

IN THIS ISSUE

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Cover

See David Balcells and Feliu Maseras, *New J. Chem.*, 2007, **31**, 333.

The modern methods of computational chemistry can provide valuable insight to experimentalists to explain their results, suggest novel interpretations, and support or disprove hypotheses. Cover designed by Gérard Calleja.

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, as well as the most significant scientific advances.

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March 2007/Volume 4/Issue 3

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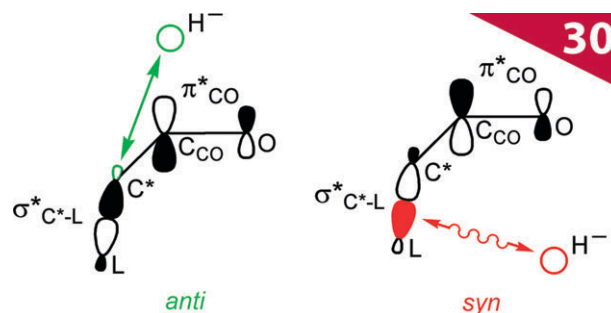
PERSPECTIVE

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Computational approaches to asymmetric synthesis

David Balcells and Feliu Maseras*

30th Anniversary article: Current computational research in asymmetric synthesis follows the lead of the pioneering work published by Nguyen Trong Anh and Eisenstein in *New J. Chem.* 30 years ago.



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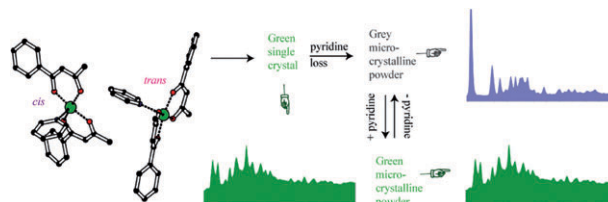
LETTERS

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***cis*- and *trans*-Bis(benzoylacetato)pyridinecopper(II): co-crystallisation of isomers and reversible pyridine loss with retention of crystallinity**

Anders Lennartson,* Mikael Håkansson* and Susan Jagner*

Bis(benzoylacetato)pyridinecopper(II) crystallises in both its *cis*- and *trans*-isomers within the same crystal; loss of pyridine yields a crystalline powder that absorbs pyridine vapour, reforming microcrystalline bis(benzoylacetato)pyridinecopper(II).

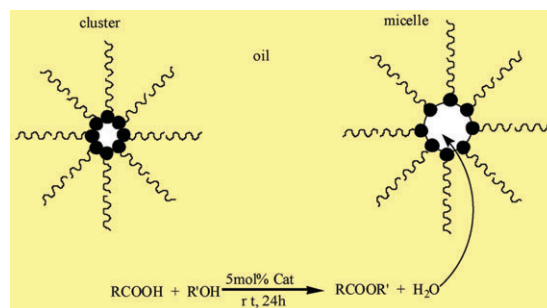


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Solvent-free esterification catalyzed by surfactant-combined catalysts at room temperature

Li Gang,* Li Xinzong and Wumanjiang Eli

Solvent-free esterifications are catalyzed by surfactant-combined catalysts at room temperature in moderate to excellent yields.

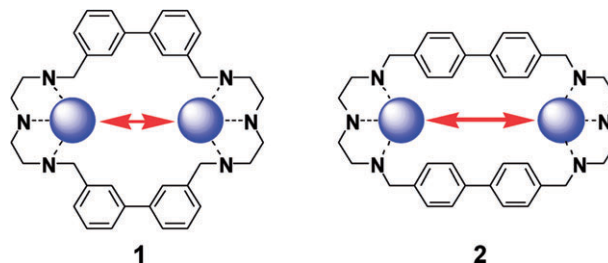


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Linear recognition of dicarboxylates by ditopic macrocyclic complexes

Massimo Boiocchi, Marco Bonizzoni, Alberto Moletti, Dario Pasini* and Angelo Taglietti*

The comparison between structurally isomeric macrocyclic ligands, whose dicopper complex acts as receptors for dianions in water at physiological pH, demonstrates that the selectivity pattern for dicarboxylate binding obeys the principles of preorganization and linear recognition.



