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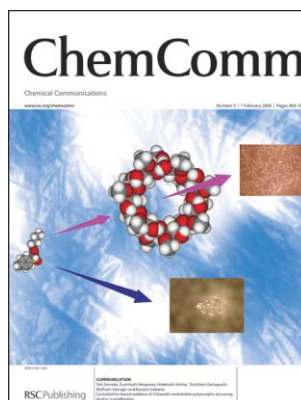
IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (5) 469–568 (2006)



Cover

See Carmen M. Atienza, Gustavo Fernández, Luis Sánchez, Nazario Martín, Inês Sá Dantas, Martijn M. Wienk, René A. J. Janssen, G. M. Aminur Rahman and Dirk M. Guldi, page 514. This light absorbing π -conjugated oligomer-tetrafullerene nanoarray undergoes an intramolecular energy transfer and has been used to fabricate a photovoltaic device with poly(3-hexylthiophene). Image reproduced by permission of Nazario Martín *et al.* from *Chem. Commun.*, 2006, 514.



Inside cover

See Yoh Sonoda, Fumitoshi Hirayama, Hidetoshi Arima, Yoshihiro Yamaguchi, Wolfram Saenger and Kaneto Uekama, page 517. A novel approach for the isolation of Ostwald's intermediate metastable polymorphs by utilizing the inclusion complexation with 2,6-di-O-methyl- β -cyclodextrin is presented. Image reproduced by permission of Kaneto Uekama *et al.* from *Chem. Commun.*, 2006, 517.

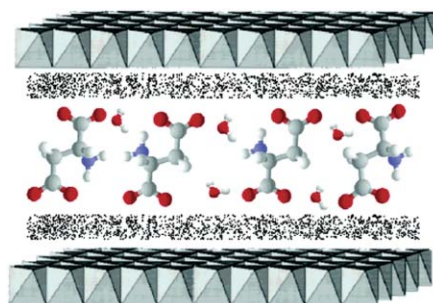
FEATURE ARTICLE

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Preparation of layered double hydroxides and their applications as additives in polymers, as precursors to magnetic materials and in biology and medicine

David G. Evans and Xue Duan*

Methods of preparing layered double hydroxides with tailored properties are described and some practical applications of the resulting materials are illustrated.



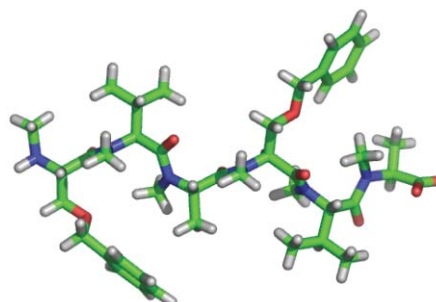
COMMUNICATIONS

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Poly-N-methylated α -peptides: synthesis and X-ray structure determination of β -strand forming foldamers

Suode Zhang, Samran Prabpai, Palangpon Kongsaree and Per I. Arvidsson*

The first high resolution structure determination of poly-N-methylated α -peptides – a class of compounds widely used in medicinal chemistry – shows that these molecules adopt a β -strand conformation in the solid state.



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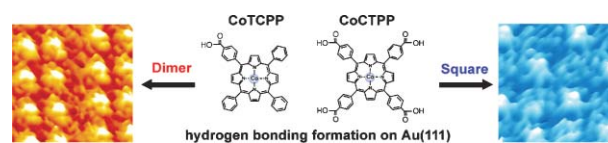
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Formation of highly ordered porphyrin adlayers induced by electrochemical potential modulation

Soichiro Yoshimoto,* Nozomi Yokoo, Takamitsu Fukuda, Nagao Kobayashi* and Kingo Itaya*

Molecular self-assembly of porphyrin derivatives formed with intermolecular hydrogen bonding on the surface of Au(111) electrode in acidic solution can be controlled by varying the number of peripheral carboxy groups and the applied electrochemical potential.

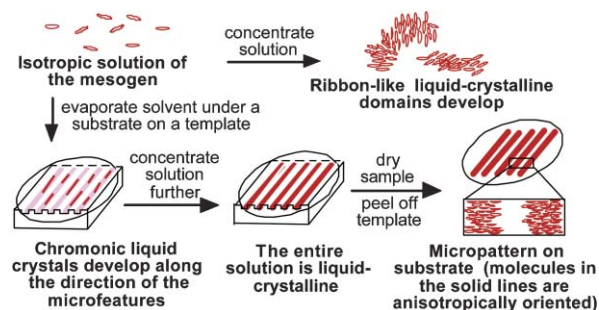


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Template-guided organization of chromonic liquid crystals into micropatterned anisotropic organic solids

Suk-Wah Tam-Chang,* Jennifer Helbley, Travis D. Carson, Wonewoo Seo and Isaac K. Iverson

An approach has been developed to generate micropatterns of anisotropic organic materials by exploiting the self-organization of an ionic perylenebis(dicarboximide) in aqueous solutions.

