

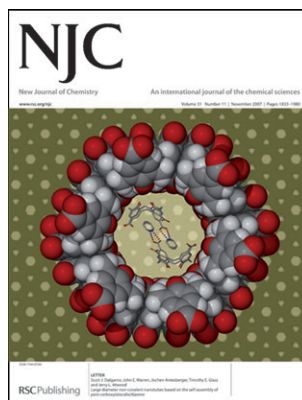
## IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 31(11) 1833–1980 (2007)



### Cover

See Malrieu *et al.*, pp. 1918–1927. The cover presents an alternative version of the famous dream of Kekulé - envisaging the benzene ring as the mythological Ouroboros snake. Cover design by Rémi Chauvin. Image reproduced by permission of Jean-Paul Malrieu, Christine Lepetit, Mickaël Gicquel, Jean-Louis Heully, Patrick W. Fowler and Remi Chauvin from *New J. Chem.*, 2007, **31**, 1918.



### Inside Cover

See Dalgarno *et al.*, pp. 1891–1894. *p*-Carboxylatocalix[4]arene, when crystallised from pyridine, forms large diameter non-covalent nanotubes through back-to-back stacking of the cone shaped host molecule. Image reproduced by permission of Scott J. Dalgarno, John E. Warren, Jochen Antesberger, Timothy E. Glass and Jerry L. Atwood from *New J. Chem.*, 2007, **31**, 1891.

## CHEMICAL SCIENCE

### C81

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## Chemical Science

November 2007/Volume 4/Issue 11

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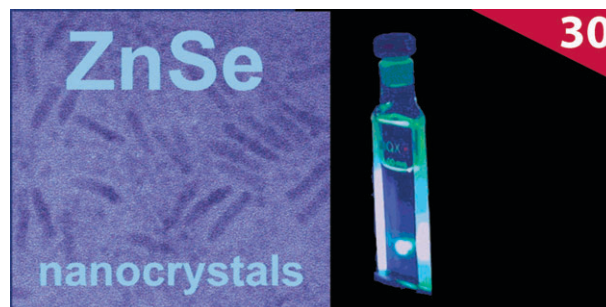
## PERSPECTIVE

### 1843

#### ZnSe based colloidal nanocrystals: synthesis, shape control, core/shell, alloy and doped systems

Peter Reiss

**30th Anniversary article:** The chemical synthesis of size- and shape-controlled ZnSe based nanostructures is reviewed with special emphasis on their application in optoelectronic devices, either as environmental friendly blue emitters or as host materials for divalent transition metal ions.



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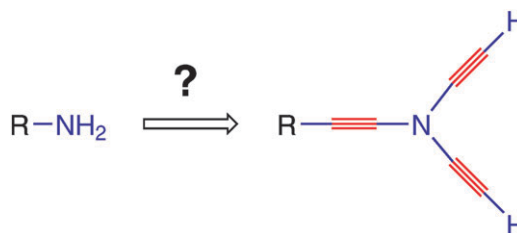
## PERSPECTIVE

1853

**Carbo-mers: from skeleton to function**

Valérie Maraval\* and Remi Chauvin\*

Beyond skeletal units such as rings, chemically reactive units, currently referred to as “chemical functions”, can be treated by the *carbo-mer* principle. Some of the resulting *carbo-meric* functions are “mysteriously” stable, while others remain “surprisingly” unknown in spite of their structural simplicity.



## LETTERS

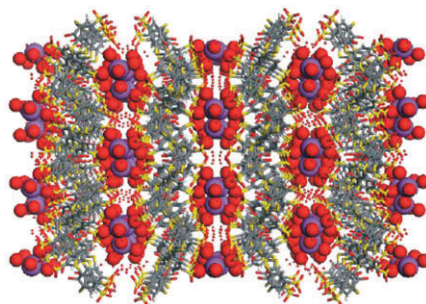


1874

**Supramolecular assembly based on *p*-sulfonatothiacalix[6]arene with sodium and water molecules**

Manabu Yamada, Yoshihiko Kondo, Kazuhiko Akimoto, Chizuko Kabuto and Fumio Hamada\*

A water-soluble *p*-sulfonatothiacalix[6]arene has been prepared in high yield and the inclusion complex with hydrated sodium cations and water has been investigated by X-ray crystal analysis.

