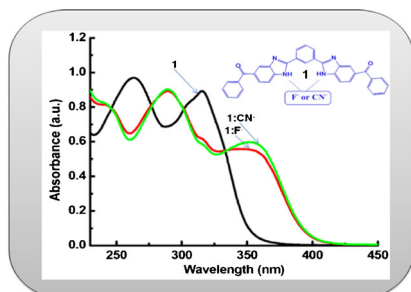


CONTENTS

General Editorial on Publication Ethicsiv

Rapid Communication

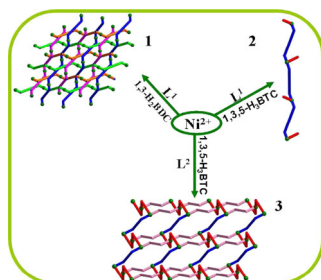


A Novel Benzimidazolyl-based Receptor for the recognition of Fluoride and Cyanide Anion

Eramoni Saikia, Pankaj Dutta and Bolin Chetia 1–7

A novel benzimidazole based ligand (**1**) has been synthesized and studied its anion recognition properties. The binding of anion with **1** was studied using UV-Visible spectroscopy, fluorescence spectroscopy and ^1H -NMR techniques at very low concentrations. The results obtained from the spectroscopic studies indicate that ligand **1** is an efficient anion receptor providing changes in chemical shift and optical signals for the detection of two most environmentally important anions, fluoride and cyanide.

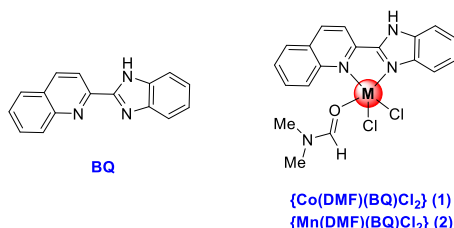
Regular Articles



Self-assembly, structures and properties of three new Ni(II) coordination polymers derived from two different bis-pyridyl-bis-amide ligands and two aromatic polycarboxylates

Hongyan Lin, Junjun Sun, Guocheng Liu, Xiang Wang and Panwen Chen. 9–20

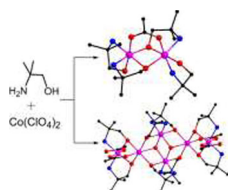
Three new Ni(II) coordination polymers have been hydrothermally synthesized by self-assembly of two bis-pyridyl-bis-amide ligands (L^1 , L^2) and two aromatic polycarboxylates (1,3- H_2BDC , 1,3,5- H_3BTC). The thermal stability, fluorescent properties and the photocatalytic activities of polymers **1–3** have been studied.



Synthesis, X-ray structure and theoretical investigation of 2-(2'-quinolyl)benzimidazole metal complexes

Feriel Aouatef Sahki, Lyamine Messaadia, Hocine Merazig, Aissa Chibani, Abdelmalek Bouraiou and Sofiane Bouacida . . . 21–29

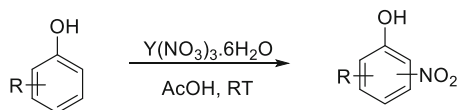
Synthesis, characterization and DFT analysis of 2-(1*H*-benzo[d]imidazol-2-yl)quinoline (BQ) and its cobalt and manganese coordination compounds $\{\text{Co}(\text{DMF})(\text{BQ})\text{Cl}_2\}$ and $\{\text{Mn}(\text{DMF})(\text{BQ})\text{Cl}_2\}$ have been described. Theoretically calculated frontier molecular orbitals (HOMO-LUMO) of both complexes indicate intermolecular charge transfer and delocalization of electron density within the molecule.



