

## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(3) 369–556 (2008)



### Cover

See Pischel *et al.*, pp. 395–400. Space filling model of a molecule, whose fluorescence depends on input information. The logic behaviour is compatible with a half-subtractor, represented in the right corner. The background shows a drawing of the calculating clock (1623) by Wilhelm Schickard. Image reproduced with permission from Uwe Pischel and Barbara Heller from *New J. Chem.*, 2008, **32**, 395.



### Inside Cover

See Ceroni *et al.*, pp. 401–406. Acid/base controlled encapsulation of a fluorescent guest into a photoactive dendritic box. Cover artwork by Dr Fausto Puntoriero. Reproduced with permission from Fausto Puntoriero, Giacomo Bergamini, Paola Ceroni, Vincenzo Balzani and Fritz Vögtle from *New J. Chem.*, 2008, **32**, 401.

## CHEMICAL SCIENCE

### C17

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 and significant scientific advances.

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March 2008/Volume 5/Issue 3

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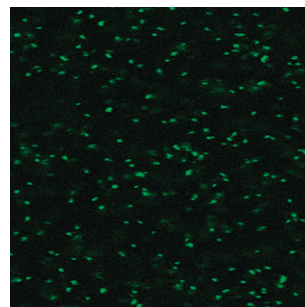
## LETTERS

### 383

#### Efficient strategy to increase the surface functionalization of core-shell superparamagnetic nanoparticles using dendron grafting

Karine Heuzé,\* Daniel Rosario-Amorin, Sylvain Nlate, Manuel Gaboyard, Anthony Bouter and Rodolphe Clérac

Core-shell superparamagnetic nanoparticles functionalized by fluorescent dendrons show an increase in the surface functionalization of such particles compared to their grafting by a linear fluorescent analogue.



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Tel (+44) (0) 191 384 2085  
E-mail [jon.steed@dur.ac.uk](mailto:jon.steed@dur.ac.uk)

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Gainesville  
FL 32611  
USA  
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## LETTERS

388

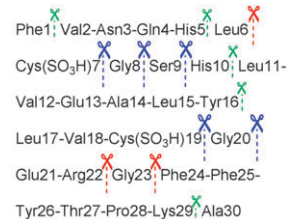
**Hydrolysis of insulin chain B using zirconium(IV) at neutral pH**

Sarah S. Cepeda and Kathryn B. Grant\*

Zr<sup>IV</sup> produces significant levels of amide bond hydrolysis at Gly8-Ser9, Gly20-Glu21, Ser9-His10, Cys(SO<sub>3</sub>H)7-Gly8, and Cys(SO<sub>3</sub>H)19-Gly20 (blue), intermediate levels at Leu6-Cys(SO<sub>3</sub>H)7, Arg22-Gly23, and Gly23-Phe24 (red), and trace levels at sites in green.

Hydrolysis of a 30-mer oligopeptide:

oxidized bovine insulin chain B

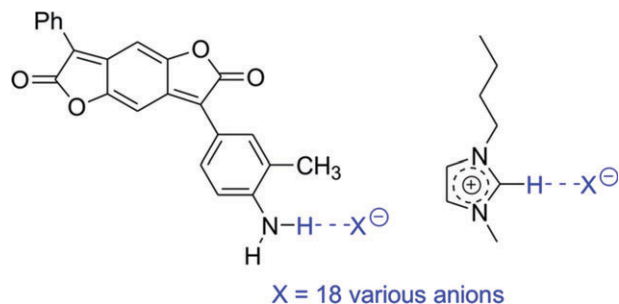


392

**A hydrogen bond accepting (HBA) scale for anions, including room temperature ionic liquids**

Ralf Lungwitz and Stefan Spange\*

A hydrogen bond accepting (HBA) ability scale for anions of room temperature ionic liquids (RTILs) has been determined by means of <sup>1</sup>H NMR spectroscopy and a solvatochromic UV/vis probe.



