

IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 29(3) 401–516 (2005)

In this issue...

Letters from Yuan-Gen Yao,
Laura Valencia and Rufina Bastida,
Gary B. Hix, Eric Clot and Alceo Macchioni.



Chemical biology articles published
in this journal also appear in the
Chemical Biology Virtual Journal:
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Cover

See Christophe Chipot and János G. Ángyán,
page 411.

The front cover shows polarization potential isosurfaces of benzene in the presence of a positive polarizing charge located 3 Å above the aromatic ring. The highly anisotropic nature of the polarization requires that the electric polarization response of the molecular charge distribution be described in a distributed fashion. Rigorous treatment of induction phenomena in statistical simulations of similar cation- π assemblies is now within reach using optimally partitioned electric properties.

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Christophe Chipot and János G. Ángyán
from *New J. Chem.*, 2005, **29**, 411.

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 2005/Volume 2/Issue 3

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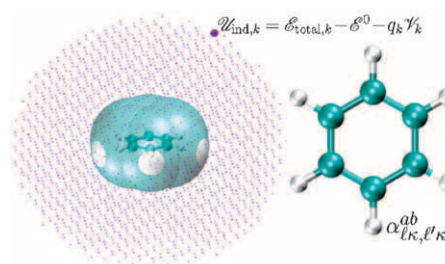
PERSPECTIVE

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Continuing challenges in the parametrization of intermolecular force fields. Towards an accurate description of electrostatic and induction terms

Christophe Chipot* and János G. Ángyán

Exploitation of the symmetry and transferability properties of a molecule is used to parametrize the induction forces in molecular systems.



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Departments of Chemistry and
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Washington University Medical
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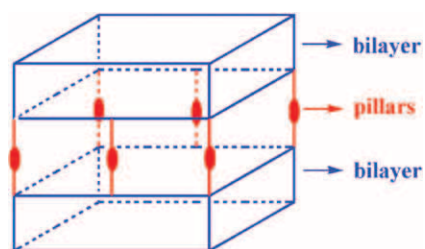
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A novel 3D framework generated by unusual pillared 2D bilayer motifs

Jian Zhang, Zhao-Ji Li, Jian-Kai Cheng, Yao Kang, Ye-Yan Qin and Yuan-Gen Yao*

A Co coordination polymer with polycarboxylate and pyrazine ligands presents a novel 3D architecture generated by an unusual 2D bilayer motif linked up by molecular pillars.

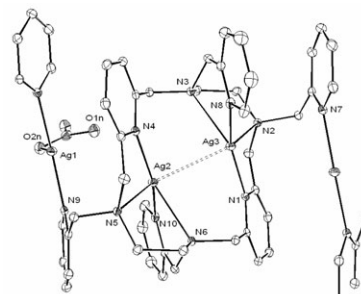


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Synthesis and helical polymeric structure of a luminescent pendant-armed macrocyclic silver(I) complex with Ag–Ag interactions

Laura Valencia,* Rufina Bastida,* Alejandro Macías, Manuel Vicente and Paulo Pérez-Lourido

The complex shows luminescence in both the solid and solution states at room temperature due to the existence of intermetallic interactions.

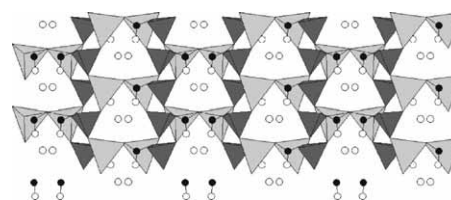


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Polymorphism in nickel phosphonates: synthesis of layered and microporous $\text{Ni}(\text{O}_3\text{PCH}_2\text{C}(\text{O})\text{NH}_2) \cdot \text{H}_2\text{O}$

Rakesh Modi, Gary B. Hix,* Maryjane Tremayne and Elizabeth MacLean

Two new polymorphic nickel phosphonates, one lamellar and one microporous, have been prepared by a reaction between nickel acetate and diethyl cyanomethylphosphonate, in which the acidity of the nickel solution affects the hydrolysis of the phosphonate to produce the phosphonic acid *in situ*.

