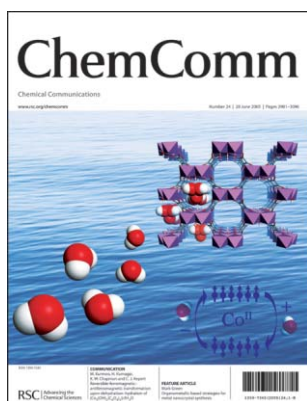


IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (24) 2981-3096 (2005)



Cover

See Mohamedally Kurmoo, Hitoshi Kumagai, Karena W. Chapman and Cameron J. Kepert, page 3012. Reversible ferromagnetic-antiferromagnetic transformation upon dehydration-hydration of the nanoporous coordination framework $[\text{Co}_3(\text{OH})_2(\text{C}_4\text{O}_4)_2] \cdot 3\text{H}_2\text{O}$. Image reproduced by permission of Dr. Mohamedally Kurmoet *et al.* from *Chem. Commun.*, 2005, 3012.



Inside cover

See Andrew M. Beale, Ad M. J. van der Eerden, Kaisa Kervinen, Mark A. Newton and Bert M. Weckhuysen, page 3015. Combined *operando* Raman, UV-Vis and energy dispersive XAFS set-up for studying heterogeneous catalysts at work with an unprecedented time-resolution. Image reproduced by permission of Professor Bert M. Weckhuysen *et al.* from *Chem. Commun.*, 2005, 3015.

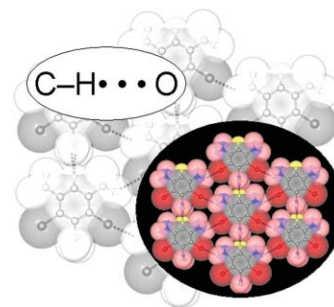
40TH ANNIVERSARY ARTICLE

2995

C-H...O and other weak hydrogen bonds. From crystal engineering to virtual screening

Gautam R. Desiraju

What is a weak hydrogen bond? With hydrogen bonds becoming increasingly important, the special features of the weaker varieties of this interaction are outlined in this review. The C-H...O hydrogen bond is significant not only in the crystal structures of small organic molecules but also in the large biological macromolecules. The spin-off in rational drug design and lead optimisation is highlighted.



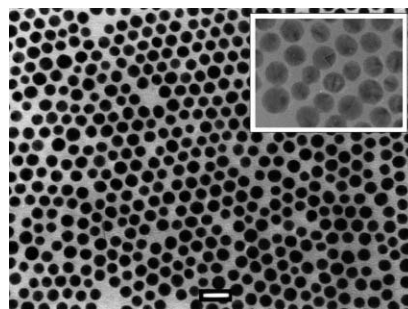
FEATURE ARTICLE

3002

Organometallic based strategies for metal nanocrystal synthesis

Mark Green

Metal nanoparticles are of immense interest due to applications in medicine, magnetic data storage and catalysis. This review covers recent advances in the preparation of high quality metal nanoparticles using organometallic strategies originally designed for the synthesis of semiconductor nanoparticles.



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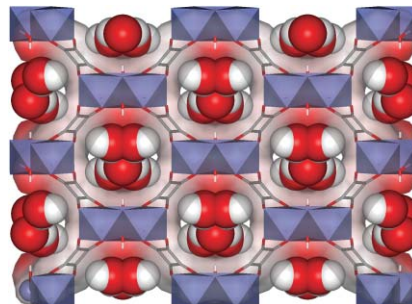
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3012

Reversible ferromagnetic–antiferromagnetic transformation upon dehydration–hydration of the nanoporous coordination framework, $[\text{Co}_3(\text{OH})_2(\text{C}_4\text{O}_4)_2] \cdot 3\text{H}_2\text{O}$

Mohamedally Kurmoo,* Hitoshi Kumagai, Karena W. Chapman and Cameron J. Kepert*

Reversible crystal-to-crystal transformation accompanied by change from ferromagnetic to antiferromagnetic ground states at 8 K upon dehydration–rehydration of the nanoporous coordination framework $[\text{Co}^{\text{II}}_3(\text{OH})_2(\text{C}_4\text{O}_4)_2] \cdot 3\text{H}_2\text{O}$.



3015

Adding a third dimension to operando spectroscopy: a combined UV-Vis, Raman and XAFS setup to study heterogeneous catalysts under working conditions

Andrew M. Beale, Ad M. J. van der Eerden, Kaisa Kervinen, Mark A. Newton and Bert M. Weckhuysen*

A powerful new multi-technique operando setup, which focuses on using millisecond UV-Vis, Raman and XAFS for studying the catalytic behaviour of supported molybdenum oxide catalysts during propane dehydrogenation reactions, is described.