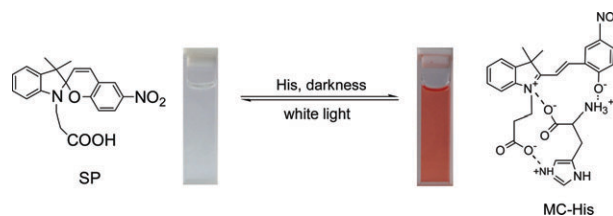


1878

**Basic amino acid induced isomerization of a spiropyran: towards visual recognition of basic amino acids in water**

Yuanyuan Liu, Meigong Fan, Shuxiao Zhang, Xiaohai Sheng and Jiannian Yao\*

Basic amino acids (BAA) induced a spiropyran derivative (SP) isomerization to its open form (MC), and its complexation with BAA in water was reported for the first time, which may provide a potential application for *in situ* recognition of BAA.

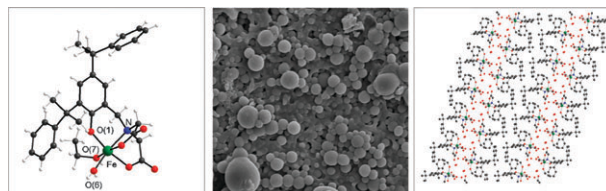


1882

**Self-assembly of Fe<sup>III</sup> complexes *via* hydrogen bonded water molecules into supramolecular coordination networks**

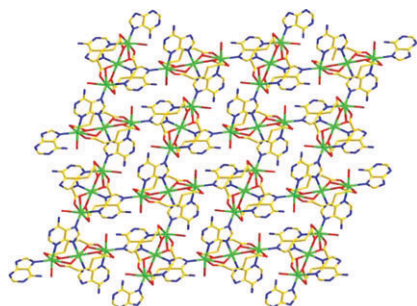
Ian McKeogh, Jonathan P. Hill, Emily S. Collins, Thomas McCabe, Annie K. Powell and Wolfgang Schmitt\*

Fe<sup>III</sup> complexes are assembled *via* hydrogen bonded water aggregates to give coordination networks that contain hydrophobic organic and hydrophilic inorganic areas.



## LETTERS

1887

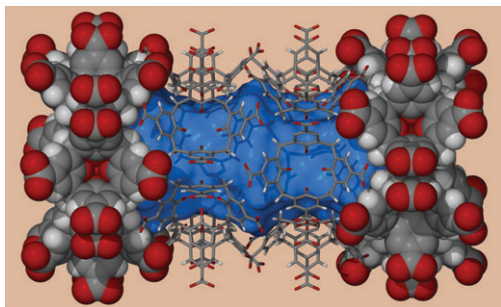


**The first 2D trinuclear Cd(II)-complex with adenine nucleobase: hydrothermal synthesis, crystal structure and fluorescent properties**

En-Cui Yang, Hong-Kun Zhao, Bin Ding, Xiu-Guang Wang and Xiao-Jun Zhao\*

The first 2D aggregate,  $\{[\text{Cd}_3(\mu_3\text{-ade})_2(\text{ap})_2(\text{H}_2\text{O})_2] \cdot 1.5\text{H}_2\text{O}\}_n$  (**1**), with trinuclear Cd(II) as secondary building units shows scarce coordination modes and a novel crystal packing arrangement.

1891

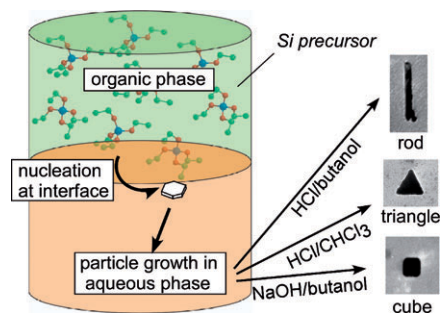


**Large diameter non-covalent nanotubes based on the self-assembly of *para*-carboxylatocalix[4]arene**

Scott J. Dalgarno,\* John E. Warren, Jochen Antesberger, Timothy E. Glass\* and Jerry L. Atwood\*

Non-covalent nanotubular arrays of *para*-carboxylatocalix[4]arene have been isolated by crystallisation from pyridine. These nanotubular arrays are amongst the widest such assemblies reported to date and possess large solvent channels running through the cores of the array (shown in blue).