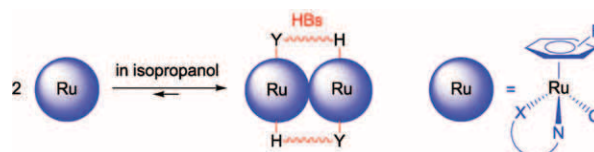


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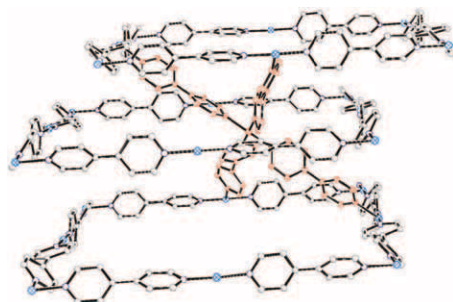
Aggregation in solution of neutral half-sandwich Ru(II) precatalysts for transfer hydrogenation

Daniele Zuccaccia, Eric Clot* and Alceo Macchioni*

PGSE NMR measurements and ONIOM calculations indicate that amino amidate and acidate half-sandwich precatalysts for transfer hydrogenation have a marked tendency to form dimers and larger aggregates in various solvents, including isopropanol.



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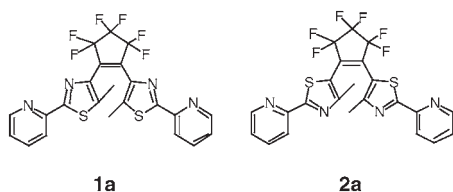


A novel two-fold interpenetrating 3D 4² · 8⁴ network self-assembled from a new 1D coordination polymer

Jack Y. Lu,* Wifredo A. Fernandez, Zhenghua Ge and Khalil A. Abboud

A new 3D coordination polymer has been synthesized, using the functional open metal (OM) sites of a new metastable 1D coordination polymer, and characterized by X-ray single-crystal structure determination (view of the 3D open-framework linkages in $[[\text{Cu}(4,4'\text{-bipy})_2(\text{H}_2\text{O})_2][\text{Cu}(4,4'\text{-bipy})_2(\text{H}_2\text{O})(\text{NO}_3)]](\text{NO}_3)_3 \cdot 12\text{H}_2\text{O}$; the “bending” part of the square-grid is in red and the copper atoms are in blue.)

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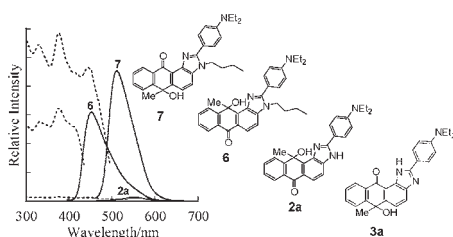


Synthesis and photochromism of two new 1,2-bis(thiazolyl)-perfluorocyclopentenes with chelating sites

Marion Giraud, Anne Léaustic, Marie-France Charlot, Pei Yu,* Michèle Césario, Christian Philouze, Robert Pansu, Keitaro Nakatani and Eléna Ishow

A new thiazole-based diarylethene exhibits crystalline phase photochromism, the first such compound to do so.

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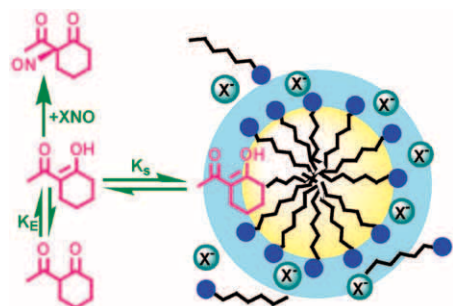


Heterocyclic quinol-type fluorophores. Synthesis of novel imidazoanthraquinol derivatives and their photophysical properties in benzene and in the crystalline state

Yousuke Ooyama, Takato Nakamura and Katsuhira Yoshida*

Novel imidazoanthraquinol-type fluorescent compounds exhibiting intense solid-state fluorescence have been prepared by control of both the tautomeric form and the crystal structure.

