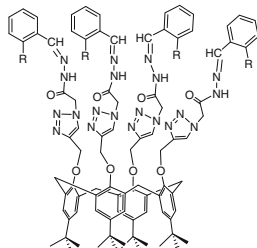
A rare linear, discrete, hexa-cationic trinuclear zinc triazole cluster has been synthesized and structurally characterized.



### DNA binding and cleavage activity of a structurally characterized Ni(II) Schiff base complex

Sarat Chandra Kumar, Abhijit Pal, Merry Mitra, V M Manikandamathavan, Chia -Her Lin, Balachandran Unni Nair and Rajarshi Ghosh . . 1375–1381

Synthesis and characterization of a mononuclear Ni(II) complex  $[\text{Ni}(\text{L})_2(\text{H}_2\text{O})_2](\text{NO}_3)_2$  [ $\text{L} = \text{N},\text{N}'\text{-bis}(\text{pyridine-2-yl})\text{phenylidene-1,3-diaminopropan-2-ol}$ ] (**1**) is reported. **1** crystallizes in P-1 space group. Spectroscopic and hydrodynamic investigations on the binding property of the complex with DNA have revealed groove or electrostatic nature of binding of **1** with DNA. **1** is also found to induce oxidative cleavage of the supercoiled pUC 18 DNA to its nicked circular form in a concentration dependent manner.



### Thiacalix[4]arene derivatives containing multiple aromatic groups: Highly efficient extractants for organic dyes

Chuang Yang, Zusheng Wang, Hongyu Guo, Ziyu Jiao and Fafu Yang . . . . . 1383–1388

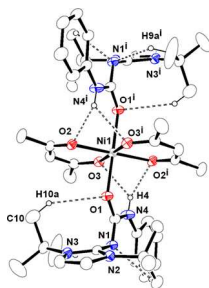
Two novel thiacalix[4]arene derivatives containing multiple aromatic groups were synthesized in yields of 86% and 90%. These complexation experiments showed that thiacalix[4]arene receptors possess excellent complexation capabilities for four tested dyes.



### Sulfanilic acid functionalized mesoporous SBA-15: A water-tolerant solid acid catalyst for the synthesis of uracil fused spirooxindoles as antioxidant agents

Robabeh Baharfar and Razieh Azimi . . . . . 1389–1395

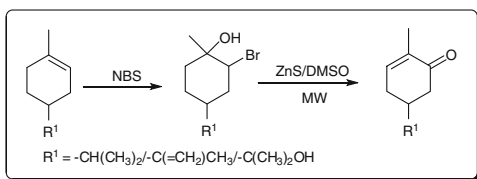
Green synthesis of uracil-fused spirooxindoles using sulfanilic acid-functionalized SBA-15 as a reusable heterogeneous acid catalyst and the antioxidant activity of the synthesized compounds are described.



### Nickel(II) complexes having Imidazol-2-ylidene-N'-phenylurea ligand in the coordination sphere – syntheses and solid state structures

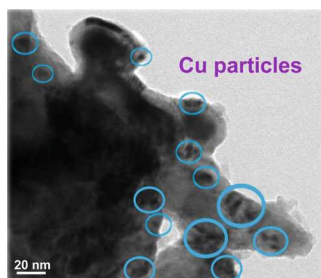
Kishor Naktode, Abhinanda Kundu, Sudeshna Saha, Hari Pada Nayek and Tarun K Panda . . . . . 1397–1404

We report the synthesis and structures of two octahedral nickel(II) complexes supported by imidazol-2-ylidene-N'-phenylureate ligand.

