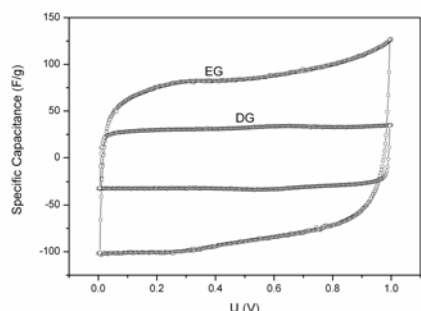


CONTENTS

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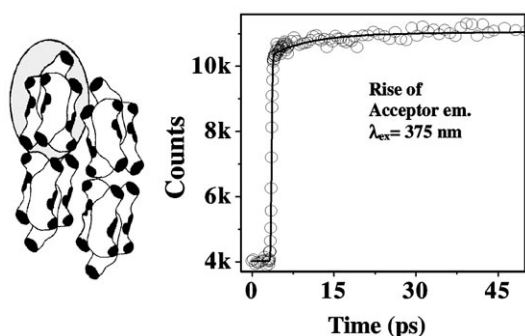
Foreword 7



Graphene-based electrochemical supercapacitors

S R C Vivekchand, Chandra Sekhar Rout, K S Subrahmanyam, A Govindaraj and C N R Rao 9–13

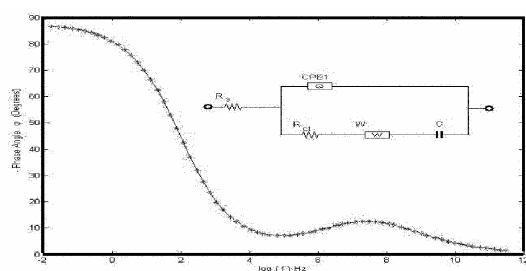
Graphenes prepared by the exfoliation of graphitic oxide and by the transformation of nanodiamond are good electrode materials for supercapacitors. The performance characteristics of the graphenes, which are directly related to the quality in terms of the number of layers and the surface area, are superior to that of carbon nanotubes.



Ultrafast fluorescence resonance energy transfer in a bile salt aggregate: Excitation wavelength dependence

Ujjwal Mandal, Subhadip Ghosh, Dibyendu Kumar Das, Aniruddha Adhikari, Shantanu Dey and Kankan Bhattacharyya 15–23

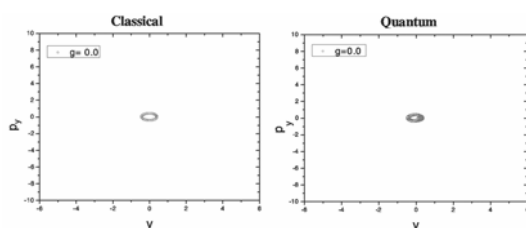
FRET from coumarin 153 to rhodamine 6G in a bile salt (NaDC) aggregate is studied by femtosecond up-conversion. With increase in excitation wavelength, contribution of the 4 ps component of FRET increases and that of the 3700 ps component decreases. This is attributed to the presence of donors at different locations.



Analysis of polypyrrole-coated stainless steel electrodes – Estimation of specific capacitances and construction of equivalent circuits

R Ramya and M V Sangaranarayanan 25–31

The feasibility of polypyrrole-coated stainless steel electrodes as electrochemical supercapacitors is investigated using impedance spectroscopy, galvanostatic charge–discharge studies and cyclic voltammetric experiments. The system parameters are obtained by constructing an appropriate equivalent circuit pertaining to the experimental Nyquist and Bode plots.



