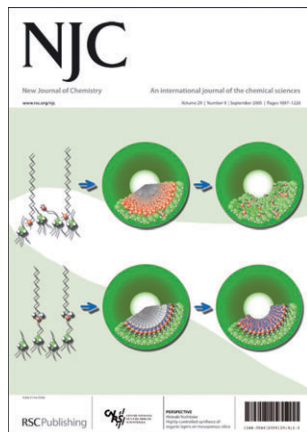


## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 29(9) 1097-1220 (2005)

**Cover**

See Hideaki Yoshitake, page 1107. The front cover picture illustrates that when functionalization is associated with templating, aminopropyl groups are dispersed more uniformly on a mesoporous silica surface than those prepared by a co-condensation method where some amino groups are inactivated, probably by binding strongly with the surface or by being buried in the silica framework. Image reproduced by permission of Hideaki Yoshitake from *New J. Chem.*, 2005, **29**, 1107.

**Inside Cover**

See Leroy Cronin *et al.*, page 1118. The inside front cover depicts a YES/NO DNA binding assay for small molecules using size exclusion filtration and UV vis spectroscopy. This means that it is extremely simple to gain information about the DNA-interactive nature of a library of molecules and it is easy, using this methodology, to examine many compounds very quickly. Image reproduced by permission of Louise V. Smith, Jesus M. de la Fuente, Kevin M. Guthrie, Alexis D. C. Parenty and Leroy Cronin from *New J. Chem.*, 2005, **29**, 1118.

## CHEMICAL SCIENCE

C65

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.

**Chemical Science**

September 2005/Volume 2/Issue 9

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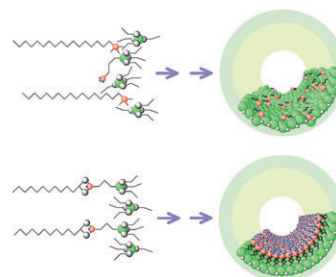
## PERSPECTIVE

1107

**Highly-controlled synthesis of organic layers on mesoporous silica: their structure and application to toxic ion adsorptions**

Hideaki Yoshitake\*

We reveal potential problems in the synthesis of modified mesoporous silica for achieving a uniform structure, developing new synthetic routes to highly-functionalized solids and elucidating the mechanism where they work as an adsorbent, which are discussed both on the mesoscopic and microscopic scales.



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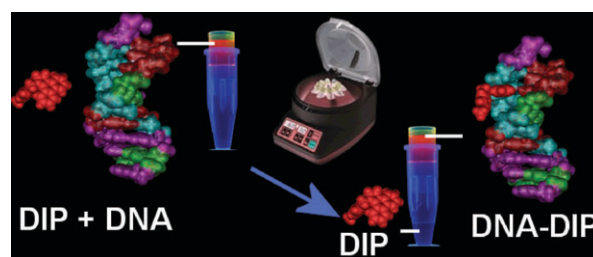
## LETTERS

1118

**Does it bind? An instant binding assay for DNA oligonucleotide interactive small molecules**

Louise V. Smith, Jesus M. de la Fuente, Kevin M. Guthrie, Alexis D. C. Parenty and Leroy Cronin\*

Ultrafiltration analysis has been used to screen DNA oligonucleotide interactive small molecules for the first time, providing a straightforward yes/no answer to small molecule DNA binding, and this was used to discover a new class of binders based on dihydro-imidazo-phenanthridinium.

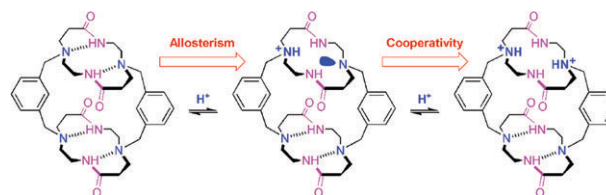


1121

**Synthesis, characterization and X-ray crystal structures of cyclam derivatives. 7. Hydrogen-bond induced allosteric effects and protonation cooperativity in a macrotricyclic bisdioxocyclam receptor**

Michel Meyer, Laurent Frémond, Enrique Espinosa, Stéphane Brandès, Guy Yves Vollmer and Roger Guillard\*

The unprecedented cooperative protonation of a barrel-shaped macrotricyclic tetraamine is rationalized in terms of allosteric effects triggered by the disruption of intramolecular hydrogen bonds upon binding of the first and third protons.