1895



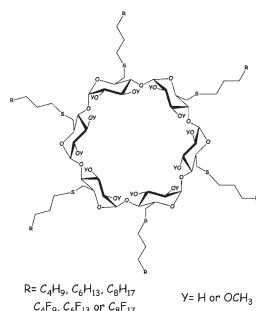
**Catalytic growth of silica nanoparticles in controlled shapes at planar liquid/liquid interfaces**

Nurxat Nuraje, Kai Su and Hiroshi Matsui\*

The shape of silica nanoparticles is controlled when they are synthesized at liquid/liquid interfaces. The combination of organic and aqueous phases that form the interface can change the shape of silica into a triangle, cube, or rod.

## PAPERS

1899



**Synthesis and characterisation of *O*-6-alkylthio- and perfluoroalkylpropanethio- $\alpha$ -cyclodextrins and their *O*-2-, *O*-3-methylated analogues**

Bernard Bertino Ghera, Florent Perret, Anne Baudouin, Anthony W. Coleman and H  l  ne Parrot-Lopez\*

The synthesis of a series of *O*-6-alkylthio- and perfluoroalkylpropanethio- $\alpha$ -cyclodextrins and their methylated analogues is described. The methylated compounds show higher stabilities of monolayers of the fluorinated derivatives, and increasing stability with chain length.

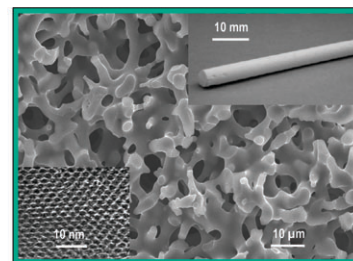


1907

### MCM-41 silica monoliths with independent control of meso- and macroporosity

Jérôme Babin, Julien Iapichella, Benoît Lefèvre, Christine Biolley, Jean-Pierre Bellat, François Fajula and Anne Galarneau\*

**30th Anniversary article:** Centimetre sized MCM-41 macroporous monoliths with tunable textural characteristics have been prepared by pseudomorphic transformation of silica bicontinuous skeletons produced by a sol–gel process accompanied by phase separation.



30

1918

### Evaluating the cyclic $\pi$ -electron delocalization energy through a double cut of conjugated rings

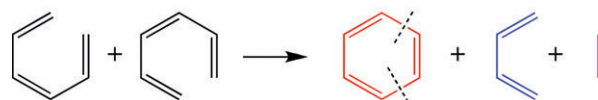
Jean-Paul Malrieu,\* Christine Lepetit, Mickaël Gicquel, Jean-Louis Heully, Patrick W. Fowler and Remi Chauvin

**30th Anniversary article:** Estimation of cyclic  $\pi$ -electron delocalization energy requires separation of a cycle into two parts, and hence two cuts, not one as in traditional methods.



30

$$\epsilon_{\text{cyc}}(\text{AB}) = E(\text{AB}) + E^0(\text{A}) + E^0(\text{B}) - E(\text{A} \sim \text{B}) - E(\text{A} \sim \text{B})$$

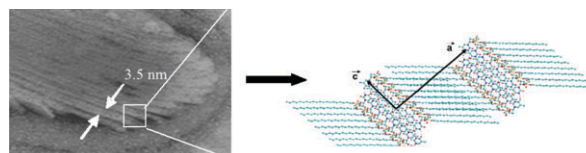


1928

### Nanostructured assemblies from nucleotide-based amphiphiles

Nathalie Campins, Philippe Dieudonné, Mark W. Grinstaff and Philippe Barthélémy\*

Synthetic nucleotide-based amphiphiles derived from thymidine and adenosine provide assemblies, which are structured at the nanoscale.