Quantum–classical correspondence of a field induced KAM-type transition: A QTM approach

P K Chattaraj, S Sengupta and S Giri 33–37

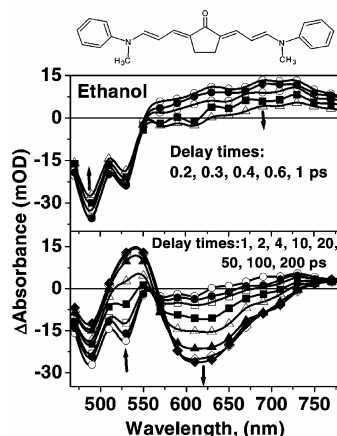
Quantum theory of motion provides a reasonable recipe for analysing the quantum signature of the classical field induced KAM transition in an anharmonic oscillator.



Self assembly of *C*-methyl resorcin[4]arene with coumarin and thiocoumarin: A nanotubular array with a near perfect lock and key fit

Lepakshaiha Mahalakshmi, Partha P Das and Tayur N Guru Row 39–44

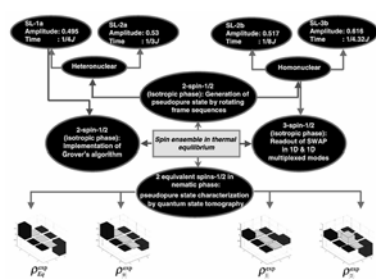
The host-guest complex of *C*-methyl resorcin[4]arene with coumarin and thiocoumarin has been characterised by single crystal X-ray diffraction technique. Structural analysis shows the host forms an infinite nanotubular array in which the guest adopts a ‘head to tail’ arrangement of dimers held together by weak $\pi \dots \pi$ interaction.



Relaxation dynamics in the excited states of a ketocyanine dye probed by femtosecond transient absorption spectroscopy

Jahur A Mondal, Sandeep Verma, Hirendra N Ghosh and Dipak K Palit 45–55

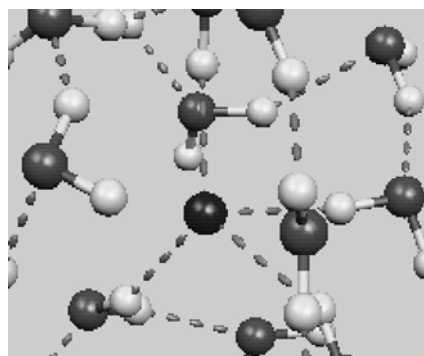
Following photoexcitation of 2,5-*bis*-(*N*-Methyl-*N*-1,3-Propdienylaniline)-cyclopentanone (MPAC), a ketocyanine dye, using 400 nm light, the molecule is excited to the S_2 state, which has a very short lifetime (0.5 ± 0.2 ps). In aprotic solvents, the S_1 state follows a complex multi-exponential relaxation dynamics consisting of torsional motion of the donor groups, solvent re-organization as well as photoisomerization processes. However, in alcoholic solvents, solvent re-organization via intermolecular hydrogen-bonding interaction is the major relaxation process observed in the S_1 state.



General approaches in ensemble quantum computing

V Vimalan and N Chandrakumar 57–69

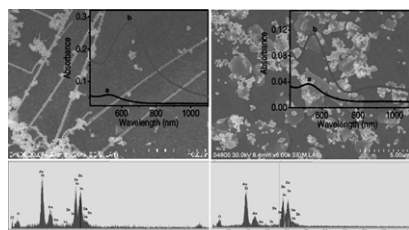
We report methodology for NMR quantum computing focusing on enhancing the efficiency of initialization, logic gate implementation and readout. Our strategy involves application of rotating frame pulse sequences to prepare pseudopure states and perform logic operations on homo- and hetero-nuclear spin systems. We also demonstrate a multiplexed 1D readout strategy.