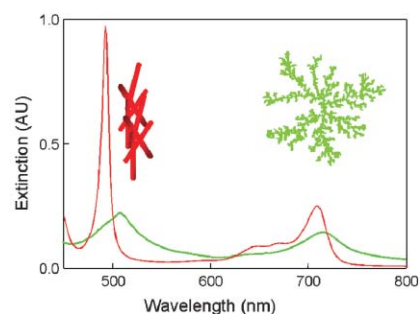


3018

Unusual optical properties of porphyrin fractal J-aggregates

Luigi Monsù Scolaro,* Andrea Romeo, Maria Angela Castriciano and Norberto Micali*

Supramolecular assembling of 5,10,15,20-tetrakis(4-sulfonatophenyl)porphyrin with spermine leads to monodispersed fractal J-aggregates exhibiting peculiar enhancement of scattered light and absorption properties, exploitable for designing non-covalent resonating systems.

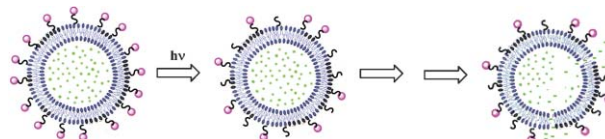


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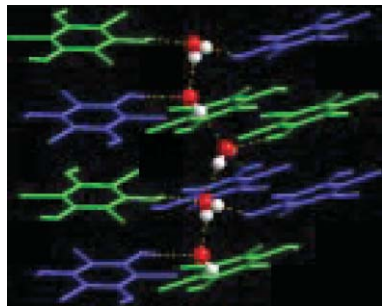
Design of photocleavable lipids and their application in liposomal “uncorking”

Binita Chandra, Sanku Mallik* and D. K. Srivastava*

The design of *o*-nitrobenzyl containing photocleavable lipid–amino acid conjugates, and their application in liposomal uncorking are described.



3024

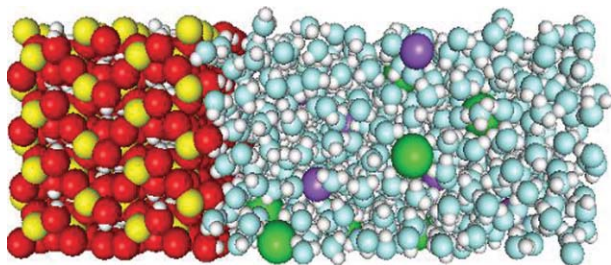


Helical water chains in aquapores of organic hexahost: remarkable halogen-substitution effect on the handedness of water helix

Binoy K. Saha and Ashwini Nangia*

The handedness of water helices in the spiral staircase (green and blue) channels of hexahosts trichlorophloroglucinol and tribromophloroglucinol (shown here) is directed by weak $\text{Cl}\cdots\text{Cl}$ and $\text{Br}\cdots\text{Br}$ interactions.

3027

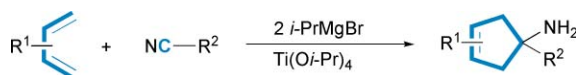


Atomistic simulation of charged iron oxyhydroxide surfaces in contact with aqueous solution

Sebastien Kerisit, David J. Cooke, Arnaud Marmier and Stephen C. Parker*

A snapshot of a longtime scale molecular dynamics simulation of the (100) surface of goethite (α -FeOOH) in contact with a 1.2M aqueous solution of NaCl.

3030

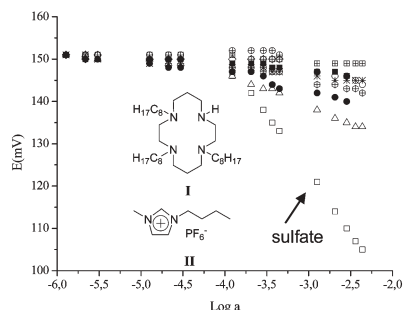


Titanium-mediated [4 + 1] assembly of 1,3-dienes and nitriles: formation of 3-cyclopentenyl amines and cyclopentenones

Christophe Laroche, Philippe Bertus* and Jan Szymoniak*

In the presence of $\text{Ti(O}^i\text{Pr)}_4$ and $^i\text{PrMgCl}$, dienes couple with nitriles to afford the title products in good yields.