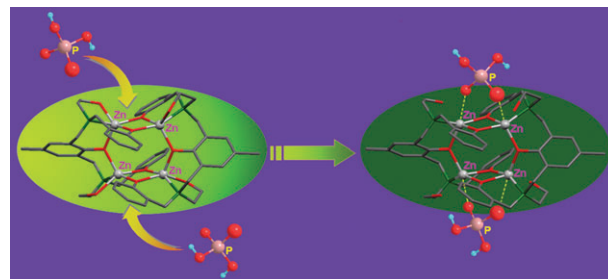
PAPERS

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Selective sensing of dihydrogen phosphate anion by a fluorescent tetranuclear pentacoordinated zinc(II) complex

Zhanfen Chen, Xiaoyong Wang,* Jingwen Chen, Xiaoliang Yang, Yizhi Li and Zijian Guo*

A tetranuclear complex $[\text{Zn}^{\text{II}}_4(\text{L}-3\text{H})_2](\text{ClO}_4)_2 \cdot 3.5\text{H}_2\text{O}$, with cresolic oxygen bridging ligands, can selectively sense the dihydrogen phosphate anion in solution. The binding phenomenon can be monitored *via* UV-vis absorption changes and fluorescence quenching effects.



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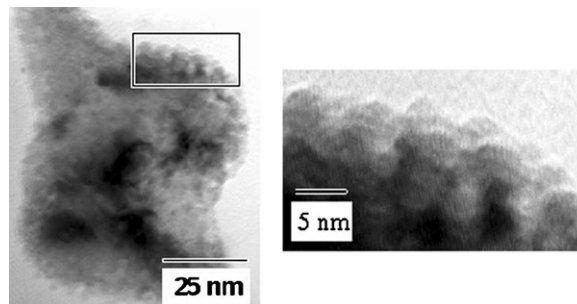
PAPERS

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Morphology evolution of GaPO₄ mesocrystals in a nonionic triblock copolymer system by pH-dependent control

Chung-Sung Yang,* Chun-Jung Chen and Xin-Hong Lin

In the synthesis of GaPO₄ crystals by pH-dependent control, the morphology of crystals is varied from the mesoscale assembly of nanoparticles (pH = 7.34) with porosity, so-called porous mesocrystals, to colloidal crystalline nanoparticles (pH = 11.54).

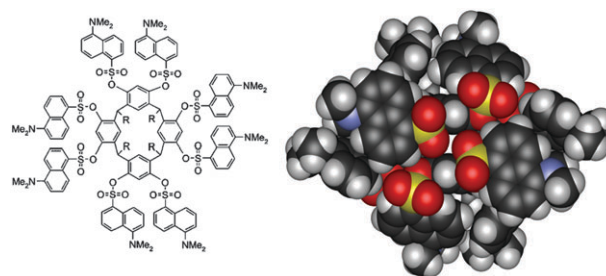


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Dansylated resorcinarenes

Ngong Kodiah Beyeh, Jukka Aumanen, Antti Åhman, Minna Luostarinen, Heidi Mansikkamäki, Maija Nissinen, Jouko Korppi-Tommola* and Kari Rissanen*

The synthesis, X-ray crystal structures and spectroscopic characterization (UV-Vis absorption and fluorescence emission) of a regioselective tetradansylated resorcinarene and octadansylated resorcinarene are described.

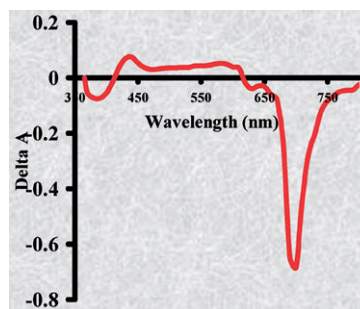


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Syntheses and photophysics of new phthalocyanine derivatives of zinc, cadmium and mercury

Wadzanai Chidawanyika, Abimbola Ogunsipe and Tebello Nyokong*

The presence of pyridyloxy substituents in novel tetra{2,(3)-pyridyloxyphthalocyaninato} complexes of zinc, cadmium and mercury results in increased quantum yields of the triplet state and decreased triplet lifetimes.

