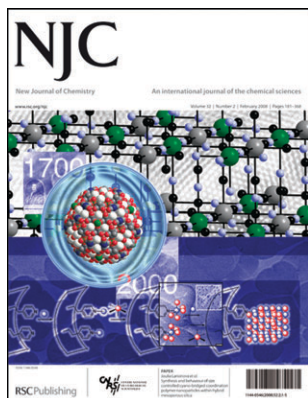


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ISSN 1144-0546 CODEN NJCHES 32(2) 181-368 (2008)



Cover

300 years after the discovery of Prussian blue, cyano-bridged metal coordination polymers are synthesised as nanoparticles and organised by using meso-structured hybrid silica hosts. Cover designed by Paolo ParrilImage. Reproduced with permission from Claudio Sangregorio.

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Inside Cover

The ethanol content of hydroalcoholic beverages (like the whisky in these barrels) and gasoline-ethanol blends can be accurately determined thanks to a fluoruous colorimetric copper(II)-based indicator-displacement assay. Photo reproduced with permission from Tim Rogers. Image reproduced by permission of Jean-Marc Vincent from *New J. Chem.*, 2008, **32**, 193-196.

CHEMICAL SCIENCE

C9

Drawing together the research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences showcasing newsworthy articles, as well as the most significant scientific advances.

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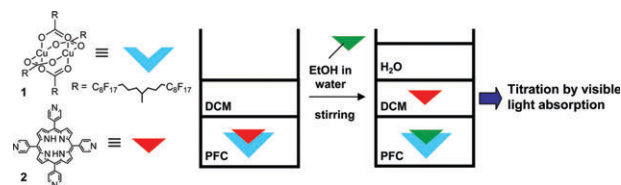
LETTERS

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A copper(II)-based multiphasic fluoruous colorimetric ethanol assay

Mounir El Bakkari, Raymond Luguia, Rosenildo Correa da Costa and Jean-Marc Vincent*

A copper(II)-based multiphasic colorimetric assay exhibiting selectivity for ethanol over water and linear aliphatic alcohols has been developed and applied in the titration of aqueous, organic and gasoline-ethanol blends (bioethanol).



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FL 32611
USA
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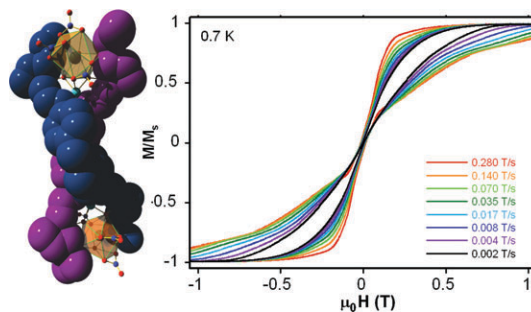
LETTERS

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A single molecule magnet (SMM) with a helicate structure

Ghenadie Novitchi, Jean-Pierre Costes,* Jean-Pierre Tuchagues, Laure Vendier and Wolfgang Wernsdorfer*

Structural determination confirms that a tetranuclear [Cu–Gd]₂ complex is a genuine double-stranded helicate with active Cu–Gd ferromagnetic interactions, while the equivalent [Cu–Tb]₂ helicate behaves as a single molecule magnet (SMM).



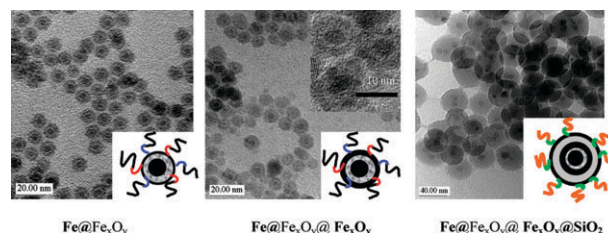
PAPERS

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Surface protected and modified iron based core-shell nanoparticles for biological applications

Kanchana Somaskandan, Teodor Veres, Mereck Niewczas and Benoit Simard*

Excellent quality superparamagnetic Fe_xO_y@Fe nanoparticles were prepared and intentionally coated with different shell materials to give long term protection. Surface modifications of these particles showed excellent stability and solubility in water and different buffer solutions which reveals the suitability of these nanoparticles for biomedical research.