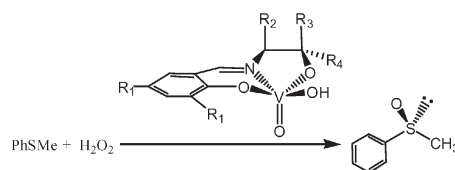


1125

**Substituent effects and mechanism elucidation of enantioselective sulfoxidation catalyzed by vanadium Schiff base complexes**

Qingle Zeng,\* Heqing Wang, Wen Weng, Wenshi Lin, Yuxing Gao, Xiantong Huang and Yufen Zhao\*

The substituent effects of vanadium-catalyzed enantioselective sulfoxidation were first systematically studied. A rational mechanism of enantioselective sulfoxidation is proposed.



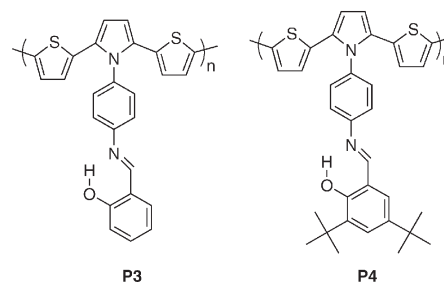
## PAPERS

1128

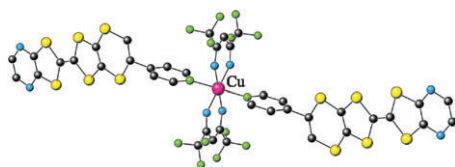
**Electrochromic conjugated *N*-salicylidene-aniline (anil) functionalized pyrrole and 2,5-dithienylpyrrole-based polymers**

Barry C. Thompson, Khalil A. Abboud, John R. Reynolds,\* Keitaro Nakatani and Pierre Audebert\*

The electrochromic and photochromic response of anil functionalized pyrrole and bis-thiophene-pyrrole monomers and polymers represents a route to a new class of multifunctional materials.



1135

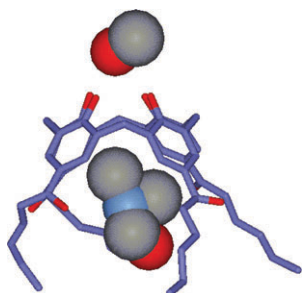


**Paramagnetic transition metal complexes with a redox-active ligand:  $M(\text{hfac})_2(\text{EDO-EDT-TTF-py})_n$ ;  $[M = \text{Cu}^{\text{II}}, n = 1, 2; M = \text{Mn}^{\text{II}}, n = 2]$**

Akira Ota, Lahcène Ouahab,\* Stéphane Golhen, Olivier Cador, Yukihiro Yoshida and Gunzi Saito

Synthesis, crystal structures and physical properties of the new TTF derivative ligand, EDO-EDT-TTF-py and three of its paramagnetic transition metal coordination complexes  $M(\text{hfac})_2(\text{EDO-EDT-TTF-py})_n$ ; ( $M = \text{Cu}^{\text{II}}$  with  $n = 1, 2$  and  $M = \text{Mn}^{\text{II}}$  with  $n = 2$ ) are reported.