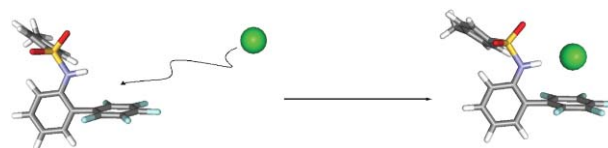


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Anion- π interaction augments halide binding in solution

Orion B. Berryman, Fraser Hof, Michael J. Hynes and Darren W. Johnson*

^1H NMR spectroscopic data and complementary theoretical predictions suggest that a designed receptor exhibits the anion- π interaction in solution.

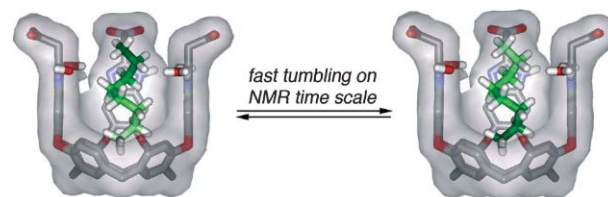


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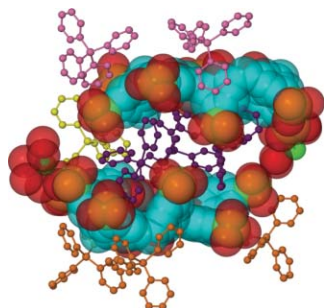
Normal hydrocarbons tumble rapidly in a deep, water-soluble cavitand

Richard J. Hooley, Shannon M. Biros and Julius Rebek, Jr.*

A deep, water-soluble cavitand extracts *n*-alkanes into its cavity *via* hydrophobic forces. The guests bind in a helical manner, and tumble rapidly on the NMR timescale inside the binding pocket.



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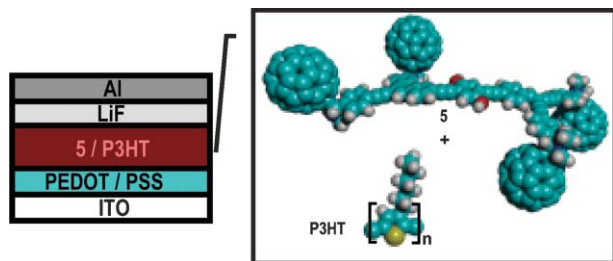


Constructing 2D porous material based on the assembly of large organic ions: *p*-sulfonatocalix[8]arene and tetraphenylphosphonium ions

Mohamed Makha,* Alexandre N. Sobolev and Colin L. Raston*

In the presence of tetraphenylphosphonium and aquated ytterbium(III) ions conformationally flexible *p*-sulfonatocalix[8]arene forms an extended structure with two dimensional porosity.

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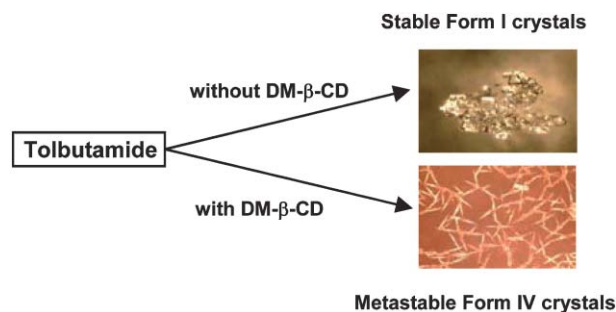


Light harvesting tetrafullerene nanoarray for organic solar cells

Carmen M. Atienza, Gustavo Fernández, Luis Sánchez, Nazario Martín,* Inês Sá Dantas, Martijn M. Wienk, René A. J. Janssen,* G. M. Aminur Rahman and Dirk M. Guldi*

A new tetrafullerene nanoarray (**5**) has been synthesized and the PV devices fabricated by blending **5** with P3HT show an external quantum efficiency of 15%.