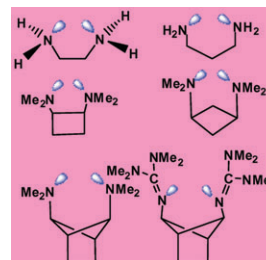


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Strategic design of small and versatile bicyclic organic superbases: a density functional study

Ajeet Singh and Bishwajit Ganguly*

With reliable DFT calculations, we have predicted organic superbases with a bicyclo framework, which are versatile in anchoring different functional groups.

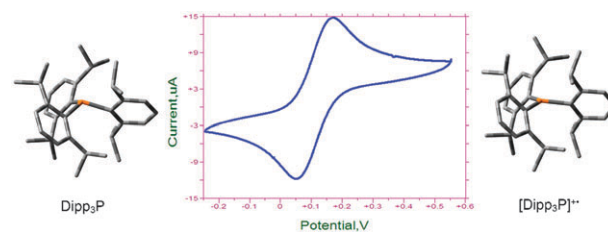


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Photophysical, dynamic and redox behavior of tris(2,6-diisopropylphenyl)phosphine

René T. Boéré,* Alan M. Bond,* Steve Cronin, Noel W. Duffy, Paul Hazendonk, Jason D. Masuda, Kyle Pollard, Tracey L. Roemmele, Peter Tran and Yuankui Zhang

Three bulky 2,6-diisopropylphenyl groups substituted on phosphorus flatten the geometry ($\angle \text{C-P-C}$ open up to $111.88(5)^\circ$); the radical cation is stable indefinitely in a dry, de-oxygenated environment.



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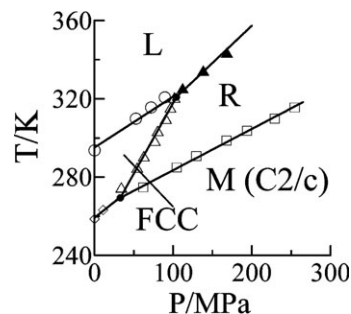


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Polymorphism of CBr_2Cl_2

Maria Barrio, Josep Ll. Tamarit,* Philippe Negrier, Luis C. Pardo, Nestor Veglio and Denise Mondieig

New rhombohedral high-pressure phase for CBr_2Cl_2 .

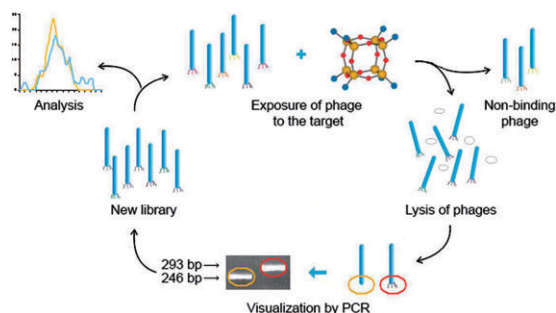


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The use of silsesquioxane cages and phage display technology to probe silicone–protein interactions

Alan R. Bassindale,* Antonio Codina-Barrios, Nunzianda Frascione and Peter G. Taylor*

Phage display technology was used to present a combinatorial library of peptides to series of substituted cage silsesquioxanes that acted as models for investigating peptide binding to silicone surfaces.

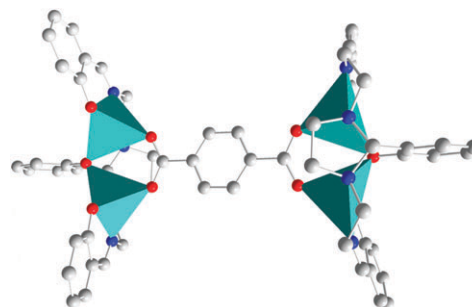


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From dinuclear to tetranuclear zinc complexes through carboxylate donors: structural and luminescence studies

Matilde Fondo,* Ana M. García-Deibe, Noelia Ocampo, Jesús Sanmartín, Manuel R. Bermejo, Elisabete Oliveira and Carlos Lodeiro

Dinuclear and tetranuclear zinc complexes, showing solid state fluorescence, are constructed by means of dinuclear $[\text{Zn}_2\text{L}]^+$ tectons and carboxylate donors.

