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## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(12) 2053-2304 (2008)



### Cover

See Bertrand Siboulet *et al.*, pp. 2080–2094.  
Surprising geometries are proposed here for the aqueous species of protactinium, based on quantum mechanics. Picture by Alastair Magnaldo (almagnus.com) reproduced by permission of Bertrand Siboulet, Colin J. Marsden and Pierre Vitorge from *New J. Chem.*, 2008, **32**, 2080.



### Inside Cover

See Takuji Ikeda *et al.*, pp. 2108–2115.  
The pseudo-micropore structure in a low dimensional caesium silicate LDS-1 is composed of strong hydrogen bonding between adjacent terminal silanols, which was elucidated by the MEM electron density analysis. Image reproduced by permission of Takuji Ikeda, Toshikazu Nishide, Hiroko Nakajima, Akiko Kawai, Yoshimichi Kiyozumi, Tetsuya Kodaira and Fujio Mizukami from *New J. Chem.*, 2008, **32**, 2108.

## CHEMICAL SCIENCE

### C89

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

## Chemical Science

December 2008/Volume 5/Issue 12

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## LETTER

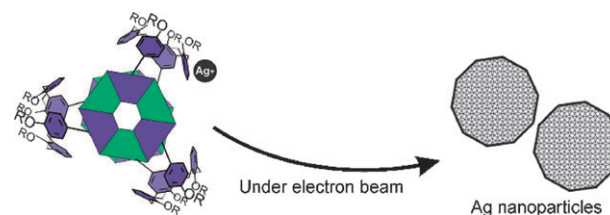


### 2071

#### Silver nanoparticles from hydrogen-bonded supramolecular scaffolds

Sachin Kinge,\* Mercedes Crego-Calama\* and David Reinhoudt

Silver nanoparticles were generated *in situ* under a TEM electron beam from hydrogen-bonded double rosette-silver complexes.



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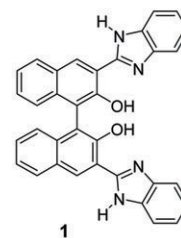
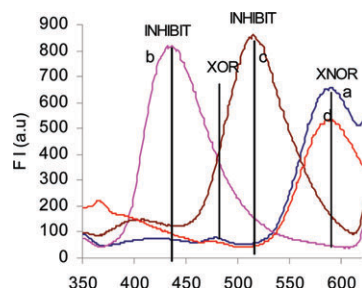
## PAPERS

2074

**Molecular half-subtractor based on 3,3'-bis(1*H*-benzimidazolyl-2-yl)[1,1']binaphthalenyl-2,2'-diol**

Vijay Luxami and Subodh Kumar\*

The emission maxima at different wavelengths arising from interactions of fluorophore **1** with HClO<sub>4</sub> and TBAOH have been elaborated as XNOR, XOR, INHIBIT logic gates and their combinatorial molecular half-subtractor with both positive and negative logic functions.

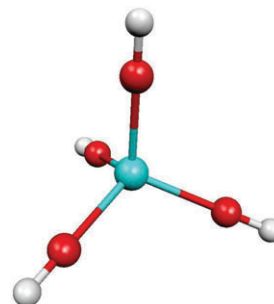


2080

**What can quantum chemistry tell us about Pa(v) hydration and hydrolysis?**

Bertrand Siboulet, Colin J. Marsden and Pierre Vitorge

“On hydration, PaO<sub>2</sub><sup>+</sup> can rearrange to give tetrahedral Pa(OH)<sub>4</sub><sup>+</sup>, a species that has not previously been considered and that could very well be one of the major Pa(v) aqueous cations in acidic conditions.”

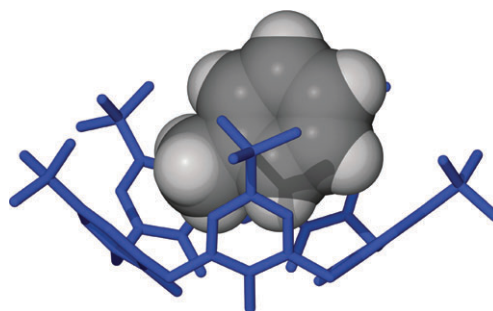


2095

**Pseudo-polymorphism in the toluene solvate of *p*-tert-butylcalix[5]arene: structural and gas sorption investigation**

Scott J. Dalgarno, Praveen K. Thallapally, Jian Tian and Jerry L. Atwood\*

Pseudo-polymorphs of the toluene solvate of *p*-tert-butylcalix[5]arene have been characterised and have been examined for ‘frustration’ in the organic solid to afford porous materials that can be used for the sorption of various gases.