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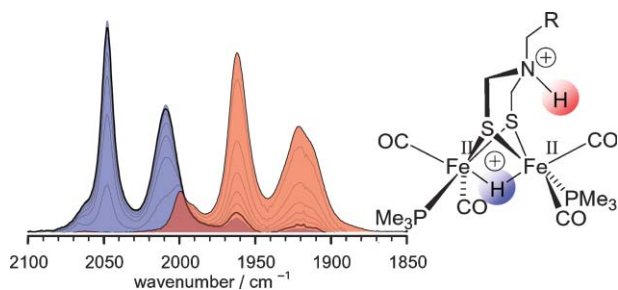


Cyclodextrin-based isolation of Ostwald's metastable polymorphs occurring during crystallization

Yoh Sonoda, Fumitoshi Hirayama, Hidetoshi Arima, Yoshihiro Yamaguchi, Wolfram Saenger and Kaneto Uekama*

A novel approach for the selective isolation of Ostwald's intermediate metastable polymorphs occurring during an early stage of crystallization by utilizing the inclusion complex formed with 2,6-di-*O*-methyl- β -cyclodextrin is reported.

520



Iron hydrogenase active site mimic holding a proton and a hydride

Lennart Schwartz, Gerriet Eilers, Lars Eriksson, Adolf Gogoll, Reiner Lomoth* and Sascha Ott*

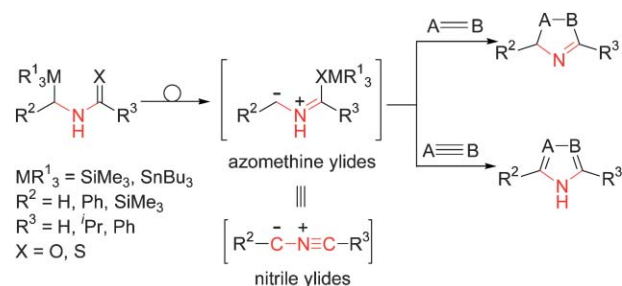
The first model of the iron hydrogenase active site which concomitantly carries a proton and a hydride has been prepared and was characterized by IR and NMR spectroscopy.

526

Unprecedented 1,4-stannatropy: effective generation of azomethine ylides as nitrile ylide equivalents from *N*-(stannylmethyl)thioamides

Mitsuo Komatsu,* Yukihiro Kasano, Jin-ichi Yonemori, Yoji Oderaotoshi and Satoshi Minakata

Generation and cycloaddition of less- or non-stabilized azomethine ylides, or nitrile ylide equivalents, *via* 1,4-stannatropy of *N*-(tributylstannylmethyl)thioamides were achieved. The reactions with dipolarophiles, such as electron-deficient alkenes and alkynes, afforded corresponding pyrrolidine and pyrrole derivatives effectively.

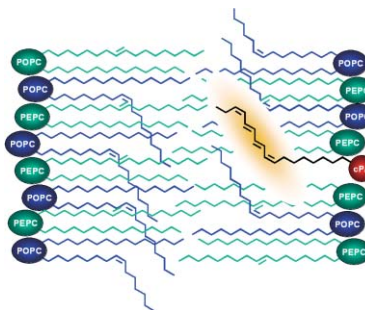


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Probing the influence of *cis*-*trans* isomers on model lipid membrane fluidity using *cis*-parinaric acid and a stop-flow technique

Carla Ferreri,* Silvia Pierotti, Chrysostomos Chatgililoglu, Andrea Barbieri* and Francesco Barigelletti

We describe the development of a stop-flow method using the environment-sensitive fluorescence probe *cis*-parinaric acid for examining the effect of *cis* : *trans* ratios on lipid membrane fluidity/diffusibility.

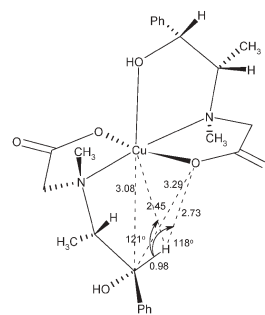


532

Misassigned C-H...Cu agostic interaction in a copper(II) ephedrine derivative is actually a weak, multicentred hydrogen bond

Tejender S. Thakur and Gautam R. Desiraju*

A recently reported 'agostic' interaction is more correctly described as a weak hydrogen bond.