3033



Ionic liquids promote selective responses towards the highly hydrophilic anion sulfate in PVC membrane ion-selective electrodes

Carmen Coll, Roberto H. Labrador, Ramón Martínez Mañez,* Juan Soto,* Félix Sancenón, María-Jesús Seguí and Enrique Sanchez

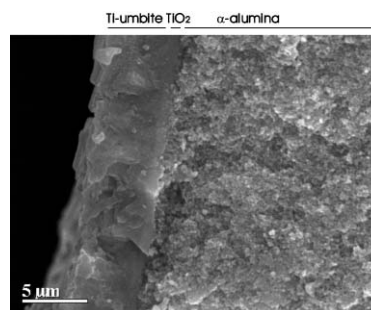
A remarkable enhanced response towards the hydrophilic anion sulfate using plasticized PVC membranes containing the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate and a polyazacycloalkane derivative as ionophore has been found.

3036

A new titanosilicate umbite membrane for the separation of H₂

Víctor Sebastián, Zhi Lin, João Rocha, Carlos Téllez, Jesús Santamaría and Joaquín Coronas*

A new microporous titanosilicate umbite (K₂TiSi₃O₉·H₂O) tubular membrane has been synthesized that can separate H₂/N₂ mixtures (with selectivities as high as 48) even in the presence of water.

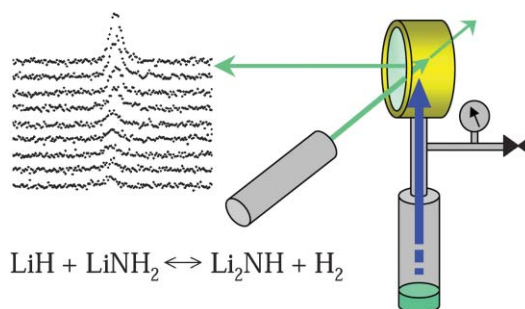


3038

Quantitative estimation of NH₃ partial pressure in H₂ desorbed from the Li–N–H system by Raman spectroscopy

Satoshi Hino, Takayuki Ichikawa,* Norio Ogita, Masayuki Udagawa and Hironobu Fujii

The partial pressure estimated by Raman spectroscopy indicates that ~0.1% NH₃ inevitably contaminates the H₂ desorbed from a mixture of LiH and LiNH₂ in a closed system.

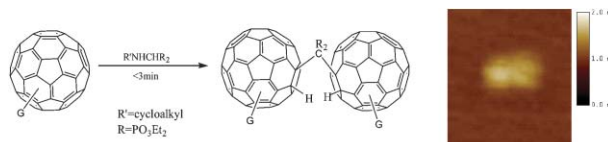


3041

Facile and potent synthesis of carbon bridged fullerene dimers (HC₆₀–CR₂–C₆₀H type)

Juan-Juan Yin, Yu-Guo Li, Bin Li, Wen-Xin Li,* Li-Mei Jin, Jin-Ming Zhou and Qing-Yun Chen*

Novel carbon bridged fullerene dimers (HC₆₀–CR₂–C₆₀H type) are obtained in high yield by the reaction of aminomethylenebis(phosphonate) anions with [60]fullerene. A single dimer molecule is observed clearly using AFM.

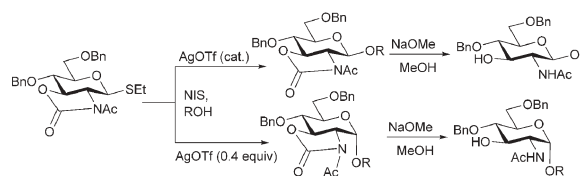


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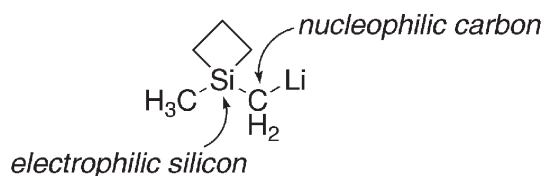
Ethyl 2-acetamido-4,6-di-O-benzyl-2,3-N,O-carbonyl-2-deoxy-1-thio-β-D-glycopyranoside as a versatile GlcNAc donor

Mike Boysen, Emiliano Gemma, Martina Lahmann and Stefan Oscarson*

By simply changing the amount of AgOTf added in NIS-promoted glycosylations with the title donor either the α- or the β-linked glycoside is produced in high yields.



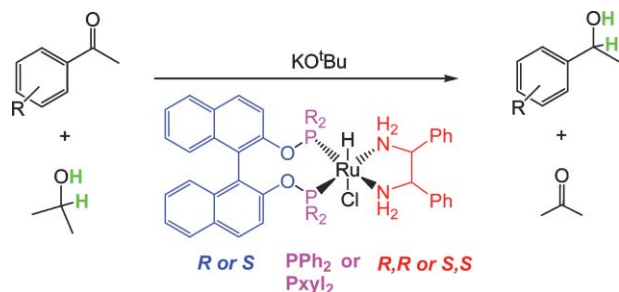
3047

**Siletanymethyl lithium: an ambiphilic organosilane**

Mariya V. Kozytska and Gregory B. Dudley*

Siletanymethyl lithium displays centres of both electrophilicity and nucleophilicity, leading to interesting chemical reactivity.