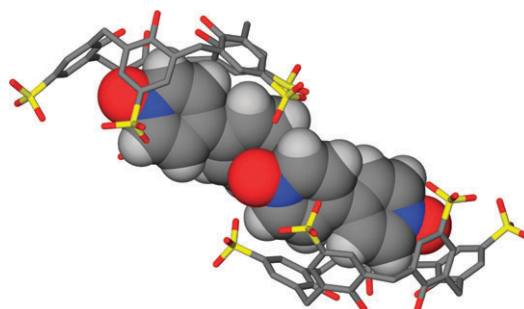


2100

**Versatility of *p*-sulfonatocalix[5]arene in building up multicomponent bilayers**

Scott J. Dalgarno, John E. Warren, Jerry L. Atwood and Colin L. Raston\*

The formation of pyridine *N*-oxide host–guest complexes with lanthanide *p*-sulfonatocalix[5]arene assemblies was probed with larger potential guest species. Three new supramolecular motifs incorporating 2- or 4-picoline *N*-oxide and 4,4'-dipyridine *N,N'*-dioxide are described with a critical analysis of *p*-sulfonatocalix[5]arene packing in bilayer arrays.





# 42nd IUPAC CONGRESS Chemistry Solutions

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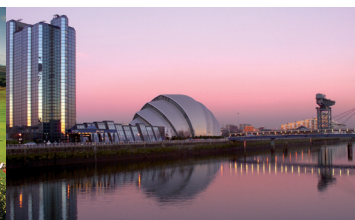
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- Analysis & Detection
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- Energy & Environment
- Industry & Innovation
- Materials
- Synthesis & Mechanisms

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 Ben L Feringa, University of Groningen  
 Sir Harold Kroto, Florida State University  
 Klaus Müllen, Max-Planck Institute for Polymer Research  
 Sir J Fraser Stoddart, Northwestern University  
 Vivian W W Yam, The University of Hong Kong  
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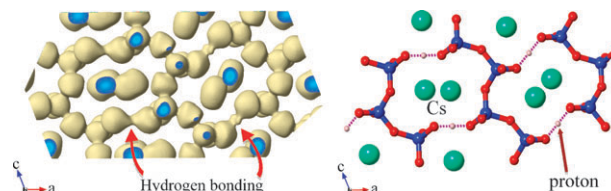


2108

### Pseudo-micropores formed by one-dimensional framework with hydrogen bonding in $\text{CsHSi}_2\text{O}_5$ observed by synchrotron powder diffraction and solid-state MAS NMR

Takuji Ikeda,\* Toshikazu Nishide, Hiroko Nakajima, Akiko Kawai, Yoshimichi Kiyozumi, Tetsuya Kodaira and Fujio Mizukami

A caesium silicate LDS-1 with strong hydrogen bonds between adjacent terminal silanols (right). The hydrogen bonds are clearly observed in the MEM electron density image (left).

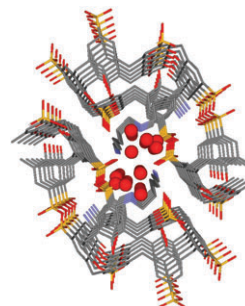


2116

### Stepped layers in the complexes of *para*-sulfonatocalix[6]arene with dimethylammonium and bis-6-aminoethylammonium cations

Adina N. Lazar, Oksana Danylyuk, Kinga Suwinska, Rima Kassab and Anthony W. Coleman\*

The structures of two complexes of *para*-sulfonatocalix[6]arene with the dimethylammonium and bis-6-aminoethylammonium organic cations, show chair conformations for the calixarene anions, in both structures channels are formed filled with solvent molecules.

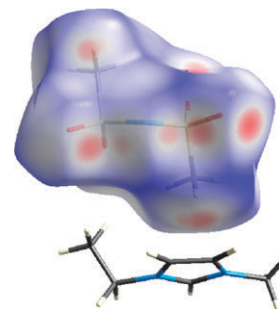


2121

### Interactions in bisamide ionic liquids—insights from a Hirshfeld surface analysis of their crystalline states

Pamela M. Dean,\* Jennifer M. Pringle, Craig M. Forsyth, Janet L. Scott and Douglas R. MacFarlane

The intermolecular interactions of a series of crystallised bisamide ionic liquids are qualitatively investigated and compared using Hirshfeld surfaces, demonstrating the applicability of this approach in elucidating the molecular origins of the physical properties.