Synthesis and structures of two cobalt compounds of 2-amino-2-methyl-1-propanol

Yongjie Qin, Shanshan Yang, Long Liu, Yuning Liang and Zilu Chen 31–37

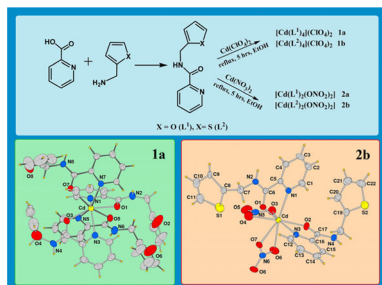
We present here two Cobalt clusters of 2-amino-2-methyl-1-propanol, which feature dinuclear and hexanuclear structures.



Yttrium Nitrate mediated Nitration of Phenols at room temperature in Glacial Acetic acid

Mohabul A Mondal, Debashis Mandal and Kanchan Mitra . . . 39–43

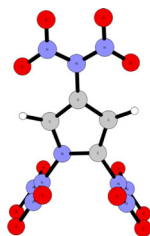
A convenient and facile nitration of aromatic phenols using $\text{Y}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ in glacial acetic acid at room temperature has been observed. The method is very simple, rapid, and specific for phenols.



Synthesis, characterization, crystal structure and DNA-binding study of four cadmium(II) pyridine-carboxamide complexes

Biplab Mondal, Buddhadeb Sen, Sandipan Sarkar, Ennio Zangrando and Pabitra Chattopadhyay 45–55

Synthesis and characterization of four mononuclear eight coordinated cadmium(II) complexes with newly explored carboxamide derivatives and study of interaction with calf-thymus DNA are reported. The results suggest that neutral complexes **2a** and **2b** bind to DNA in an intercalative mode. On the other hand, cationic complexes **1a** and **1b** interact with DNA *via* weak intercalative or groove binding mode.

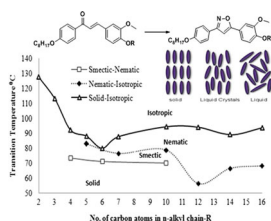


D=9.04 km/s P= 40.36 GPa

Molecular design and performance prediction of poly-dinitroamino pyrrole compounds as energetic materials

Mei Li, Feng-Min Wu and Hang Xu. 57–65

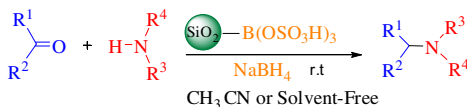
To identify superior and safe energetic materials, eighteen poly-dinitroamino pyrrole derivatives were studied at the B3LYP/6-311G** level of density functional theory (DFT). One of the compounds, C2(N-R), is the most promising energetic compound due to its superior energetic properties (D=9.04 km/s, P= 40.36 GPa) and lower sensitivity among all poly-dinitroamino pyrrole derivatives.



Synthesis and characterization of new homologous series of unsymmetrical liquid crystalline compounds based on chalcones and 3, 5-disubstituted isoxazoles

Sowmya P T and K M Lokanatha Rai 67–73

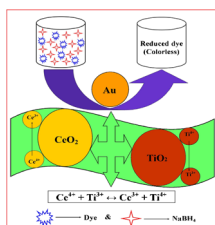
Two homologous series of unsymmetrical alkylated chalcogens and 3,5-diaryl isoxazoles were synthesized and characterized by polarizing optical microscopy (POM) and differential scanning calorimetry (DSC).



One-pot Reductive Amination of Carbonyl Compounds with $\text{NaBH}_4\text{-B(OSO}_3\text{H)}_3/\text{SiO}_2$ in Acetonitrile and in Solvent-free Condition

Hosein Hamadi and Samira Javadi 75–80

An efficient one-pot procedure for the direct reductive amination of aldehyde and ketones in the presence of sodium borohydride by using $\text{B(OSO}_3\text{H)}_3/\text{SiO}_2$ (SBSA) as the reusable solid catalyst in acetonitrile and under solvent-free conditions is described.