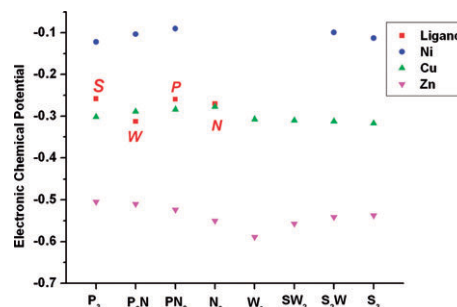


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Is copper(I) hard or soft? A density functional study of mixed ligand complexes

Chinnappan Sivasankar, Nabanita Sadhukhan, Jitendra K. Bera* and Ashoka G. Samuelson*

DFT calculations on Ni(0), Cu(I) and Zn(II) complexes with a combination of hard and soft ligands reveals the intermediate behaviour of Cu(I) with regard to its hardness.

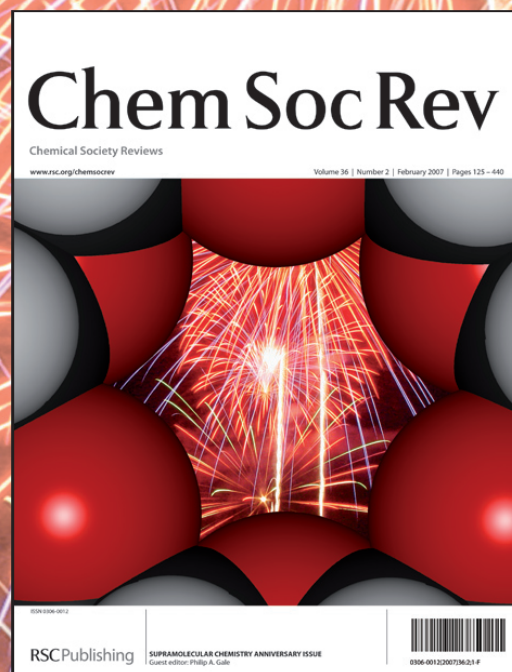


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In its February 2007 special issue *Chem Soc Rev* celebrates two landmark anniversaries in the field of Supramolecular Chemistry:

1967: Charles Pedersen's first paper on the synthesis and metal binding properties of crown ethers is published in the *Journal of the American Chemical Society*.

1987: the Nobel prize in chemistry is awarded to Charles Pedersen, Jean-Marie Lehn and Donald Cram in recognition of their pioneering work in Supramolecular Chemistry.

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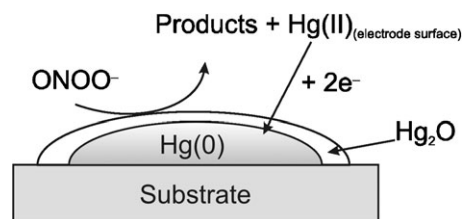
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The voltammetric determination of peroxynitrite at a mercury film electrode

Elza A. Zakharova,* Tatyana A. Yurmazova, Boris F. Nazarov, Gregory G. Wildgoose* and Richard G. Compton

Peroxynitrite can be voltammetrically detected *via* an “inverted” cathodic peak in the oxidative scan direction at a mercury film electrode. The unusual behaviour can be attributed to an ECE mechanism.

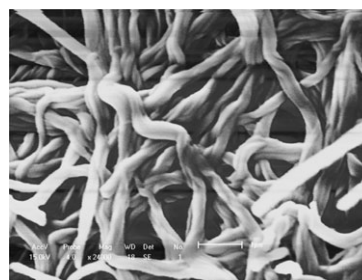


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Hydrazide-based organogels and liquid crystals with columnar order

Binglian Bai, Haitao Wang, Hong Xin, Fenglong Zhang, Beihong Long, Xiaobing Zhang, Songnan Qu and Min Li*

A series of achiral compounds form a stable thermotropic columnar phase and twist fibrous organogel.