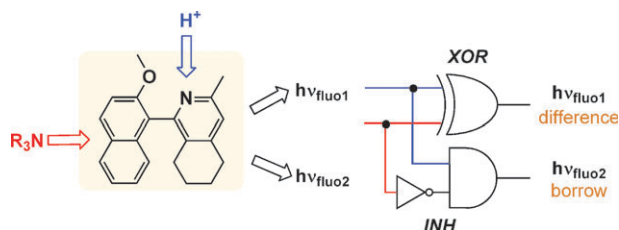
## PAPERS

395

**Molecular logic devices (half-subtractor, comparator, complementary output circuit) by controlling photoinduced charge transfer processes**

Uwe Pischel\* and Barbara Heller

The fluorescence modulation of a naphthalene derivative by several chemical inputs can be used to implement advanced reconfigurable logic circuits in a unimolecular manner.

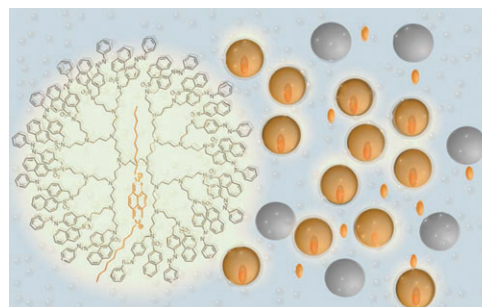


401

**A fluorescent guest encapsulated by a photoreactive azobenzene dendrimer**

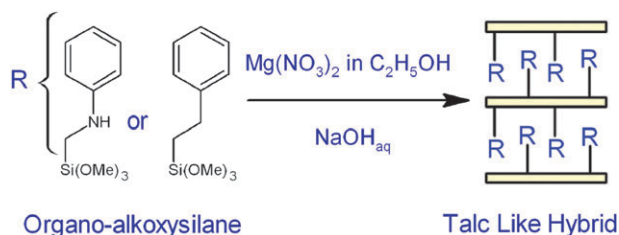
Fausto Puntoriero, Giacomo Bergamini, Paola Ceroni,\* Vincenzo Balzani and Fritz Vögtle\*

A poly(propylene amine) dendrimer functionalized with 16 naphthyl and 16 azobenzene units in the periphery forms a stable adduct with *N,N'*-2,7-didecyldiazapyrenium. The adduct is fluorescent both in fluid solution and in rigid matrix and can be reversibly disassembled upon addition of acid.



## PAPERS

407

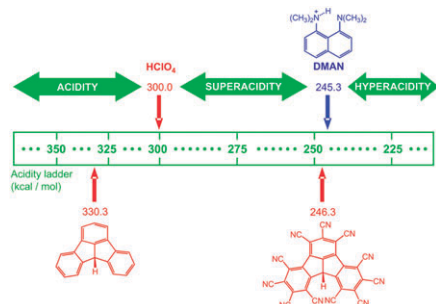


### Synthesis of new lamellar inorganic–organic talc-like hybrids

Jean-Christophe Gallégo, Maguy Jaber,\*  
Jocelyne Miehé-Brendlé and Claire Marichal

One-step synthesis of new phenethyl- and phenylaminomethyl-talc like hybrids as nanocomposite precursors: the mobility of both organic moieties within the layers was probed by solid-state NMR.

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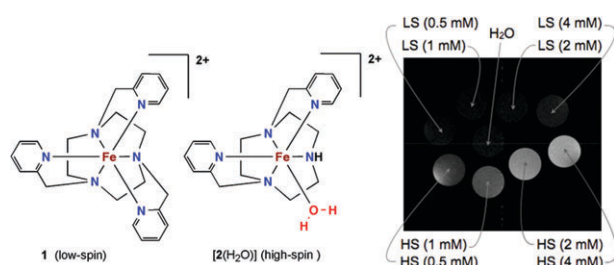


### Rees polycyanated hydrocarbons and related compounds are extremely powerful Brønsted superacids in the gas-phase and DMSO—a density functional B3LYP study

Robert Vianello\* and Zvonimir B. Maksić

The peryano derivative of fluoradene is a hyperstrong neutral organic acid.