1141

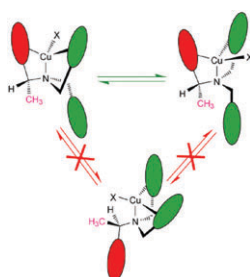


**Guest-induced chain folding in amphiphilic calixarene structures**

Alix Dubes, Kostantin A. Udachin, Patrick Shahgaldian, Adina N. Lazar, Anthony W. Coleman and John A. Ripmeester\*

By derivatization of *p*-H-calix[4]arene with hexanoyl chains, amphiphilic calixarenes are formed. The grafted chains extend the calixarene cavity and alter their geometry to aid encapsulation of a variety of guest molecules.

1147

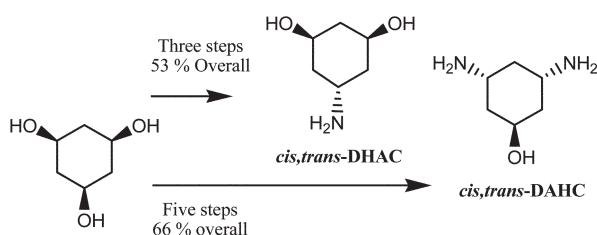


**Conformational dynamics of Cu(I) complexes of tripodal ligands: steric control of molecular motion**

Jing Zhang, Kam Siu, Chin H. Lin and James W. Canary\*

The dynamics of molecular conformational changes for Cu(I) complexes of two tripodal ligands were studied by variable-temperature NMR and circular dichroism in combination with two-dimensional NMR experiments.

1152

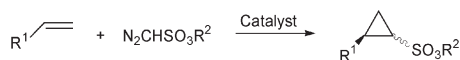


**Design and stereospecific synthesis of modular ligands based upon *cis*-1,3-*trans*-5-substituted cyclohexanes**

John Fielden, Joanna Sprott and Leroy Cronin\*

A range of eight novel ligands, based on the *cis*-1,3-*trans*-5-substituted cyclohexane framework, have been synthesized by a stereospecific route starting from *cis*-1,3,5-cyclohexanetriol.

1159



**Enantiocontrol in intermolecular cyclopropanations: use of diazosulfonate esters**

Tao Ye\* and Congying Zhou

The novel use of diazosulfonate esters as cyclopropanating agents is investigated; effects of ligand and substrate structure on diastereo- and enantioselectivity are reported.

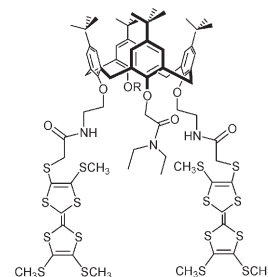
1164



### A calixarene–amide–tetrathiafulvalene assembly for the electrochemical detection of anions

Bang-Tun Zhao, María-Jesús Blesa, Nicolas Mercier, Franck Le Derf and Marc Sallé\*

The electroactive tetrathiafulvalene unit has been attached to a calix[4]arene scaffold through amide junctions, leading to a receptor able to electrochemically respond to  $\text{H}_2\text{PO}_4^-$  anion ( $\text{A}^-$ ).

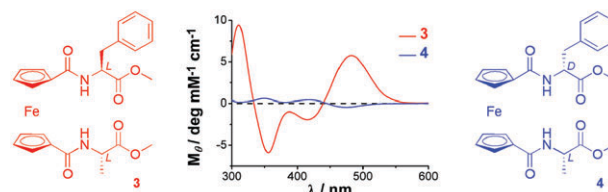


1168

### Unsymmetrical 1,*n*'-disubstituted ferrocenoyl peptides: convenient one pot synthesis and solution structures by CD and NMR spectroscopy

Srećko I. Kirin, Dirk Wissenbach and Nils Metzler-Nolte\*

The interdependence between amino acid chirality and the helical chirality at the ferrocene core is investigated in solution for a series of ferrocenoyl peptides with two different amino acids on each Cp ring.