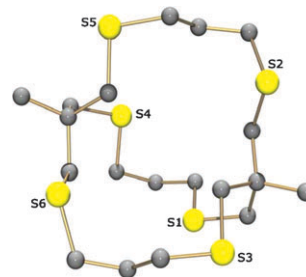


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Syntheses of a series of S₆ thioether cages and their coordination chemistry with Ag⁺

Roger Alberto, Daniela Angst, Kirstin Ortner, Ulrich Abram, P. August Schubiger and Thomas A. Kaden*

The syntheses of four S₆ cages with different cavity sizes and their complexation potential towards Ag(I) in solution and in the solid state are described.

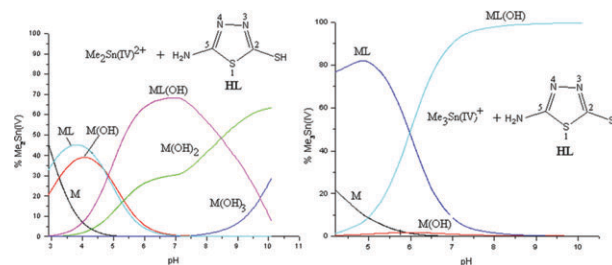


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Potentiometric and multinuclear NMR investigations of di-/trimethyltin(IV) cations with some heterocyclic thiones in aqueous media

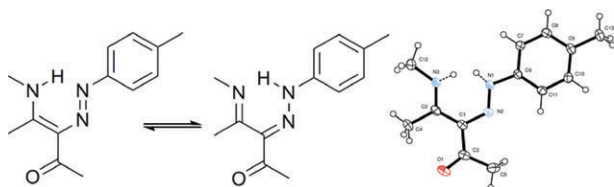
Mala Nath* and Sulaxna

The interaction of Me₂Sn(IV)²⁺ and Me₃Sn(IV)⁺ with some heterocyclic thiones has been performed by means of potentiometric titrations in aqueous solution at *I* = 0.1 M KNO₃ and 298 K in the pH range 2–10.5. The possible geometry of the complex species formed in aqueous solution has been suggested by multinuclear NMR spectroscopic studies.



PAPERS

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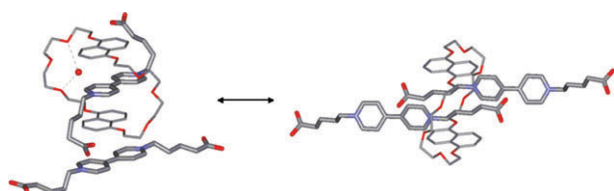


Structure and tautomerism of azo coupling products from *N*-alkylenaminones derived from acetylacetone and benzoylacetone in solid phase and in solution

Petr Šimůnek,* Markéta Svobodová, Valerio Bertolasi, Loretta Pretto, Antonín Lyčka and Vladimír Macháček

The structure and tautomerism of the products formed by reaction of some benzenediazonium tetrafluoroborates with some *N*-alkyl enaminones were studied both in solution and in the solid state.

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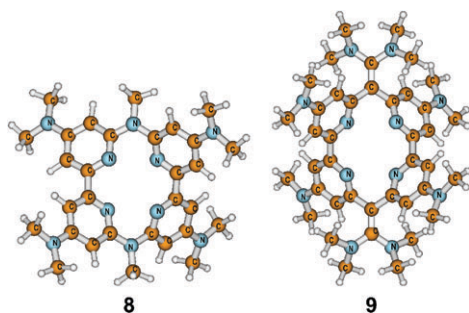


Temperature-, molar ratio- and counterion-effects on the crystal growth of bipyridinium-bis(alkylcarboxylic acid)-crown ether pseudorotaxanes

Gellert Mezei, Jeff W. Kampf and Vincent L. Pecoraro*

The crystallization of different polymorphs of pseudorotaxanes can be controlled by temperature, molar ratio between the rod- and ring-components and the availability of one or more different counterions.

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Pyridine and *s*-triazine as building blocks of nonionic organic superbases—a density functional theory B3LYP study

Ines Despotović, Borislav Kovačević and Zvonimir B. Maksić*

The supramolecular structures **8** and **9** are strong neutral organic superbases in the gas phase and MeCN.

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