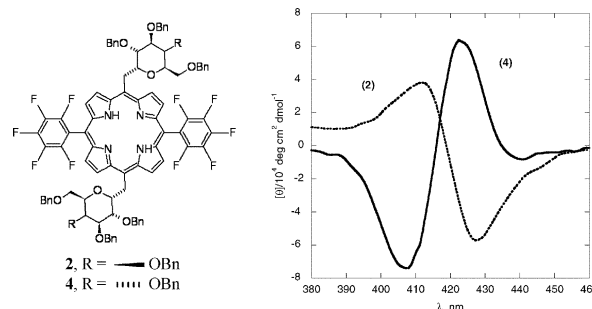


2127

### Study of the supramolecular chiral assembly of *meso*-“C-glucoside”-porphyrin derivatives in aqueous media

Donato Monti,\* Mariano Venanzi, Emanuela Gatto, Giovanna Mancini, Alessandro Sorrenti, Petr Štěpánek and Pavel Drašar\*

The solvent driven self-aggregation studies of several *meso*-“C-glycoside”-porphyrin derivatives have been carried out, showing the effect of bulk solvent properties, and of the structure of the molecular framework, on the supramolecular chirality of the mesoscopic final architectures.



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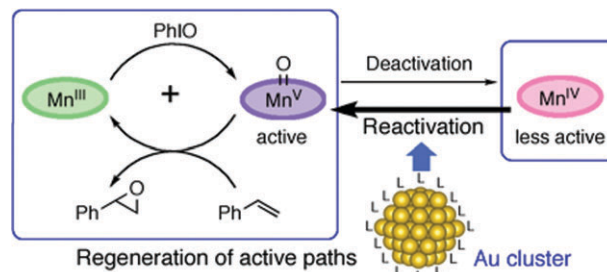
## PAPERS

2134

**Mechanistic insights into the co-catalyst effect of Au clusters in Mn-porphyrin-catalyzed olefin oxidation**

Yoshitaka Murakami and Katsuaki Konishi\*

Promoting effects of thiolate-, phosphine- and polymer-protected Au clusters on styrene oxidation with iodosylbenzene (PhIO) catalyzed by Mn porphyrins were investigated from several aspects, and mechanistic discussions associated with the nature of the unique positive effect of Au clusters are provided.

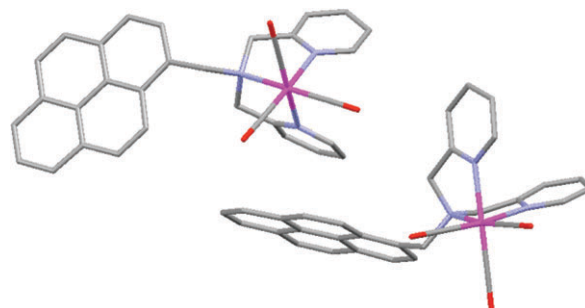


2140

**Rhenium complexes of chromophore-appended dipicolylamine ligands: syntheses, spectroscopic properties, DNA binding and X-ray crystal structure**

Lucy A. Mullice, Rebecca H. Laye, Lindsay P. Harding, Nikolaas J. Buurma\* and Simon J. A. Pope\*

Cationic  $\text{Re}^{\text{I}}$  complexes of chromophore-appended dipicolylamine ligands possess intra-ligand emission. The pyrene-functionalised complex binds to DNA ( $K = 1.5 \times 10^5 \text{ M}^{-1}$ ,  $\Delta H = -14 \text{ kcal mol}^{-1}$ ).

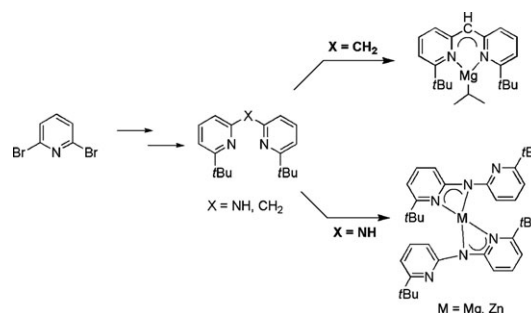


2150

**Synthesis of new dipyridinylamine and dipyridinylmethane ligands and their coordination chemistry with  $\text{Mg}(\text{II})$  and  $\text{Zn}(\text{II})$** 

Zhanjiang Zheng, Mohammed Kamal Elmkaddem, Cédric Fischmeister, Thierry Roisnel, Christophe M. Thomas,\* Jean-François Carpentier\* and Jean-Luc Renaud\*

A short, simple, and flexible access to functionalized bispyridylamines 2,2'-*tert*-butyldipyridylamine and 2,2'-*tert*-butyldipyridylmethane *via* a Cu and Pd catalysis is described.