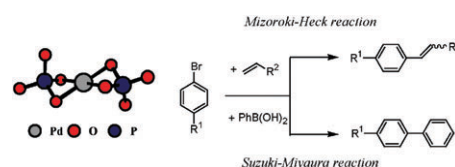


1174

### Catalytic investigations of carbon–carbon bond-forming reactions by a hydroxyapatite-bound palladium complex

Kohsuke Mori, Takayoshi Hara, Michitaka Oshiba, Tomoo Mizugaki, Kohki Ebitani and Kiyotomi Kaneda\*

A new type of hydroxyapatite-bound palladium complex (PdHAP-1) displayed outstanding catalytic activities for the Mizoroki–Heck reaction and Suzuki–Miyaura coupling reaction of aryl bromides.



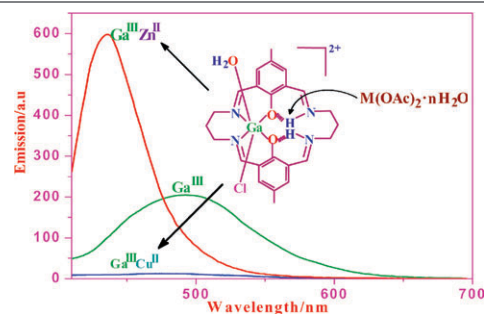
1182



### Mononuclear $\text{Al}^{\text{III}}$ , $\text{Ga}^{\text{III}}$ and $\text{In}^{\text{III}}$ , and heterodinuclear $\text{Ga}^{\text{III}}\text{M}^{\text{II}}$ ( $\text{M} = \text{Zn}, \text{Cu}, \text{Ni}, \text{Co}$ ) complexes of a tetraiminodiphenol macrocyclic ligand

Bula Dutta, Pradip Bag and Kamalaksha Nag\*

Synthetic and spectroscopic studies have been made of the macrocyclic complexes  $[\text{M}^{\text{III}}(\text{LH}_2)(\text{H}_2\text{O})\text{Cl}](\text{ClO}_4)_2 \cdot n\text{H}_2\text{O}$  ( $\text{M} = \text{Al}, \text{Ga}, \text{In}$ ) and  $[\text{Ga}^{\text{III}}\text{M}^{\text{II}}\text{L}(\mu\text{-OAc})(\text{OAc})](\text{ClO}_4)_2 \cdot n\text{H}_2\text{O}$  ( $\text{M} = \text{Zn}, \text{Cu}, \text{Ni}, \text{Co}$ ).



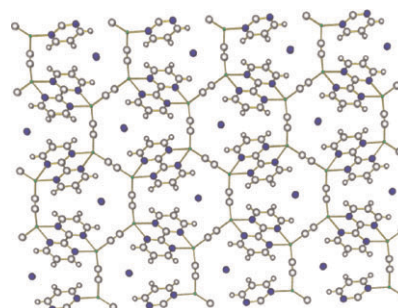
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### 2D and 3D coordination polymers based on 2,2'-bipyrimidine and cyanide bridging ligands incorporating coordinated and guest ammonia molecules. Synthesis, crystal structures, magnetic properties and thermal analysis of $[\{\text{Ni}(\text{CN})_4\}_2\text{-(Ni}(\text{NH}_3)_2(\text{bpym})\}\cdot 2\text{H}_2\text{O}]_n$ and $[\{\text{Cu}_2(\text{CN})_2(\text{bpym})\}\cdot \text{NH}_3]_n$

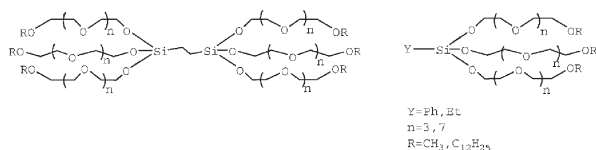
Enrique Colacio,\* Francesc Lloret, Miguel Navarrete, Antonio Romerosa, Helen Stoeckli-Evans and José Suarez-Varela

2D and 3D coordination polymers,  $[\{\text{Ni}(\text{CN})_4\}_2\text{-(Ni}(\text{NH}_3)_2(\text{bpym})\}\cdot 2\text{H}_2\text{O}]_n$  and  $[\{\text{Cu}_2(\text{CN})_2(\text{bpym})\}\cdot \text{NH}_3]_n$ , respectively, containing 2,2'-bipyrimidine and cyanide bridging ligands and incorporating coordinated or guest ammonia molecules have been prepared and structurally, magnetically and thermally characterized.