Effects of ion concentration on the hydrogen bonded structure of water in the vicinity of ions in aqueous NaCl solutions

A Nag, D Chakraborty and A Chandra 71–77

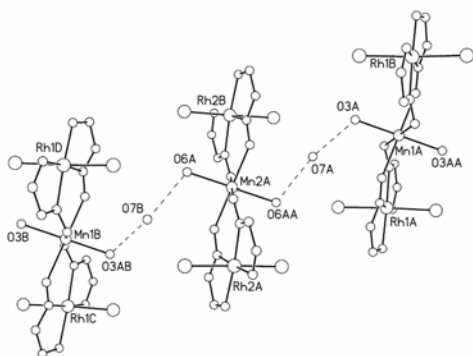
Molecular dynamics simulations of dilute and concentrated aqueous NaCl solutions are carried out to investigate the changes of the hydrogen bonded structures in the vicinity of ions for different ion concentrations. An analysis is made for the hydrogen bond distributions in the first and second solvation shells of the ions and also in the bulk water.



Growth of anisotropic gold nanostructures on conducting glass surfaces

P R Sajanlal and T Pradeep 79–85

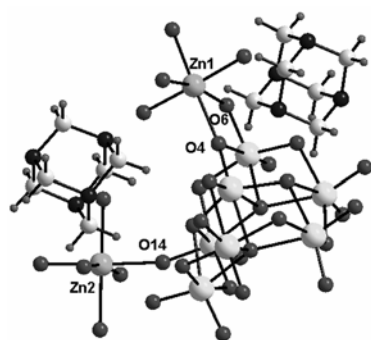
A simple method for the growth of gold nanoplates and nanowires on ITO substrates starting from a bilayer assembly of gold nanoparticle seeds is demonstrated.



Oximate bridged $\text{Rh}^{\text{III}}_2\text{M}^{\text{II}}$ and $\text{Rh}^{\text{III}}\text{M}^{\text{I}}$ species ($\text{M}^{\text{II}} = \text{Mn}, \text{Co}, \text{Ni}$; $\text{M}^{\text{I}} = \text{Cu}, \text{Ag}$)

Indranil Bhattacharyya, Sanjib Ganguly, Bikash Kumar Panda and Animesh Chakravorty 87–93

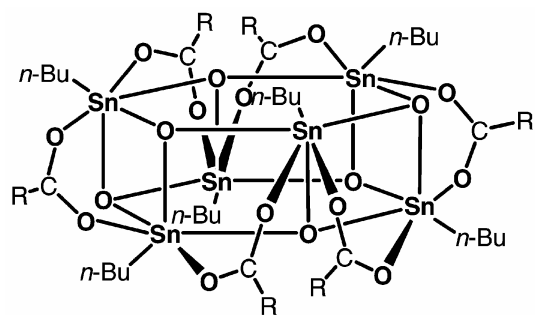
The title species incorporate azooxime bridging which binds Rh^{III} at N and M^{II} or M^{I} at O. The $\text{Mn}^{\text{II}}\text{O}_6$ coordination spheres of neighbouring molecules in the $\text{Rh}_2^{\text{III}}\text{Mn}^{\text{II}}$ system are held in a zigzag chain by hydrogen bonded water trimers. In $\text{Rh}^{\text{III}}\text{Cu}^{\text{I}}$ the copper geometry is distorted tetrahedral.



Two different zinc(II)-aqua complexes held up by a metal-oxide based support: Synthesis, crystal structure and catalytic activity of $[\text{HMTAH}]_2\{\{\text{Zn}(\text{H}_2\text{O})_5\}\{\text{Zn}(\text{H}_2\text{O})_4\}\{\text{Mo}_7\text{O}_{24}\}\cdot 2\text{H}_2\text{O}$ (HMTAH = protonated hexamethylenetetramine)

T Arumuganathan, A Srinivasarao, T Vijay Kumar and Samar K Das 95–103

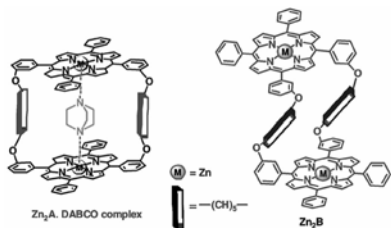
The title compound consisting of two Zn(II)-aqua complexes, $[\text{Zn}(\text{H}_2\text{O})_5]^{2+}$ and $[\text{Zn}(\text{H}_2\text{O})_4]^{2+}$ supported by an isopolyanion $[\text{Mo}_7\text{O}_{24}]^{6-}$, exhibits an interesting supramolecular architecture in its crystal structure and is found to catalyse the oxidation of benzyl alcohol to benzaldehyde using hydrogen peroxide as an oxidant.