428

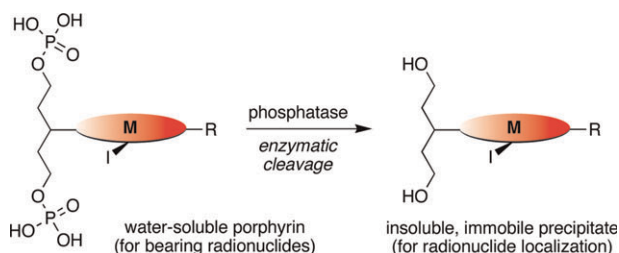


### Significant relaxivity gap between a low-spin and a high-spin iron(II) complex of structural similarity: an attractive off-on system for the potential design of responsive MRI probes

Vitalie Stavila, Mustapha Allali, Laurence Canaple, Yvon Stortz, Cécile Franc, Philippe Maurin, Olivier Beuf, Olivier Dufay, Jacques Samarut, Marc Janier and Jens Hasserodt\*

Compounds **1** and **2** have been characterized in solution to assess their usefulness in the design of a responsive MRI probe.

436



### Soluble precipitable porphyrins for use in targeted molecular brachytherapy

Zhen Yao, K. Eszter Borbas and Jonathan S. Lindsey\*

A porphyrin is designed to undergo a water soluble-to-insoluble conversion upon enzymatic action, a transformation that can form the basis for localization of immobile radionuclides in solid tumors.

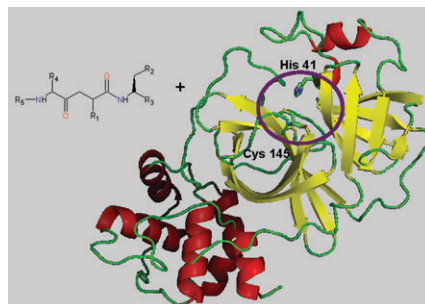
## PAPERS

452

**Molecular design of inhibitors against the M<sup>pro</sup> protein of the severe acute respiratory syndrome (SARS) virus**

Jesús Olivero-Verbel, Isaías Lans, Emiliano Martínez, Isaura Ospino, Angelica Padilla and Ricardo Vivas-Reyes\*

The main proteinase of SARS coronavirus (3CL<sup>pro</sup> or M<sup>pro</sup>) is crucial for its replication process, and therefore it is a potential target for the development of anti-SARS drugs.

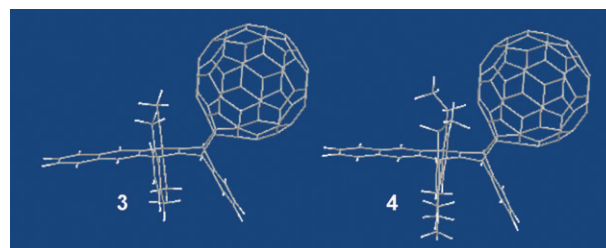


459

**[60]Fullerene cycloaddition across hindered acenes**

Irvinder Kaur and Glen P. Miller\*

[60]Fullerene cycloadds across sterically hindered pentacenes to produce fullerene–acene monoadducts that readily add <sup>1</sup>O<sub>2</sub>.

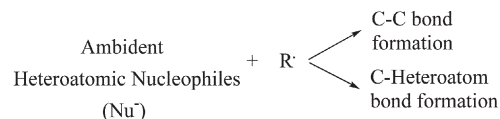


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**Regioselectivity of the coupling between radicals and ambident nucleophiles. A theoretical study**

María T. Baumgartner,\* Guillermo A. Blanco and Adriana B. Pierini

We here report a theoretical study on the reaction of the anions of phenol, 2-naphthol, pyrimidine bases, pyrrole, imidazole and benzimidazole with phenyl and 4-nitrobenzyl radicals with the aim of interpreting the factors that control the regiochemical outcome of these reactions.