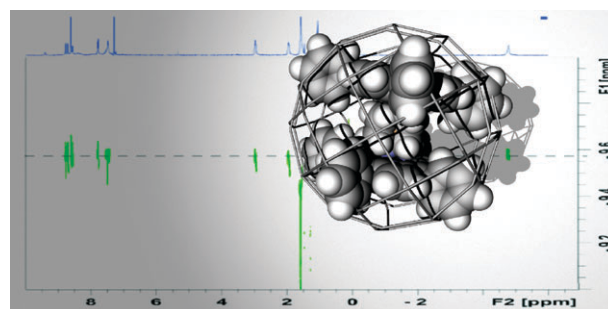


2159

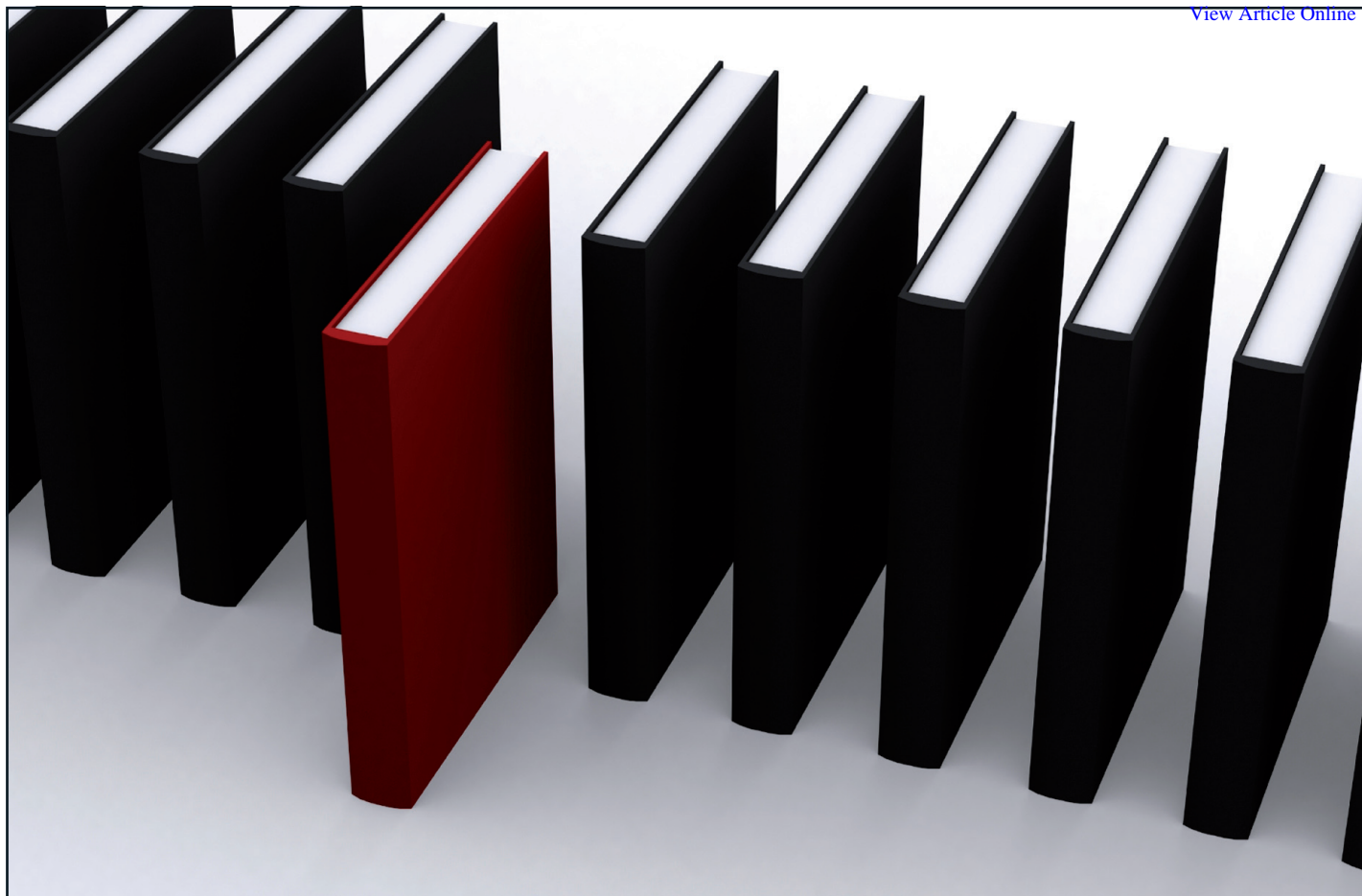
**Diffusion-ordered spectroscopy ( $^1\text{H}$ -DOSY) of Zn-porphyrin assemblies induced by coordination with DABCO**

Ana I. Oliva, Kerman Gómez, Gabriel González and Pablo Ballester\*

$^1\text{H}$ -DOSY experiments carried out on multicomponent architectures induced by DABCO coordination with Zn-porphyrins are used to confirm their stoichiometries and sandwich-like structure.