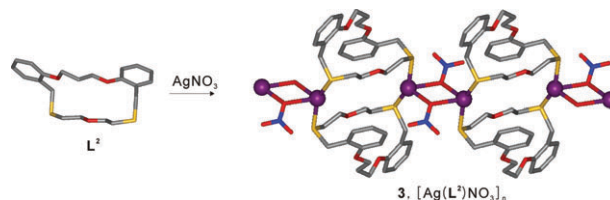


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Exo-coordinated discrete and continuous supramolecular silver(I) complexes with thioxa-macrocycles

Hyun Jee Kim, Il Yoon, So Young Lee, Kyu Seong Choi and Shim Sung Lee*

Reactions of L^1 and L^2 with silver(I) salts afforded the respective ligand- and/or anion-directed complexes **1–3** with different topologies; tetranuclear sandwich **1**, cyclic tetramer **2** and poly(bicyclic dimer) **3**.



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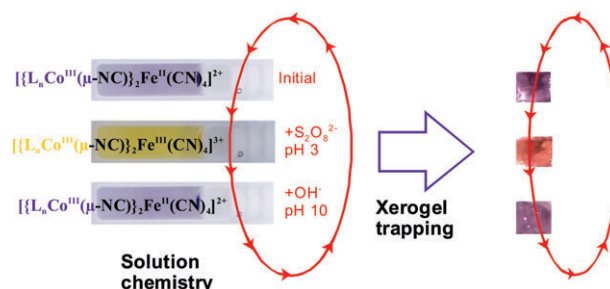
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Sol-gel materials with trapped trinuclear class-II mixed-valence macrocyclic complexes that mimic their solution redox behaviour

Manuel G. Basallote,* Fernando Bozoglian,
María J. Fernández-Trujillo and Manuel Martínez*

Trapping of di- and trinuclear mixed-valence $\text{Co}^{\text{III}}/\text{Fe}^{\text{II}}$ complexes in xerogel matrices produces a parallel redox cyclic chemistry as that observed in solution.



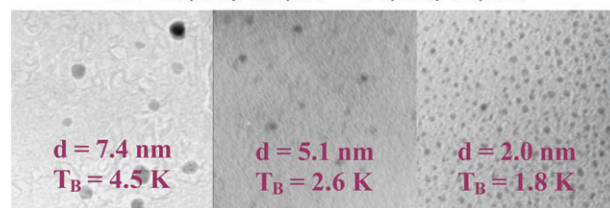
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Synthesis and behaviour of size controlled cyano-bridged coordination polymer nanoparticles within hybrid mesoporous silica

Benjamin Folch, Yannick Guari,* Joulia Larionova,*
Carlos Luna, Claudio Sangregorio,* Claudia Innocenti,
Andrea Caneschi and Christian Guérin

Size controlled cyano-bridged coordination polymer nanoparticles $\text{M}^{n+}/[\text{M}'(\text{CN})_m]^{3-}$ were synthesised into mesostructured hybrid silica hosts and their size-dependent magnetic properties were studied by using dynamic analysis.

$\text{M}^{n+}/[\text{M}'(\text{CN})_m]^{3-}$ nanoparticles $\text{M} = \text{Ni, Fe, Co}; \text{M}' = \text{Fe, Co, Cr, Mo}$

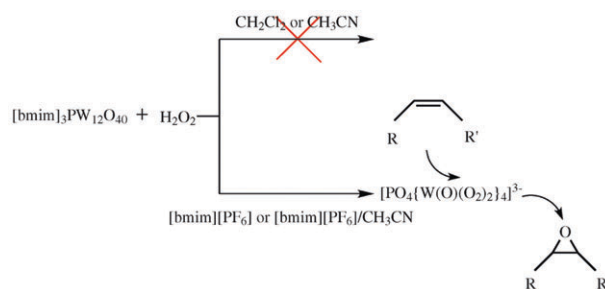


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A role of ionic liquid as an activator for efficient olefin epoxidation catalyzed by polyoxometalate

Lili Liu, Chuncheng Chen, Xuefeng Hu, Tariq Mohamood,
Wanhong Ma, Jun Lin and Jincui Zhao*

Ionic liquid (IL), such as 1-butyl-3-methylimidazolium hexafluorophosphate ($[\text{bmim}][\text{PF}_6]$), was used as an activator for the epoxidation of a wide variety of olefins with H_2O_2 catalyzed by Keggin polyoxometalate $[\text{bmim}]_3\text{PW}_{12}\text{O}_{40}$.