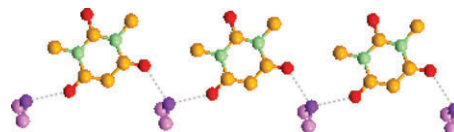


1935

### Solid–gas reactions between 1,3-dimethylbarbituric acid and amines. A structural and spectroscopic study

Dario Braga,\* Marcella Cadoni, Fabrizia Grepioni, Lucia Maini\* and Jacco van de Streek

The reactions of solid 1,3-dimethylbarbituric acid (DMBA) with vapours of  $\text{NH}_3$  and of the volatile amines  $\text{NH}_2(\text{CH}_3)$  and  $\text{NH}(\text{CH}_3)_2$  have been investigated, and the products characterized by X-ray powder and single crystal diffraction, differential scanning calorimetry, thermogravimetric analysis and UV–Vis spectroscopy in the solid state.



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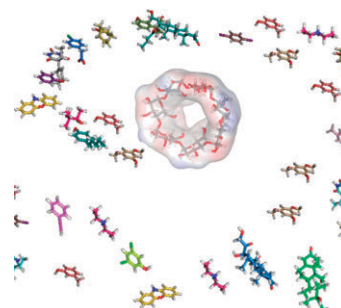


1941

### Combined similarity and QSPR virtual screening for guest molecules of $\beta$ -cyclodextrin

Andreas Steffen, Maximilian Karasz, Carolin Thiele, Thomas Lengauer, Andreas Kämper, Gerhard Wenz\* and Joannis Apostolakis\*

A high throughput, ligand-based, virtual screening approach identifies strong binding ligands of  $\beta$ -CD.

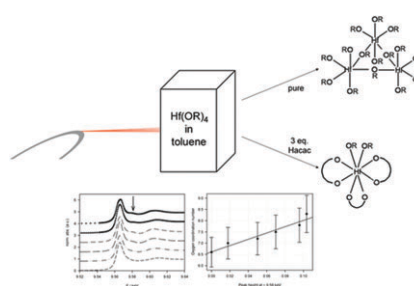


1950

### The structures of the precursor $\text{Hf}(\text{O}^i\text{Bu})_4$ and its modification in solution: EXAFS-investigation in combination with XANES- and IR-spectroscopy

Matthias Bauer,\* Sonja Müller, Guido Kickelbick and Helmut Bertagnolli

Structural characterization of the sol-gel precursor hafnium *n*-butoxide and its modification by different ligands by EXAFS spectroscopy and new insights into the XANES spectroscopy of such systems.

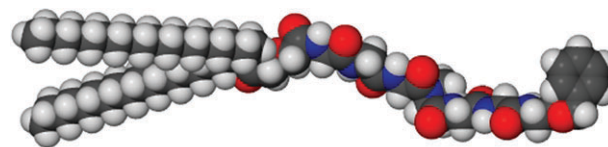


1960

### The effect of midpolar regime mimics on anion transport mediated by amphiphilic heptapeptides

Robert Pajewski, Jolanta Pajewska, Ruiqiong Li, Megan M. Daschbach, Elizabeth A. Fowler and George W. Gokel\*

Nine amphiphilic heptapeptides, synthetic anion transporters (SATs) of the form  $(\text{C}_{18}\text{H}_{37})_2\text{N}-\text{Y}-(\text{Gly})_3-\text{Pro}-(\text{Gly})_3-\text{OCH}_2\text{Ph}$  ( $\text{H}_2\text{Y}$  = succinic, glutaric, diglycolic, 3-thioglutaric, *N*-methyliminodiglycine, isophthalic and terephthalic acid) were prepared and mediated release of  $\text{Cl}^-$  from DOPC/DOPA vesicles with varying efficacy.

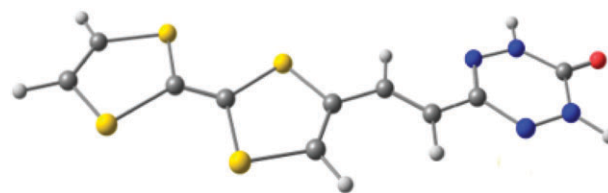


1973

### Synthesis and characterization of a TTF- $\pi$ -verdazyl radical—a new building block for conducting and/or magnetic systems

M'hamed Chahma, Keely Macnamara, Art van der Est, Antonio Alberola, Victor Polo and Melanie Pilkington\*

The synthetic strategy for the preparation of the first TTF- $\pi$ -verdazyl building block that links an organic donor molecule to a stable organic radical *via* a  $\pi$ -ethenyl spacer is presented.



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