Nu<sup>−</sup> = anions of phenol, 2-naphthol, 1-methyl-2-naphthol, cytosine, thymine, uracil, pyrrole, imidazole, benzimidazole.  
R<sup>•</sup> = phenyl, 4-nitrobenzyl.

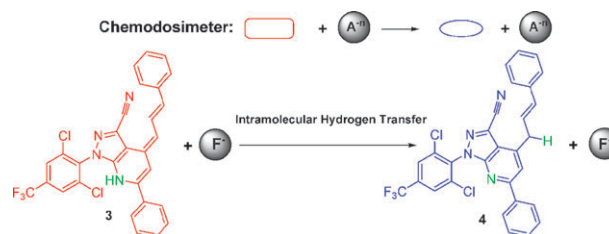


472

**Chromogenic and fluorescent chemodosimeter for fluoride ion based on novel anion-catalyzed intramolecular hydrogen transfer**

Chuanxiang Liu, Xuhong Qian,\* Guangqiang Sun, Liwei Zhao and Zhong Li\*

Novel anion-catalyzed intramolecular hydrogen transfer resulting in dosimetric fluoride ion determination through drastic changes in UV-Vis absorption and a fluorogenic “off-on” response.





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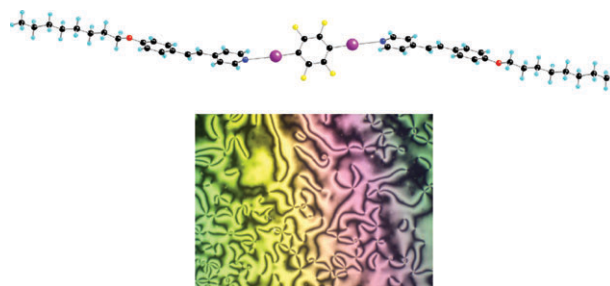
## PAPERS

477

**Mesogenic, trimeric, halogen-bonded complexes from alkoxy stilbazoles and 1,4-diiodotetrafluorobenzene**

Duncan W. Bruce,\* Pierangelo Metrangolo,\*  
 Franck Meyer, Carsten Präsang, Giuseppe Resnati,\*  
 Giancarlo Terraneo and Adrian C. Whitwood

Trimeric, halogen-bonded liquid crystals are obtained from complexation of two stilbazoles to 1,4-diiodotetrafluorobenzene. Individual complexes show monotropic phases while enantiotropic behaviour is seen with mixtures.

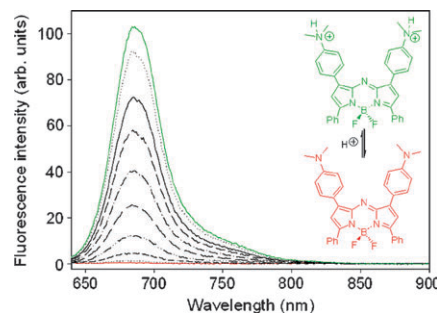


483

**A substituted BF<sub>2</sub>-chelated tetraarylazadipyrromethene as an intrinsic dual chemosensor in the 650–850 nm spectral range**

John Killoran, Shane O. McDonnell, John F. Gallagher  
 and Donal F. O'Shea\*

The synthesis and spectral analysis of a new class of long wavelength intrinsic fluorosensor is reported. Chemosensor performance reveals large off/on fluorescence intensity responses to acid analyte with low response to microenvironment polarity.

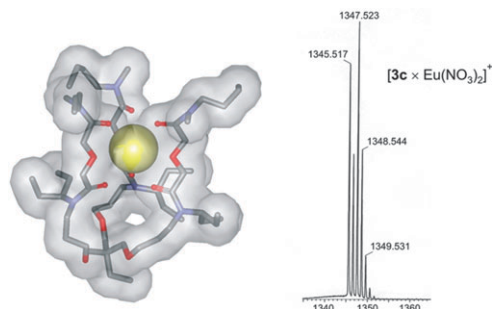


490

**Tripodal diglycolamides as highly efficient extractants for f-elements**

Dominik Jańczewski, David N. Reinhoudt,  
 Willem Verboom,\* Clément Hill, Cécile Allignol and  
 Marie-Thérèse Duchesne

Highly efficient, novel diglycolamide ligands for extraction of lanthanides and actinides coordinating Eu<sup>3+</sup> with 1 : 1 metal–ligand ratio.