Multi-functional architectures supported on organostannoxane scaffolds

Vadapalli Chandrasekhar, Palani Sasikumar, Puja Singh, Ramalingam Thirumoorthi and Tapas Senapati 105–113

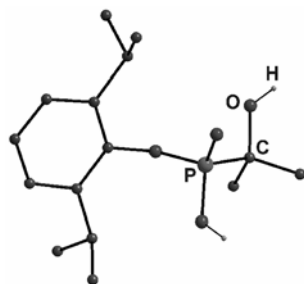
The reactions of organotin oxides/hydroxides with protic acids such as RCOOH afford a variety of organostannoxane assemblies. Utilizing this synthetic protocol it has been possible to prepare organostannoxane-cored dendrimeric structures. The periphery of such dendrimers can be varied with the incorporation of electroactive, photoactive or multi-site coordinating ligands.



Cyclic porphyrin dimers as hosts for coordinating ligands

G Vaijyanthimala, V Krishnan and S K Mandal 115–129

Synthesis and characterization of molecular hosts for complexing coordinating ligands based on cyclic porphyrin dimers Zn_2A and Zn_2B are reported.

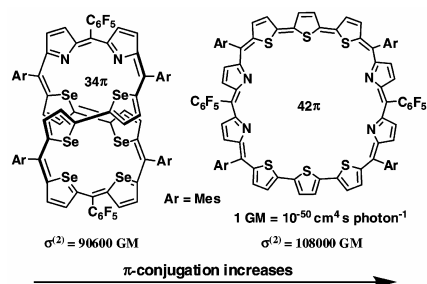


Facile one-pot synthesis of functionalized organophosphonate esters via ketone insertion into bulky aryloxy phosphites

Ramaswamy Murugavel and Subramaniam Kuppaswamy

131–136

A single step methodology has been developed for the synthesis of organophosphonate esters starting from aryloxy phosphorus(III)chlorides.



Expanded porphyrins as third order non-linear optical materials: Some structure–function correlations

Sabapathi Gokulnath and Tavarekere K Chandrashekar ... 137–142

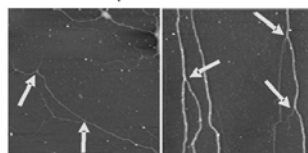
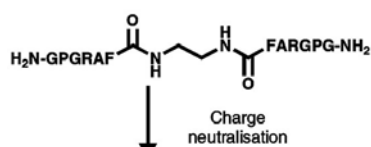
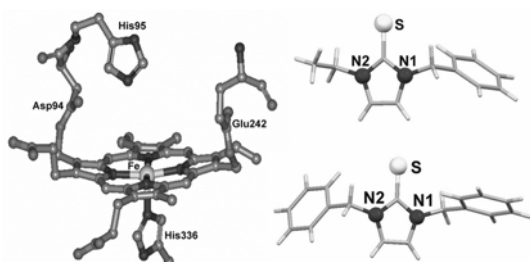
This article presents an overview of various factors that influence TPA (σ^2) values through 22 to 42 π expanded porphyrins. Significant increase in the σ^2 values are observed as a function of aromaticity and conformation of the macrocycle.

Effect of thione–thiol tautomerism on the inhibition of lactoperoxidase by anti-thyroid drugs and their analogues

P N Jayaram, Gouriprasanna Roy and Govindasamy Mugesh

143–154

The synthesis and characterization of some thiones and selones having N,N-disubstituted imidazole moiety are described. The single crystal X-ray and NMR spectroscopic studies suggest that these compounds exist as zwitterions in which the sulfur/selenium atom carries a large negative charge. While the N,N-disubstituted thiones do not inhibit LPO-catalysed oxidation reactions, the selones effectively inhibit the LPO activity. The kinetic and mechanistic studies reveal that the selones inhibit the LPO activity by scavenging the peroxide substrate, suggesting that the selenium analogues of anti-thyroid drugs may have significant antioxidant activity.