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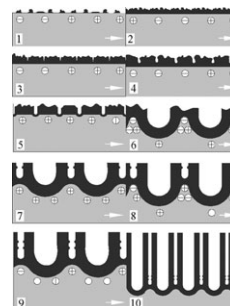
## PAPERS

2164

**Mechanism study of self-organized TiO<sub>2</sub> nanotube arrays by anodization**

Jinliang Tao, Jianling Zhao, Chengcun Tang, Yingru Kang and Yangxian Li\*

A new growth, dissolution-breakdown model, of self-organized titania nanotube arrays is presented.

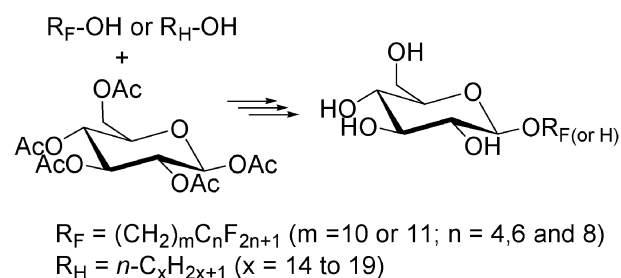


2169

**Synthesis and biocompatibility evaluation of fluorinated, single-tailed glucopyranoside surfactants**

Xueshu Li, Jaroslav Turánek,\* Pavlína Knötigová, Hana Kudláčková, Josef Mašek, D. Brant Pennington, Stephen E. Rankin, Barbara L. Knutson and Hans-Joachim Lehmler\*

The synthesis and biocompatibility assessment of partially fluorinated glucopyranoside surfactants is described.

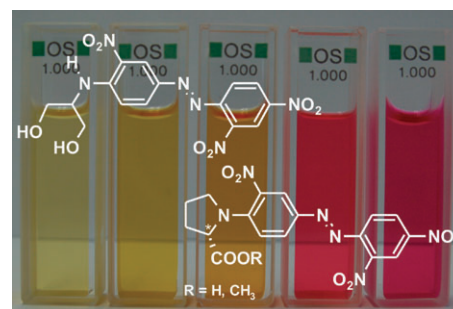


2180

**Solvatochromism and linear solvation energy relationship of diol- and proline-functionalized azo dyes using the Kamlet–Taft and Catalán solvent parameter sets**

Katja Hofmann, Katja Schreiter, Andreas Seifert, Tobias Rüffer, Heinrich Lang and Stefan Spange\*

Herein, the synthesis, crystal structure and solvatochromic behavior of the novel donor–acceptor-substituted azo dyes are reported. The solvatochromic studies were comparatively investigated by means of the well established Kamlet–Taft and Catalán solvent parameter sets.

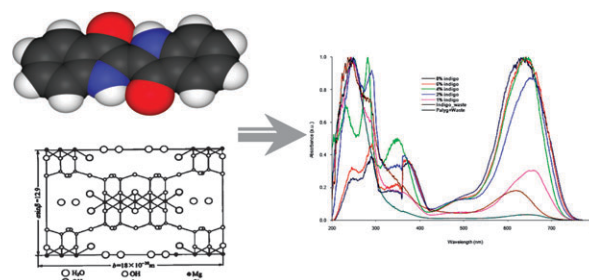


2189

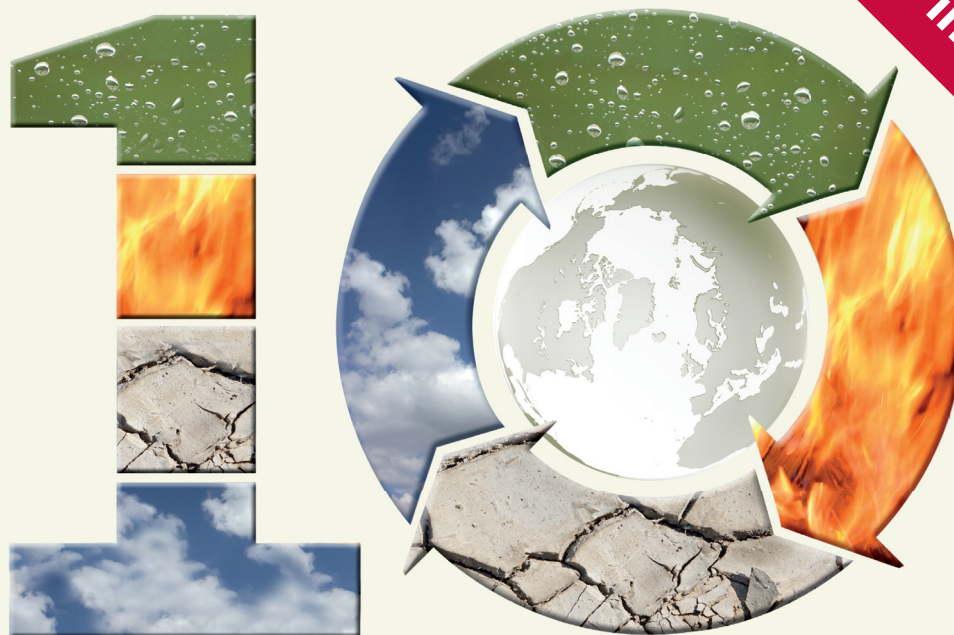
**Indigo dye waste recovery from blue denim textile effluent: a by-product synergy approach**