**Microwave assisted bi-functional activation of  $\beta$ -bromo-*tert*-alcohols**

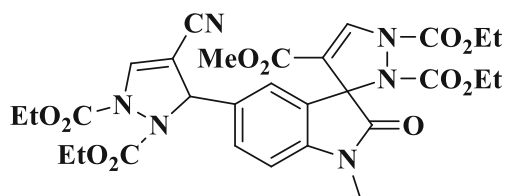
Kannan Nandini, Manjunatha Javagal Rangaswamy and Bettadaiah Bheemanakere Kemapaiah . . . . . 1405–1410

Microwave-assisted bi-functional activation of  $\beta$ -bromo-*tert*-alcohols to afford 2,3-unsaturated ketones is reported. The dehydration-oxidation of  $\beta$ -bromo-*tert*-alcohols occurs with DMSO in the presence of ZnS under solvent-free condition.

**Significant improvement of electrochemical performance of Cu-coated LiVPO<sub>4</sub>F cathode material for lithium-ion batteries**

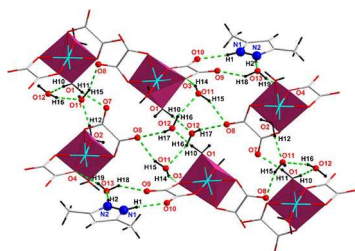
Yu Zhang, Xiaolan Bai and Cuiling Li . . . . . 1411–1416

Nano-Cu coating on the surface of pristine LiVPO<sub>4</sub>F particles is successfully synthesized for the first time via a soft chemical route with mechanical activation assistance. The effect of Cu coating on the crystalline structure, morphology and electrochemical performance of the pristine sample has been investigated in detail.

**An efficient and facile synthesis of divergent C-3/C-5 bis-functionalized 2-oxindoles from 5-formyl-Morita-Baylis-Hillman adducts of oxindole**

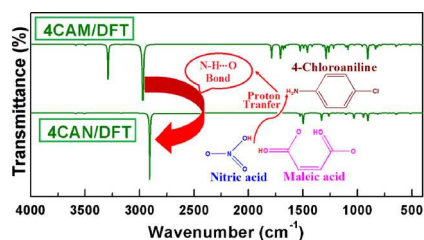
Kodirajan Selvakumar, Kandapalam Arun Prasath Lingam, Rama Varma Luxmi Varma and Poovan Shanmugavelan . . 1417–1426

An efficient and facile synthesis of divergent C-3/C-5 bis-functionalized 2-oxindoles has been achieved from 3,5-bis-Morita-Baylis-Hillman (MBH) adducts. A wider substrate scope/rate acceleration has been noted under a typical reaction condition and also the synthetic usefulness of bis-allyl derivatives has been demonstrated by the synthesis of potent bis-pyrazole *via* [3+2]-annulation strategy.

**Synthesis, Crystal structure and Characterization of a New Oxalate Chromium(III) Complex**

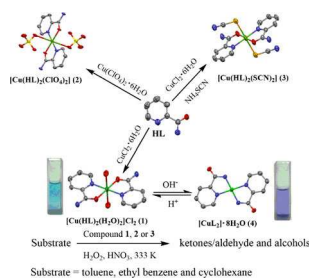
Rihab Dridi, Saoussen Cherni and Mohamed Faouzi Zid . . . 1427–1433

Fragments of the molecular structure of the complex show clearly the intermolecular N H...O and O H...O hydrogen bonds between the cation, the complex anion and the lattice water molecules which contribute to the cohesion of the ionic structure, leading to a three dimensional network.

**Structural and vibrational spectral studies on hydrogen bonded salts: 4-chloroanilinium maleate and nitrate**

R Anitha, M Gunasekaran, S Suresh Kumar and S Athimoolam . . 1435–1450

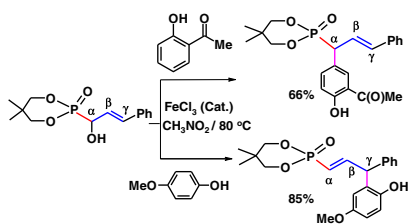
The proton transfer from the nitric and maleic acids to amine group (of 4-chloroaniline) lead to hydrogen bonded crystals of 4-chloroanilinium maleate (4CAM) and 4-chloroanilinium nitrate (4CAN). The molecular structures of these two compounds were optimized with the Density Functional Theory (DFT) and Hartree-Fock (HF) methods. Geometrical parameters of the molecules were analyzed along with their intermolecular hydrogen bond which tailors the ions. These analyses show that the molecular aggregations are stabilized through the N–H...O and O–H...O hydrogen bonds. The vibrational modes were computed by quantum chemical methods and further investigated by FT-IR and FT-Raman spectroscopy in the range of 4000–400 cm<sup>-1</sup>.