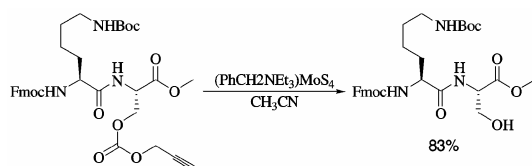


Facilitation of peptide fibre formation by arginine-phosphate/carboxylate interactions

K Krishna Prasad and Sandeep Verma 155–162

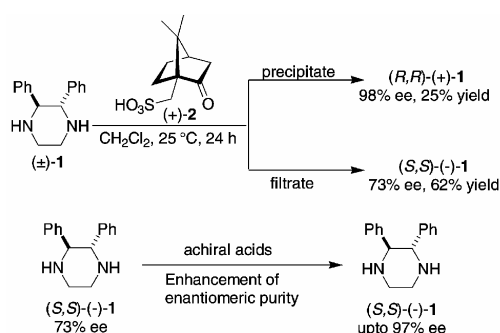
This study describes peptide fibre formation in a hexapeptide, derived from the V3 loop of HIV-1, mediated by electrostatic interactions between arginine residues and phosphate/carboxylate anions.

Propargyloxycarbonyl as a protecting group for the side chains of serine, threonine and tyrosine



Ramapanicker Ramesh, Kavita De, Shipra Gupta and Srinivasan Chandrasekaran 163–173

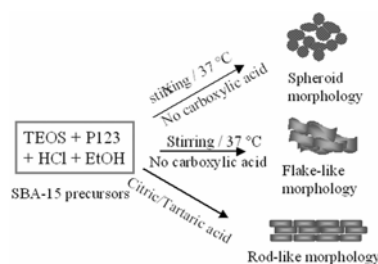
The applications of Propargyloxy-carbonyl group as an efficient protecting group for the side chain hydroxyl groups of serine, threonine and tyrosine is studied in detail and its application in solution phase peptide synthesis is demonstrated.



Efficient resolution of (\pm) -*trans*-2,3-diphenylpiperazine using $(1S)$ - $(+)$ -10-camphorsulfonic acid and enrichment of enantiomeric purity of non-racemic 2,3-diphenylpiperazine using different achiral acids

Pothiappan Vairaprakash and Mariappan Periasamy 175–179

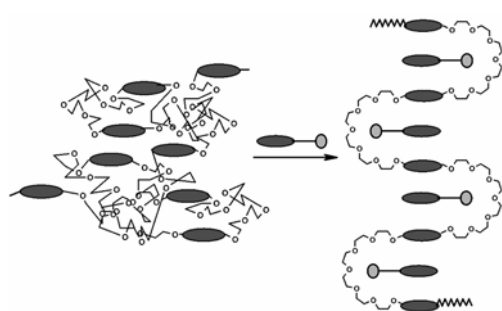
Enantiomerically pure (R,R) - $(+)$ -2,3-diphenylpiperazine with 98% ee was obtained by resolution of the corresponding racemic mixture using $(1S)$ - $(+)$ -10-camphorsulfonic acid. The partially resolved enriched sample of (S,S) - $(-)$ -2,3-diphenylpiperazine with 72% ee obtained from filtrate fraction was purified to obtain samples of 97% ee using different achiral acids via the preparation of either homochiral or heterochiral hydrogen bonded aggregates.