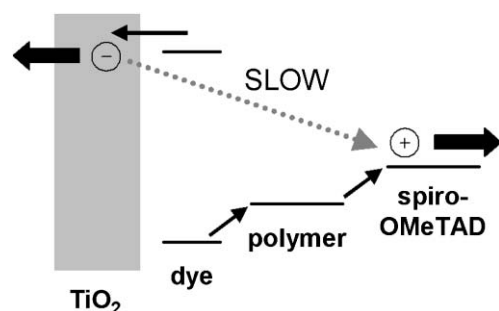


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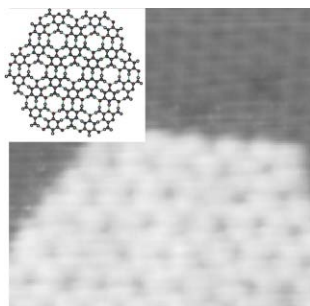
Interface engineering for solid-state dye-sensitised nanocrystalline solar cells: the use of an organic redox cascade

Narukuni Hirata, Jessica E. Kroeze, Taiho Park, David Jones, Saif A. Haque, Andrew B. Holmes* and James R. Durrant*

We demonstrate the formation of a charge transfer cascade at a nanostructured TiO_2 /dye/polymer/molecular hole transport multilayer interface. Charge recombination dynamics at this interface are shown to be retarded when the ionisation potential of the polymer layer exceeds that of the molecular hole transport layer.



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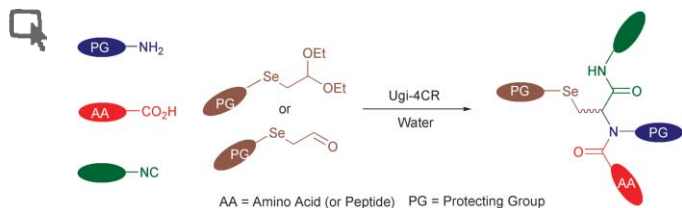


Surface self-assembly of the cyanuric acid–melamine hydrogen bonded network

Luis M. A. Perdigão, Neil R. Champness* and Peter H. Beton*

A hydrogen-bonded bimolecular network formed between cyanuric acid (CA) and melamine (M), CA·M, has been prepared by a surface-based self-assembly process under ultra-high vacuum conditions.

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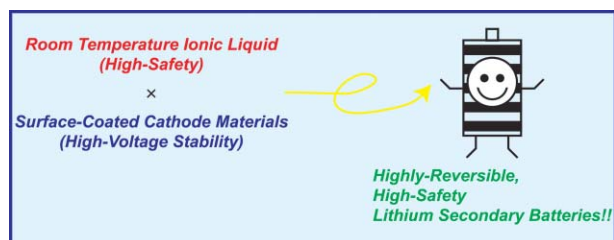


One pot synthesis of selenocysteine containing peptoid libraries by Ugi multicomponent reactions in water

Muhammad Abbas, John Bethke and Ludger A. Wessjohann*

Selenocysteine peptoids—model compounds for selenocysteine peptides and proteins—can be synthesized in one step by combinatorial Ugi multicomponent reactions using a selenoacetal in water or under microwave conditions.

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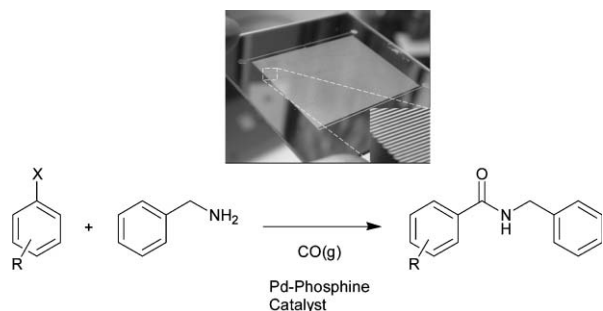


Highly reversible lithium metal secondary battery using a room temperature ionic liquid/lithium salt mixture and a surface-coated cathode active material

Shiro Seki,* Yo Kobayashi, Hajime Miyashiro, Yasutaka Ohno, Akira Usami, Yuichi Mita, Masayoshi Watanabe and Nobuyuki Terada

For realizing high-voltage, high-capacity, long-life and safe rechargeable batteries, a lithium secondary battery that uses high-voltage stable ZrO_2 -coated $LiCoO_2$ cathode and a nonvolatile high-safety rt ionic liquid was fabricated.

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Rapid formation of amides *via* carbonylative coupling reactions using a microfluidic device

Philip W. Miller, Nicholas J. Long, Andrew J. de Mello, Ramon Vilar, Jan Passchier and Antony Gee

For the first time a microstructured device has been used to perform a gas–liquid carbonylation reaction—featuring the Pd-catalysed cross-coupling reaction of arylhalides with benzylamine and CO to rapidly form a range of secondary amides.

549

Mechanistic studies of an unusual epoxide-forming elimination of a β -hydroxyalkyl rhodium porphyrin

Yuan-Zhang Han, Melanie S. Sanford,
Michael D. England and John T. Groves*

A new and remarkably facile sp^3 -C–O bond forming reaction of β -hydroxyalkyl Rh porphyrins to form epoxides has been discovered and its mechanism investigated.