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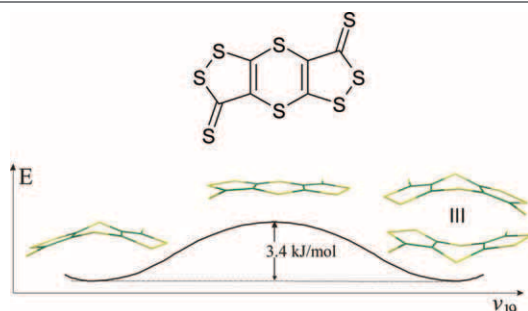


Tautomerization of 2-acetylcyclohexanone in assemblies of cationic surfactants

Emilia Iglesias

Rates of both keto-enol tautomerization and enol nitrosation of 2-acetylcyclohexanone are reduced in aqueous micellar solutions due to solvent effects that generally predominate over concentration effects.

465



Bent and planar molecules in polymorphs of the tricyclic carbon sulfide C₆S₈

Johannes Beck,* Johannes Weber,* Atashi Basu Mukhopadhyay and Michael Dolg

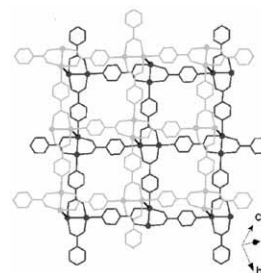
A second, nonplanar, polymorph of C₆S₈ has been discovered, in which the molecules adopt a more stable conformation than in the previously known planar structure.

474

**Synthesis, structures, and photoluminescent properties of two ligand unsupported silver(I) coordination polymers from isonicotinate anions**

Zheng Liu, Ping Liu,* Yun Chen, Jian Wang and Meihua Huang

Two novel structural coordination polymers with ligand unsupported Ag...Ag interactions have been synthesized. Compound **1** is the first example of double-layer architecture.

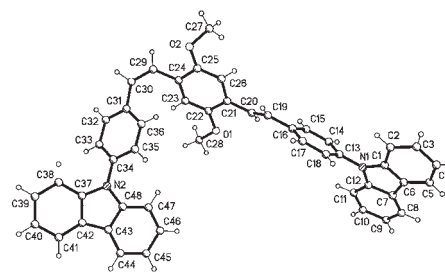


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**Structures and nonlinear optical properties of new symmetrical two-photon photopolymerization initiators**

Yun-Xing Yan,* Xu-Tang Tao, Yuan-Hong Sun, Chuan-Kui Wang, Gui-Bao Xu, Wen-Tao Yu, Hua-Ping Zhao, Jia-Xiang Yang, Xiao-Qiang Yu, Yong-Zhong Wu, Xian Zhao and Min-Hua Jiang

New centrosymmetric two-photon absorbing chromophores are good photopolymerization initiators for microfabrication.

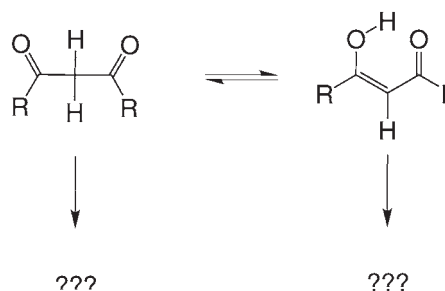


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Laser pyrolysis studies of β -diketonate chemical vapour deposition precursors. Part 1: β -diketones

Douglas K. Russell* and Anna Yee

While the thermal decomposition of acetylacetone and hexafluoroacetylacetone is dominated by molecular elimination and subsequent rearrangement, that of hexamethylacetylacetone proceeds *via* radical routes.