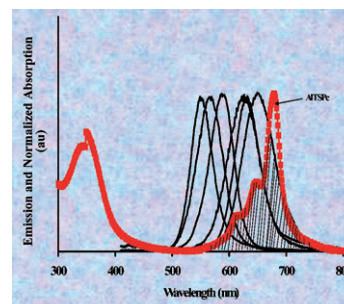


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Photoinduced energy transfer between water-soluble CdTe quantum dots and aluminium tetrasulfonated phthalocyanine

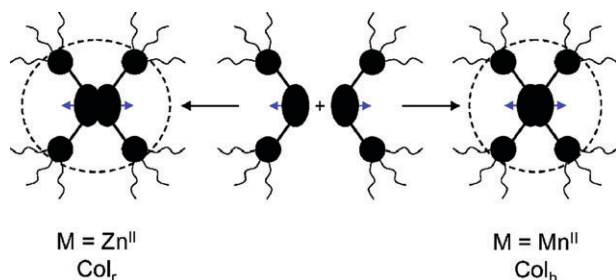
Mopelola Idowu, Ji -Yao Chen and Tebello Nyokong*

Thiol capped CdTe nanoparticles synthesized in aqueous solution have been used as energy donors to water-soluble aluminum tetrasulfonated phthalocyanine (AITSPc), due to the strong overlap between emission of the quantum dots and the absorption spectra of AITSPc.



PAPERS

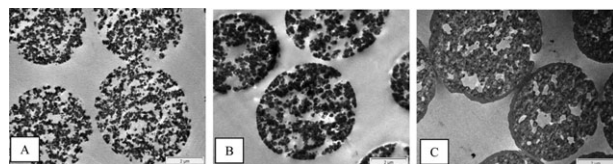
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**Metal-directed columnar phase formation in tetrahedral zinc(II) and manganese(II) metallomesogens**

Francesca Morale, Rachel L. Finn, Simon R. Collinson, Alexander J. Blake, Claire Wilson, Duncan W. Bruce,* Daniel Guillon, Bertrand Donnio* and Martin Schröder*

The complexes $[\text{MCl}_2(\text{L})]$ $\{\text{M} = \text{Mn}, \text{Zn}; \text{L} = 2,6\text{-diformyl-4-methylphenolbis}[3',4',5'\text{-tris(hexadecyloxy)phenylimine}]\}$ exhibit columnar mesophases of rectangular (for Zn) and hexagonal (for Mn) symmetries.

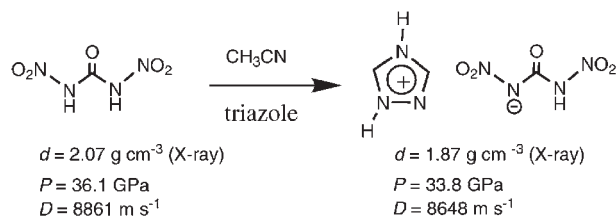
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**Redox graft polymerization of vinylic monomers on ozone-activated poly(styrene-divinylbenzene) microspheres of narrow size distribution**

Eran Partouche and Shlomo Margel*

Cross-section TEM images of porous oxidized P(S-DVB) microspheres before (A) and after graft polymerization of AN (B) and CMS (C) demonstrating the polymerization of these monomers within and on the surface of the core particles.

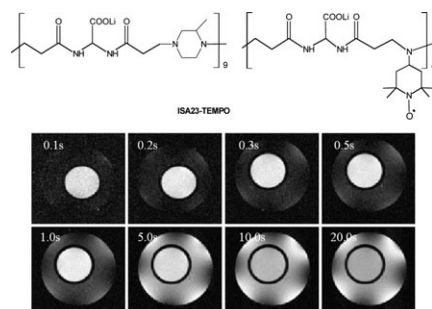
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**Dense energetic salts of *N,N'*-dinitrourea (DNU)**

Chengfeng Ye, Haixiang Gao, Brendan Twamley and Jean'ne M. Shreeve*

Eleven mono-organic salts of DNU were prepared in acetonitrile and characterized *via* NMR spectra, elemental analyses and DSC. Derivatives of 1,2,4-triazolium salts of DNU exhibit densities ranging from 1.75 to 1.86 g cm^{-3} and detonation properties comparable with those of RDX and HMX.