### 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

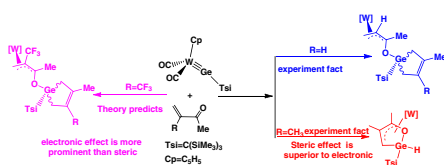
X-ray structural characterization, pH-induced co-ordination mode switching phenomenon, peroxidative oxidation catalysis and antimicrobial activity of water soluble, discrete mononuclear complexes of copper(II) using the simplest pyridine 2-carboxamide ligand (HL) and its deprotonated form have been investigated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

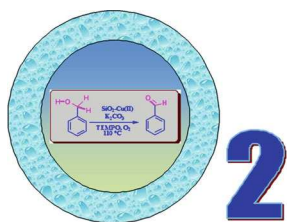
Regioselective allylation of phenolic substrates using phosphono-allyl alcohols was achieved by using even catalytic amounts of FeCl<sub>3</sub>. Both vinylphosphonates and allylphosphonates are obtained, the ratio depending upon the substrate.



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

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

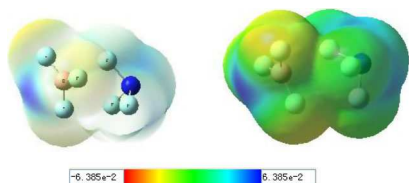
Results of theoretical analysis for the reaction mechanism involving a tungsten-germylyne complex with α, β-unsaturated ketones have been reported. The effect of substituents at the α position (H, Me and CF<sub>3</sub>) of the unsaturated ketones has been demonstrated.



### 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

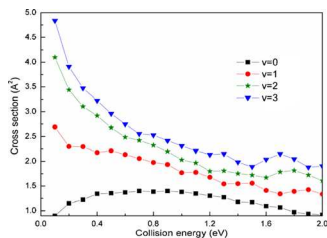
This work deals with the oxidation of benzyl alcohols catalyzed by silica functionalized copper (II) and co-catalyzed by TEMPO using molecular oxygen as an oxidant. The catalytic system works very selectively and exclusively forming only aldehydes.



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

Hongchen Du . . . . . 1491–1496

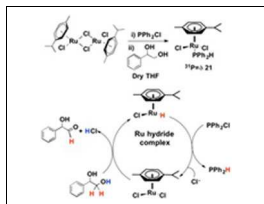
The adduct NF<sub>3</sub>·BF<sub>3</sub> exists as a complex but is not ionic. The heat of formation of the gas (–1266.09 kJ·mol<sup>-1</sup>) is slightly higher than the condensed phase (–1276.37 kJ·mol<sup>-1</sup>). Its crystal form belongs to *P21/c* space group. The calculated large band gap (6.06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



### Influence of collision energy and vibrational excitation on the dynamics for the $\text{H}+\text{HBr} \rightarrow \text{H}_2+\text{Br}$ reaction

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

A detailed dynamical study of reaction,  $\text{H}+\text{HBr} (\nu=0-3, j=0) \rightarrow \text{H}_2+\text{Br}$ , with QCT method has been performed. Both present QCT and available QM results for the  $\text{HBr} (\nu=0, j=0)$  have been found to be fairly consistent with each other. The reaction switches from activated to capture-type with increase of the quantum number  $\nu$ .



*Cover picture:* Unraveling the mysterious formation of a diphenylphosphine complex. For details, see the paper by Arun Kumar Pandiakumar and Ashoka G Samuelson (pp. 1329–1338)