Dennis Wambuguh\* and Russell R. Chianelli

The recovery process uses palygorskite clay and converts the by-products to Maya blue pigment. Because indigo is expensive and recalcitrant to biological degradation, the process has significant potential economic and ecological implications.



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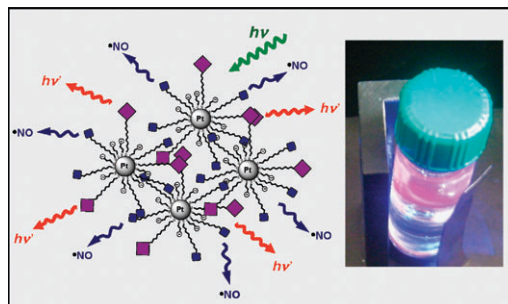
## PAPERS

2195

**Bifunctional nanoparticle assemblies: photoluminescent and nitric oxide photodelivering monolayer protected platinum clusters**

Mariarita Barone, Angela Mascali and Salvatore Sortino\*

Nanoassemblies of bichromophoric platinum nanoparticles combine light-regulated NO release and satisfactory red-fluorescence yield, representing appealing bright point sources of NO to be tested in the emerging field of nanomedical research.

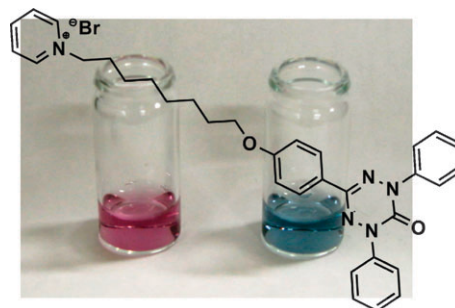


2201

**Association-mediated chromism of amphiphilic triphenyl-6-oxoverdazyl**

Kentarō Suzuki, Michio M. Matsushita, Hiroyuki Hayashi, Noboru Koga and Tadashi Sugawara\*

The color of aqueous solutions of a novel amphiphilic verdazyl radical, PyC8TOV, was found to change from red to blue in less polar environment, being associated with the aggregation of the amphiphilic radicals.

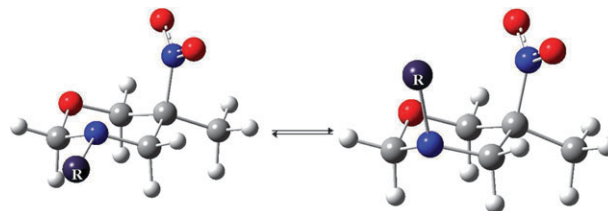


2209

**Conformational analysis, NMR properties and nitrogen inversion of N-substituted 1,3-oxazines**

Marcela Hurtado, J. Guillermo Contreras,\* Adelio Matamala, Otilia Mó and Manuel Yáñez\*

The conformational preference, axial or equatorial, of N-substituted oxazines depends on the nature of the substituent as well as on the polarity of the media. Nitrogen inversion barriers decrease with the size of the substituent.

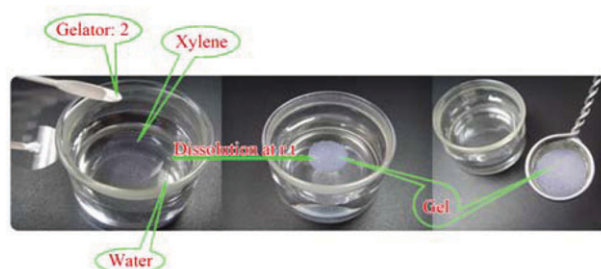


2218

**New dicholesteryl-based gelators: gelling ability and selective gelation of organic solvents from their mixtures with water at room temperature**

Junxia Peng, Kaiqiang Liu, Xufei Liu, Huiyun Xia, Jing Liu and Yu Fang\*

Four new diacid amides of dicholesteryl L-phenylalaninate have been designed and prepared. Gelation tests showed that the four compounds are versatile organogelators, and a subtle change in the length of the spacer can produce a dramatic change in the gelation behaviors.