323

**Poly(amidoamine)s carrying TEMPO residues for NMR imaging applications**

Maristella Gussoni,* Fulvia Greco, Paolo Ferruti, Elisabetta Ranucci, Alessandro Ponti and Lucia Zetta*

Relaxivity measurements and preliminary MRI determinations indicate that amphoteric bio-compatible and stealth-like PAA-TEMPO adducts have a definite potential as MRI contrast agents.

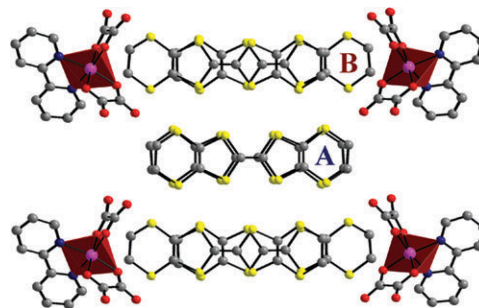
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Conducting mixed-valence salt of bis(ethylenedithio)tetrathiafulvalene (BEDT-TTF) with the paramagnetic heteroleptic anion $[\text{Cr}^{\text{III}}(\text{oxalate})_2(2,2'\text{-bipyridine})]^-$

Augustin M. Madalan, Enric Canadell, Pascale Auban-Senzier, Diana Brânzea, Narcis Avarvari* and Marius Andruh*

The new molecular crystalline paramagnetic semiconductor α' -(BEDT-TTF) $_2[\text{Cr}(\text{C}_2\text{O}_4)_2(2,2'\text{-bipy})] \cdot \text{CHCl}_2\text{CH}_2\text{Cl}$ shows a peculiar α' packing of the donor molecules.

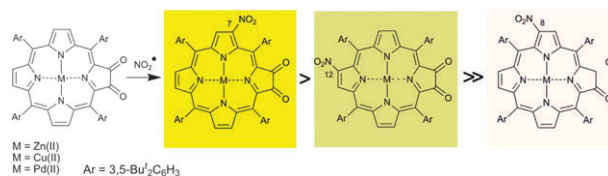


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Construction of building blocks for extended porphyrin arrays by nitration of porphyrin-2,3-diones and quinoxalino[2,3-*b*]porphyrins

Maxwell J. Crossley,* Craig S. Sheehan, Tony Khoury, Jeffery R. Reimers and Paul J. Santic

Nitration of porphyrin-2,3-diones and quinoxalino[2,3-*b*]porphyrins gave a mixture of β -pyrrolic functionalised nitroporphyrin isomers in relative abundance of 7-nitro- > 12-nitro- $\gg$ 8-nitro. The nitro compounds are useful building blocks for the synthesis of extended porphyrin arrays.

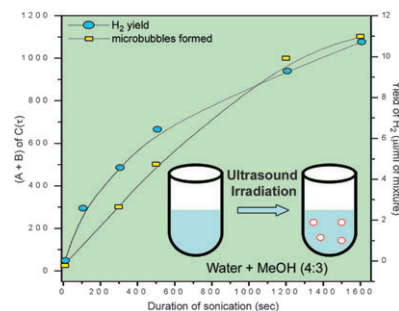


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Synergistic enhancement of microbubble formation in ultrasound irradiated H_2O – CH_3OH mixtures probed by dynamic light scattering

Mrinal R. Pai, Puthusserickal A. Hassan, Shyamala R. Bharadwaj* and Shailendra K. Kulshreshtha

Formation of microbubbles in water–methanol mixtures upon ultrasound irradiation and its correlation with the yield of H_2 obtained as a result of sonochemical splitting of water.

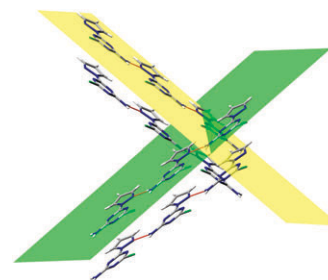


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An experimental and theoretical investigation of the molecular and electronic structure of 2-amino-4-chloro-6-pyrazolyl-[1,3,5]triazine, forming supramolecular linear tapes in the solid state

Maurizio Casarin, Federica Garau, Magda Monari,* Luciano Pandolfo,* Claudio Pettinari* and Alfonso Venzo

The molecular structure of 2-amino-4-chloro-6-pyrazolyl-[1,3,5]triazine and its H-bonded supramolecular self-assembly, generating intersecting linear tapes, is examined by combining both experimental and theoretical approaches.



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