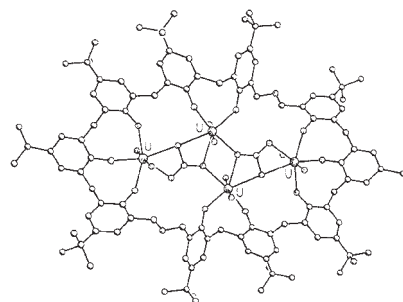


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**Synthesis of homooxalixarenes with 5 and 10 phenol units and crystal structure of their complexes with uranyl ions**

Bernardo Masci* and Pierre Thuéry*

p-tert-Butyldihomooxalix[5]arene and *p*-tert-butyltetrahomodioxalix[10]arene have been synthesized and a single crystal X-ray investigation of their complexes with uranyl ion is reported.

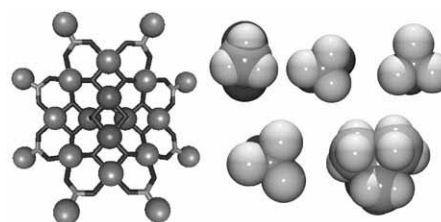


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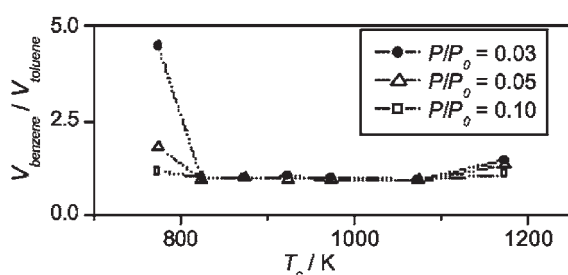
**Trihaloacetic acids: an investigation of steric and inductive ligand effects on the synthesis of $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CCX}_3)_{16}(\text{H}_2\text{O})_4]$ single-molecule magnets**

Jordi Gómez-Segura, Elsa Lhotel, Carley Paulsen, Dominique Luneau, Klaus Wurst, Jaime Veciana, Daniel Ruiz-Molina* and Philippe Gerbier*

Both steric and inductive ligand effects are critical factors in determining the thermal stability of these complexes.



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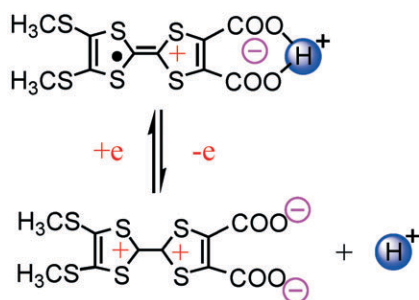


Effect of the calcination temperature of self-ordered mesoporous silicate on its adsorption characteristics for aromatic hydrocarbons

Yuko Ueno,* Tsutomu Horiuchi, Akiyuki Tate, Osamu Niwa, Hao-shen Zhou,* Takeo Yamada and Itaru Honma

Mesoporous silicate calcined at 773 K shows a high selectivity for benzene over toluene, especially at low pressures; this is due to the nature of the microporosity.

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A water-soluble derivative of tetrathiafulvalene exhibiting pH sensitive redox properties

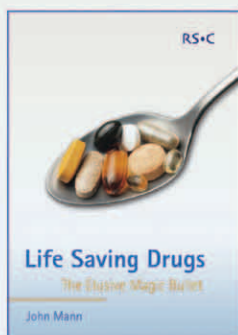
Hai-Hong Lin, Zhe-Min Yan, Jie Dai,* De-Qing Zhang, Jing-Lin Zuo, Qin-Yu Zhu and Ding-Xian Jia

A novel water-soluble and pH-sensitive TTF dicarboxylate forms a redox-active salt that shows a redox-coupled association/dissociation of the proton.

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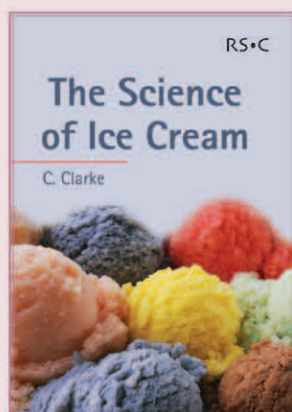
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