1195

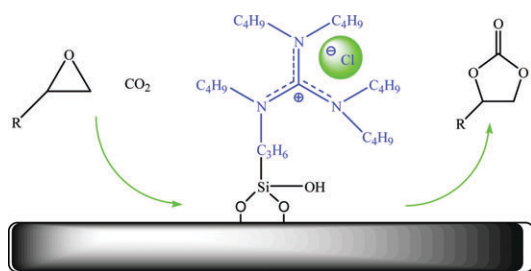


### Catalytic activity and anion activation in S<sub>N</sub>2 reactions promoted by complexes of silicon polypodands. Comparison with traditional polyethers

Angelamaria Maia,\* Dario Landini, Cecilia Betti, Boguslawa Leska and Grzegorz Schroeder

The catalytic activity of silicon polypodands was evaluated in anion-promoted reactions under solid–liquid phase-transfer catalysis (SL-PTC) conditions. Results showed that these many-armed ligands are particularly efficient catalysts.

1199

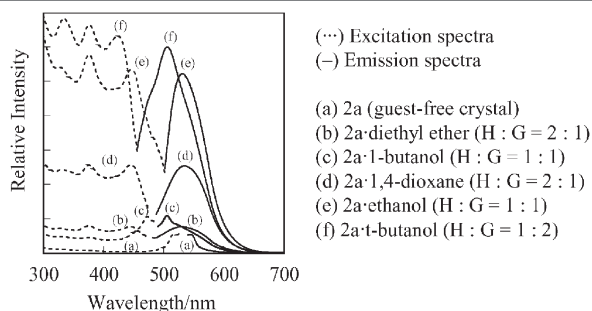


### The effective synthesis of propylene carbonate catalyzed by silica-supported hexaalkylguanidinium chloride

Haibo Xie, Haifeng Duan, Shenghai Li and Suobo Zhang\*

Both homogeneous and silica-supported hexaalkylguanidinium chloride were effective catalysts for CO<sub>2</sub> fixation to carbonate without any solvent under mild reaction conditions, the silica-supported hexaalkylguanidinium chloride showing the great advantage that it could be recycled easily at least 5 further times without any obvious decrease in its catalytic activity, after simple filtration.

1204

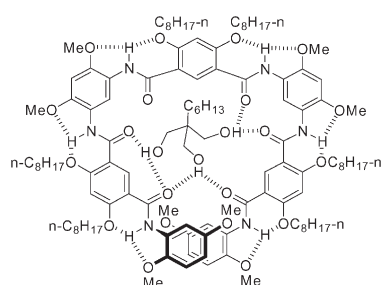


### Heterocyclic quinol-type fluorophores. Dramatic solid-state fluorescence enhancement behaviour of imidazoanthraquinol-type clathrate hosts upon inclusion of various kinds of organic solvent molecules

Yousuke Ooyama and Katsuhira Yoshida\*

Novel imidazoanthraquinol-type clathrate fluorophores which can exhibit dramatic solid-state fluorescence enhancement behaviour upon formation of guest-inclusion crystals with various organic solvent molecules have been developed.

1213



### Hydrogen bonding-mediated oligobenzamide foldamer receptors that efficiently bind a triol and saccharides in chloroform

Hui-Ping Yi, Xue-Bin Shao, Jun-Li Hou, Chuang Li, Xi-Kui Jiang and Zhan-Ting Li\*

Two hydrogen bonding-driven foldamers have been synthesized which are able to efficiently bind multi-hydroxyl molecules in chloroform.


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