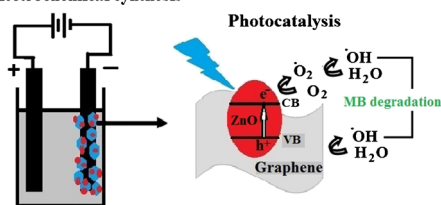


Highly efficient catalytic reductive degradation of various organic dyes by $\text{Au/CeO}_2\text{-TiO}_2$ nano-hybrid

Pranjal Saikia, Abu T Miah and Partha P Das 81–93

Nanosized Gold particles stabilized on $\text{CeO}_2\text{-TiO}_2$ nanocomposite exhibits tremendous catalytic activity in the reductive degradation of various organic dyes with good stability and reusability.

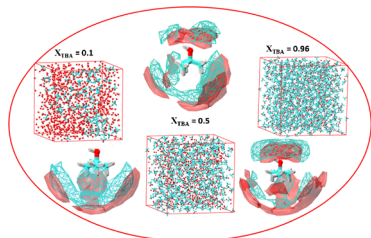
Electrochemical synthesis



Photocatalytic Activity of Graphene/ZnO Nanocomposite Fabricated by Two-step Electrochemical Route

A R Nanakkal and L K Alexander 95–102

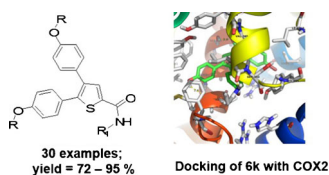
Graphene and Graphene – ZnO nanocomposite were synthesized by a two-step electrochemical route. Phase-pure samples were prepared by post heating of the electrochemically prepared samples. Graphene-ZnO exhibited enhanced photocatalytic activity over ZnO. The methodology discussed in this report suggests a facile, efficient method for the synthesis of metal oxide functionalized graphene suitable for different applications.



Three-dimensional Morphology and X-ray Scattering Structure of Aqueous *tert*-Butanol Mixtures: A Molecular Dynamics Study

Supreet Kaur and Hemant K Kashyap. 103–116

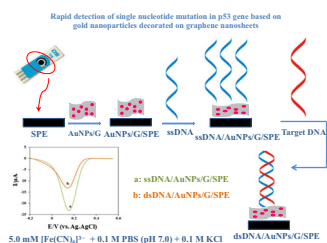
Molecular dynamics simulation results show that for less than 10% concentration of TBA, the water-like structural arrangement is apparently present and beyond 50:50 composition, TBA-like microscopic structure gradually takes over. Hydrophobic aggregation is maximum at 10% TBA concentration of the mixture.



Synthesis, *in vitro* anti-inflammatory activity and molecular docking studies of novel 4,5-diarylthiophene-2-carboxamide derivatives

T Shanmuganathan, K Parthasarathy, M Venugopal, Y Arun, N Dhatchanamoorthy and A A M Prince. 117–130

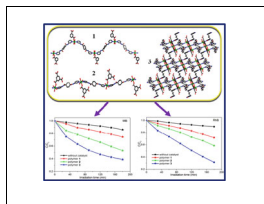
A series of 30 novel 4,5-diarylthiophene-2-carboxamide containing alkyl, cycloalkyl, aryl, aryl alkyl and heterocyclic alkyl moieties were synthesized, characterized and evaluated *in vitro* for their anti-inflammatory activity and molecular docking study.



Rapid detection of single nucleotide mutation in p53 gene based on gold nanoparticles decorated on graphene nanosheets

Seyedeh Zeinab Mousavisani, Jahan Bakhsh Raoof, Reza Ojani and Roudabeh Valiollahi 131–139

Rapid detection of DNA hybridization and single nucleotide mutation is reported by using gold nanoparticle-decorated, graphene nanosheets-modified screen printed electrode. Under optimal conditions, the peak current had a linear relation with the logarithm of the concentration of target complementary DNA in the range 0.5 fM to 0.05 nM, with a detection limit of 0.36 ± 0.04 fM.



Cover picture: Structures and photocatalytic properties of three Ni(II) polymers. For details, see the paper by H Lin *et al.* (pp. 9–20)