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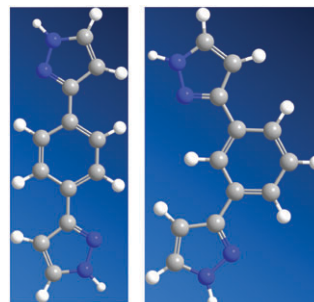
## PAPERS

2225

**A theoretical and experimental NMR study of the tautomerism of two phenylene-bis-*C*-substituted pyrazoles**

Dionisia Sanz,\* Rosa M. Claramunt, Ibon Alkorta, José Elguero, Werner R. Thiel and Tobias Rüffer

The tautomerism of *meta* and *para* bis-pyrazolylbenzenes has been determined in DMSO solution. In the solid state the *meta* is a 3,3- while the *para* is a 3,5 tautomer. This last tautomer exists in a dynamic equilibrium with the 5,3 one (proton transfer in the solid state, SSPT).

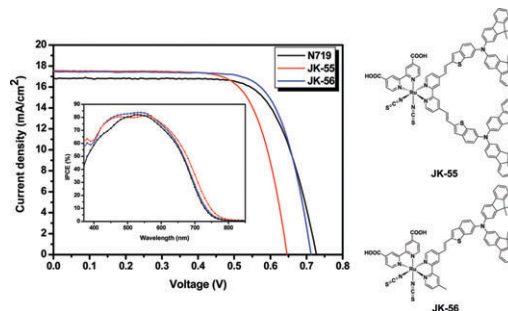


2233

**Molecular engineering of hybrid sensitizers incorporating an organic antenna into ruthenium complex and their application in solar cells**

Hyunbong Choi, Chul Baik, Sanghoon Kim, Moon-Sung Kang, Xiang Xu, Hong Seok Kang, Sang Ook Kang, Jaejung Ko,\* Md. K. Nazeeruddin\* and Michael Grätzel

Two new hybridized sensitizers incorporating the polypyridyl group and organic dye unit are synthesized and applied successfully to solar cells under AM 1.5 solar light, giving solar to electricity conversion efficiencies of 8.20–9.16%.

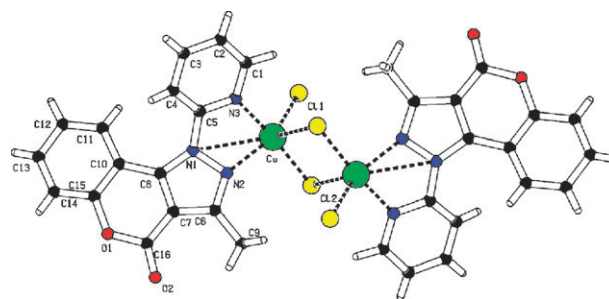


2238

**Synthesis, crystal structure, theoretical calculation and cytotoxic effect of new Pt(II), Pd(II) and Cu(II) complexes with pyridine-pyrazoles derivatives**

Elzbieta Budzisz,\* Ingo-Peter Lorenz, Peter Mayer, Piotr Paneth, Lukasz Szatkowski, Urszula Krajewska, Marek Rozalski and Magdalena Miernicka

A simple and convenient route for synthesis of neutral *cis*-oriented Pt, Pd and Cu-complexes  $MLCl_2$  is given. Pt complex **2** exhibits activity against the WM-115 melanoma cell line comparable to that of cisplatin.

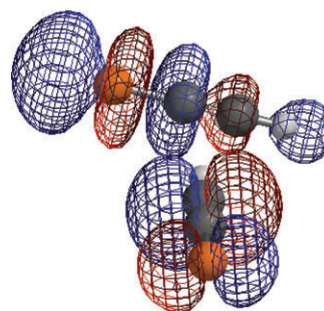


2245

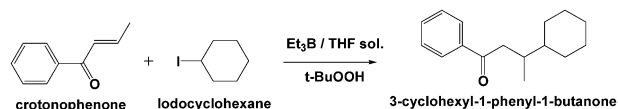
**Molecular mechanisms in the pyrolysis of unsaturated chlorinated hydrocarbons**

Grant J. McIntosh\* and Douglas K. Russell

Frontier orbitals in chlorinated acetylenes are ideally oriented for low activation energy reaction leading to adduct formation.