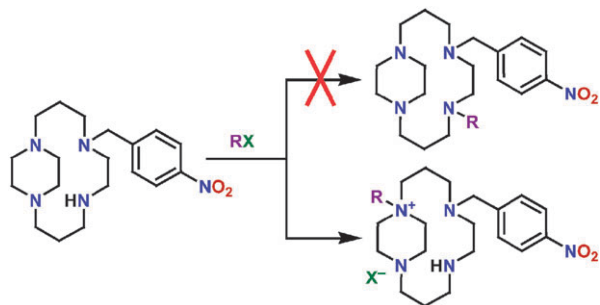


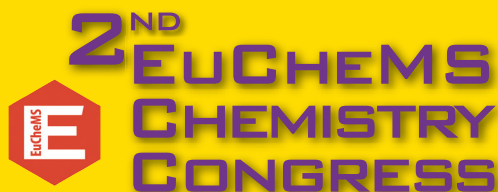
496

**Unsymmetrically substituted side-bridged cyclam derivatives and their Cu(II) and Zn(II) complexes**

Jan Plutnar, Jana Havlíčková, Jan Kotek,\* Petr Hermann  
 and Ivan Lukeš

A series of unsymmetrically substituted derivatives of 1,5,8,12-tetraazabicyclo[10.2.2]hexadecane together with an unexpected alkylation pathway is reported.





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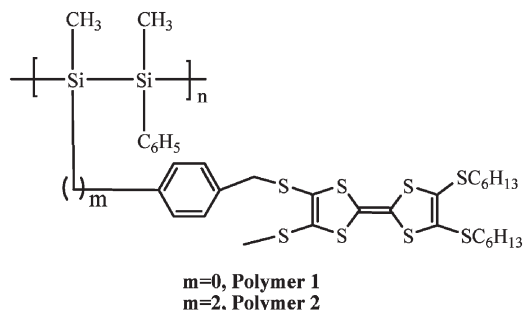
## PAPERS

505

### Synthesis and properties of polysilanes with tetrathiafulvalene as pendant group

Yibo Liu, Chengyun Wang,\* Meijiang Li, Guoqiao Lai and Yongjia Shen\*

Polysilanes with tetrathiafulvalene as pendant groups have been synthesized for the first time. These polysilanes doped by  $I_2$  exhibited high conductivities ( $10^{-2} \text{ S cm}^{-1}$ ).



511

### Computational study of the bonding structure in ylide compounds

Hsin-Yi Liao\* and Mei-Yin Yen

The ylide compounds  $H_m D=A H_n$  were examined; the geometrical planarity and bond strength of the  $D=A$  double bond can be interpreted in terms of the  $\Sigma\Delta E_{ST}$  (CGMT model) and the HOMO–LUMO gap of the two bonding fragments.

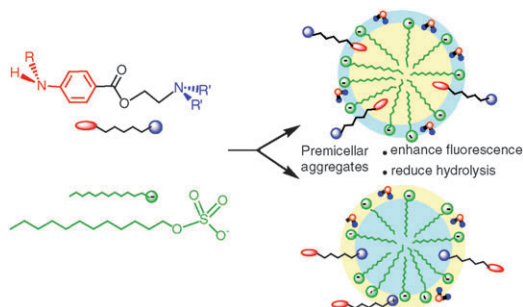


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### Investigation of physico-chemical behaviour of local anaesthetics in aqueous SDS solutions

Emilia Iglesias

Aqueous solutions of SDS, at concentrations close to the cmc, enhance the fluorescence of local anaesthetics and reduce the rate of hydrolysis of the ester function.