Significant improvement in the pore properties of SBA-15 brought about by carboxylic acids and hydrothermal treatment

Milan Kanti Naskar and M Eswaramoorthy 181–186

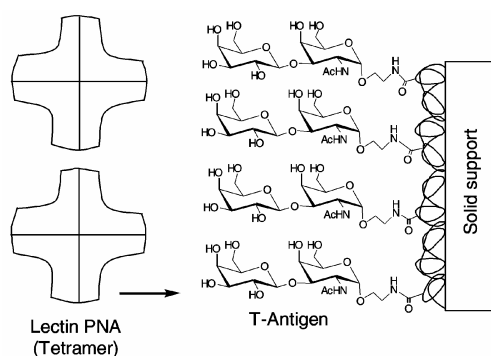
A comparative study of the pore properties of SBA-15 samples prepared under non-hydrothermal and hydrothermal conditions, in the absence and presence of carboxylic acids, shows that the carboxylic acids modify the morphology as well as the pore properties.



Understanding the folding process of synthetic polymers by small-molecule folding agents

S G Ramkumar and S Ramakrishnan 187–194

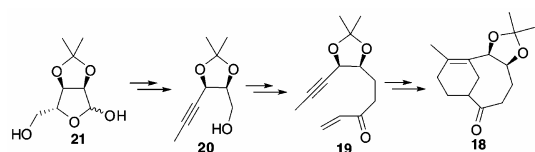
Two acceptor containing polyimides carrying either pyromellitic diimide or 1,4,5,8-naphthalene tetracarboxy diimide units, along with hexa(oxyethylene) (EO6) segments as linkers, were made to adopt a folded conformation by a two-point interaction with a suitable dialkoxy-naphthalene donor that carried a potassium carboxylate group covalently linked to it.



A kinetic analysis of the tumor-associated galactopyranosyl-(1→3)-2-acetamido-2-deoxy- α -D-galactopyranoside antigen–lectin interaction

Bandaru Narasimha Murthy and Narayanaswamy Jayaraman 195–203

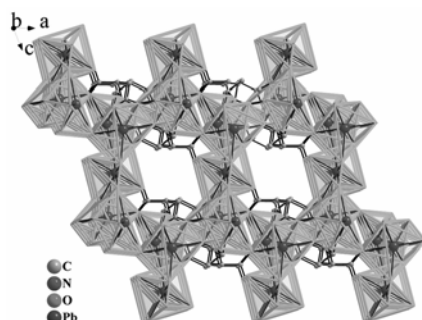
The kinetic on-off rates for the interaction of the immobilized T-antigen with lectin peanut agglutinin (PNA) as analyte are assessed by the surface plasmon resonance technique. The high-affinity interaction between the ligand and the lectin is characterized by fast first association rate constant and a slow dissociation rate constant.



Synthetic studies on taxanes: A domino–enyne metathesis/Diels–Alder approach to the AB-ring

Krishna P Kaliappan, Velayutham Ravikumar and Sandip A Pujari 205–216

A highly efficient, domino enyne cross-metathesis/intramolecular Diels–Alder reaction approach to synthesize bicyclo[5.3.1]undecene, which corresponds to the AB-ring of taxol without gem dimethyl group and our cumulative efforts towards the synthesis of functionalized BC-ring framework of taxane are described.



Three-dimensional hybrid networks based on aspartic acid

Anupama Ghosh and R A Sanguramath 217–222

Three-dimensional achiral coordination polymers of the general formula $M_2(D, L\text{-NHCH}(\text{COO})\text{CH}_2\text{COO})_2\text{-C}_4\text{H}_4\text{N}_2$, where $M = \text{Ni}$ and Co , have been prepared under hydrothermal conditions starting with $[\text{M}(\text{L-NHCH}(\text{COO})\text{CH}_2\text{COO})_3\text{H}_2\text{O}]$ and pyrazine. A three-dimensional hybrid compound of the formula $\text{Pb}_{2.5}[\text{N}\{\text{CH}(\text{COO})\text{CH}_2\text{COO}\}_2\text{H}_2\text{O}]$ has also been prepared hydrothermally starting with $\text{Pb}(\text{NO}_3)_2$ and aspartic acid where the acid undergoes *in situ* dimerisation to form a secondary amine.