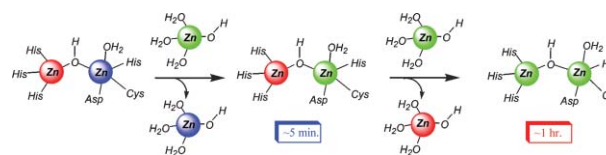


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^{68}Zn isotope exchange experiments reveal an unusual kinetic lability of the metal ions in the di-zinc form of IMP-1 metallo- β -lactamase

Stefan Siemann, Hamid R. Badiei, Vassili Karanassios,
Thammaiah Viswanatha and Gary I. Dmitrienko*

Zinc ions in the β -lactamase IMP-1 resist removal by dialysis but exchange rapidly with exogenous $^{68}\text{Zn}^{2+}$ as detected by ICP MS-based tracer-to-tracee ratio analysis. Exogenous Cd^{2+} exchanges with only one metal ion.

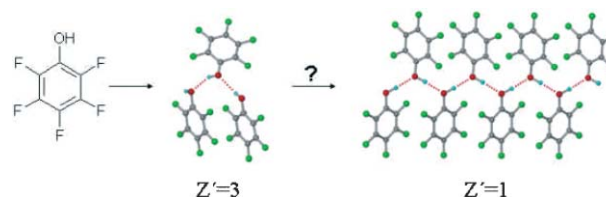


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Synthon evolution and unit cell evolution during crystallisation. A study of symmetry-independent molecules ($Z' > 1$) in crystals of some hydroxy compounds

Dinabandhu Das, Rahul Banerjee, Raju Mondal,
Judith A. K. Howard, Roland Boese and
Gautam R. Desiraju*

A kinetically favoured crystal, with many molecules in the asymmetric unit, may be a fossil relic of the crystal nucleus of a more stable polymorph.

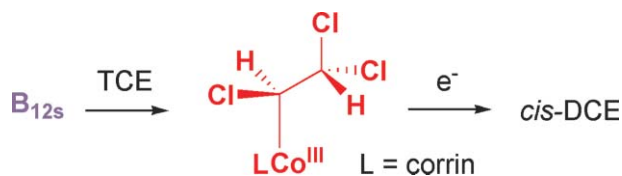


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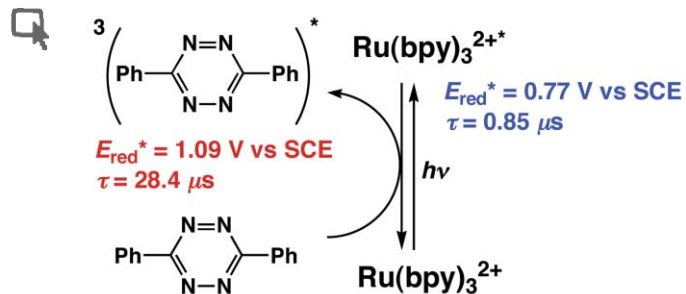
On the role of alkylcobalamins in the vitamin B_{12} -catalyzed reductive dehalogenation of perchloroethylene and trichloroethylene

Derek A. Pratt* and Wilfred A. van der Donk*

An alternative mechanism for the vitamin B_{12} -catalyzed dechlorination of the priority pollutants perchloroethylene and trichloroethylene is proposed. This mechanism involves chlorinated ethylcobalamins as intermediates.



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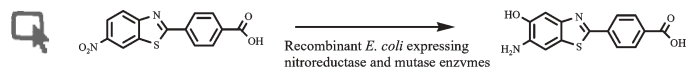


Remarkable oxidizing ability of triplet excited states of tetrazines produced by photosensitization with $\text{Ru}(\text{bpy})_3^{2+}$

Junpei Yuasa and Shunichi Fukuzumi*

An efficient energy transfer from $\text{Ru}(\text{bpy})_3^{2+*}$ (bpy = 2,2'-bipyridine, * denotes the excited state) to tetrazines occurs to yield the triplet excited states of tetrazines, which have much longer lifetimes and higher oxidizing ability as compared with those of $\text{Ru}(\text{bpy})_3^{2+*}$.

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Conversion of 2-(4-carboxyphenyl)-6-nitrobenzothiazole to 4-(6-amino-5-hydroxybenzothiazol-2-yl)benzoic acid by a recombinant *E. coli* strain

Lloyd J. Nadeau, Jim C. Spain,* Ramamurthi Kannan and Loon-Seng Tan

The biological conversion of a complex nitroaromatic compound to the corresponding *o*-aminophenol, a novel synthon of potential use for the production of thermally resistant polymers.

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