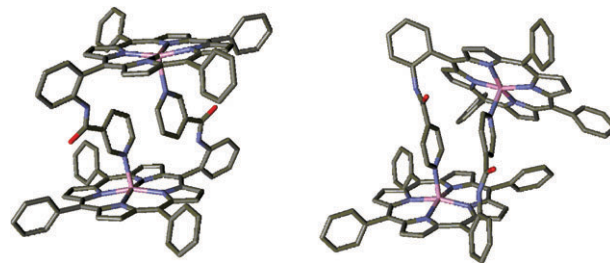


525

### Structurally-tolerant self-assembly of zinc pyridyl porphyrins

Pablo L. Bernad, Jr, Andrea J. Guerin, Richard A. Haycock, Sarah L. Heath, Christopher A. Hunter,\* Cesar Raposo, Carmen Rotger, Luke D. Sarson and Liam R. Sutton

Zinc porphyrins equipped with pyridine ligands in diverse orientations form stable self-assembled dimeric macrocycles. Expansion to larger macrocycles requires a monomer geometry that strongly destabilises the dimer.



## PAPERS

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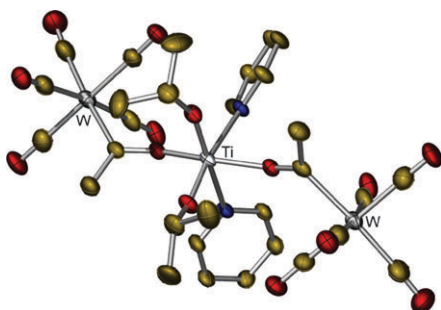


### A cytotoxic bis(carbene)gold(I) complex of ferrocenyl complexes: synthesis and structural characterisation

Ulrike E. I. Horvath,\* Gino Bentivoglio, Michael Hummel, Herwig Schottenberger, Klaus Wurst, Margo J. Nell, Constance E. J. van Rensburg, Stephanie Cronje and Helgard G. Raubenheimer\*

A stable, dinuclear N-heterocyclic gold(I) carbene complex that contains an electrophoric ferrocenyl side chain shows significant anti-tumour activity against two chosen cell lines.

540

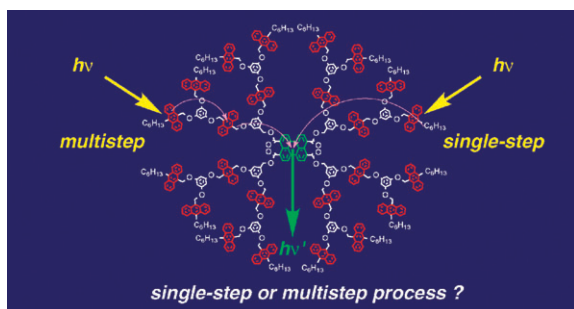


### Titanoxycarbene complexes of Ti(IV) with O- and N-donor ligands

Stefan D. Nogai, Oliver Schuster, Jocelyn Bruce and Helgard G. Raubenheimer\*

New heterobimetallic compounds,  $[(OC)_5M=C(Me)OTi(OiPr)_2](\mu-OiPr)_2$  with  $M = Cr$  (**1**),  $W$  (**2**), react with pyridine in an unprecedented way to afford bis(carbenoxide)titanium(IV) complexes. Displaying a rare behaviour, crystals of complex **1** virtually “explode” when cooled below  $-60^\circ C$ .

547



### Mechanistic investigation of energy transfer in perylene-cored anthracene dendrimers

Masaki Takahashi,\* Hironao Morimoto, Kentaro Miyake, Hideki Kawai, Yoshihisa Sei, Kentaro Yamaguchi, Tetsuya Sengoku and Hidemi Yoda\*

Inspection of energy transfer efficiencies obtained from all ten dendrimers demonstrated that single-step energy transfer should represent a key mechanism for long-range energy transport.

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