2257



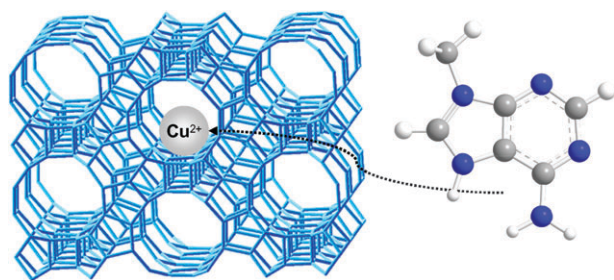
### Microwave-enhanced radical reactions at ambient temperature

#### Part 3: Highly selective radical synthesis of 3-cyclohexyl-1-phenyl-1-butanone in a microwave double cylindrical cooled reactor

Satoshi Horikoshi,\* Junichi Tsuzuki, Masatsugu Kajitani, Masahiko Abe and Nick Serpone\*

The near-quantitative synthesis of 3-cyclohexyl-1-phenyl-1-butanone is enhanced under microwave irradiation with cooling to ambient temperature with the involvement of specific non-thermal microwave effects.

2263

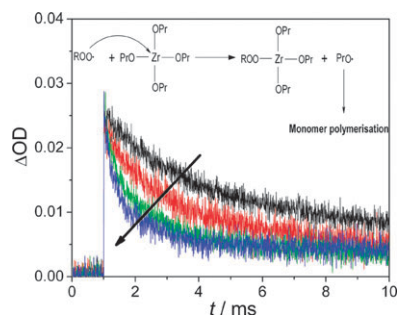


### Host(beta zeolite)-guest (copper(II)-methyladenine complex) nanomaterials: synthesis and characterization

Catarina Teixeira, Paolo Pescarmona, M. Alice Carvalho, António M. Fonseca\* and Isabel C. Neves\*

A host-guest nanomaterial was obtained by a process of sequential introduction of 9-methyladenine ligand and copper(II) in the liquid phase followed by assembly inside the void space of the zeolite.

2270

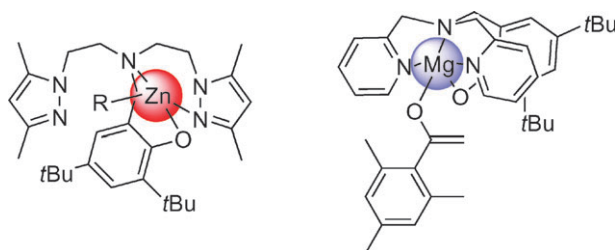


### Influence of zirconium propoxide on the radical induced photopolymerisation of hybrid sol-gel materials

Davy-Louis Versace, Olivier Soppera, Jacques Lalevée and Céline Croutxé-Barghorn\*

Peroxy radicals ( $\text{ROO}^\bullet$ ) generated upon radical induced photopolymerisation can react with  $\text{Zr}(\text{OPr})_4$  and lead to generation of  $\text{PrO}^\bullet$  that act as further initiating species. Kinetics decays of reaction of an observable peroxy radical formed from an aminoalkyl radical were observed by Laser Flash Photolysis when increasing the amount of  $\text{Zr}(\text{OPr})_4$  complex.

2279



### Zinc and enolato-magnesium complexes based on bi-, tri- and tetradentate aminophenolate ligands

Zhanjiang Zheng, Gang Zhao, Rémy Fablet, Miloud Bouyahyi, Christophe M. Thomas,\* Thierry Roisnel, Osvaldo Casagrande Jr and Jean-François Carpentier\*

The coordination chemistry of aminophenolate ligands with variable denticity onto  $\text{Zn}(\text{II})$  and  $\text{Mg}(\text{II})$ , as well as the reactivity of the resulting complexes towards polar monomers, have been studied.

## PAPERS

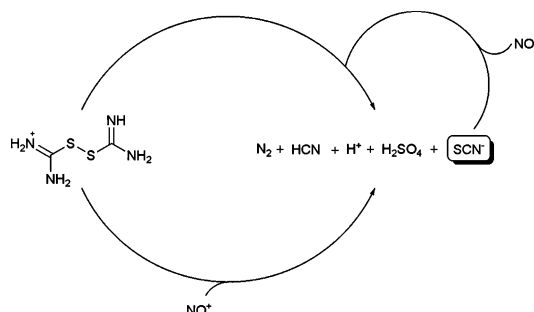


2292

**Kinetic study of an autocatalytic reaction: nitrosation of formamidine disulfide**

Vitor Francisco, Luis Garcia-Rio,\* José António Moreira and Geoffrey Stedman

The reaction kinetics for the acid nitrosation of formamidine disulfide (FDS) show an autocatalytic behavior that arises from the fact that the thiocyanate ion formed as a product acts as a powerful catalyst for the nitrosation reaction.



## ADDITIONS AND CORRECTIONS

2299

**Additions and corrections published in 2008**

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