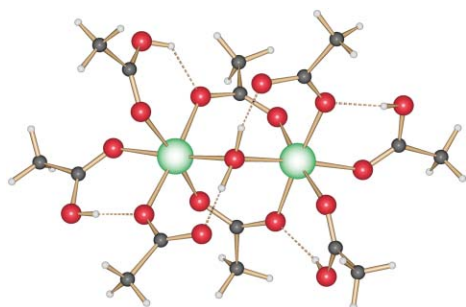
3050

**A modular design of ruthenium catalysts with diamine and BINOL-derived phosphinite ligands that are enantiomerically-matched for the effective asymmetric transfer hydrogenation of simple ketones**

Rongwei Guo, Christian Elpelt, Xuanhua Chen, Datong Song and Robert H. Morris*

A series of modular ruthenium complexes with diamine and readily-prepared phosphinite ligands are precatalysts for the asymmetric transfer hydrogenation of simple ketones to give chiral alcohols in good yield and enantioselectivity.

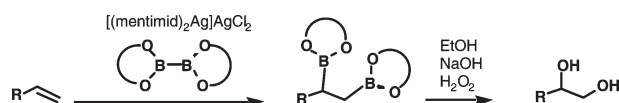
3053

**Theoretical studies on di- and tetra-nuclear Ni pivalate complexes**

Gopalan Rajaraman,* Kirsten E. Christensen, Finn K. Larsen, Grigore A. Timco and R. E. P. Winpenny*

Combined magnetic–DFT studies have been used to obtain good numerical estimates of *J* and *D* in di- and tetra-nuclear Ni pivalate clusters. Results show that the procedure can be used to obtain structural information concerning the H-bonding and solvation of clusters.

3056

**Unprecedented use of silver(I) N-heterocyclic carbene complexes for the catalytic preparation of 1,2-bis(boronate) esters**

Jesus Ramírez, Rosa Corberán, Mercedes Sanaú, Eduardo Peris* and Elena Fernandez*

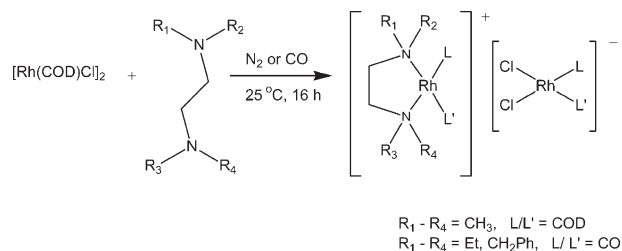
A novelty has been introduced in the scope of the catalytic diboration reaction using thermally and air-stable Ag(I)–N-heterocyclic carbene complexes as catalytic systems.

3059

Ionic diamine rhodium(I) complexes—highly active catalysts for the hydroformylation of olefins

Jai Jun Kim and Howard Alper*

Ionic diamine rhodium(I) complexes are able to catalyze the hydroformylation reaction under mild reaction conditions in excellent activity and regioselectivity, and in the absence of a phosphorus ligand.

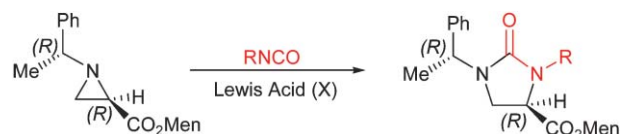


3062

Lewis acid-catalyzed stereospecific ring expansion of aziridine-2-carboxylates to imidazolidin-2-ones

Min Sung Kim, Yong-Woo Kim, Heung Sik Hahm, Jae Won Jang, Won Koo Lee* and Hyun-Joon Ha*

Lewis acid-catalyzed ring expansion reaction of chiral aziridine-2-carboxylate proceeds regio- and stereoselectively to yield enantiomerically pure 4-functionalized imidazolidin-2-ones in high yields.

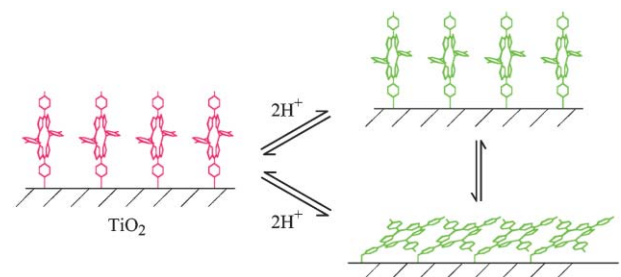


3065

pH-Dependent reversible transformation of TPPS₄ anchored on mesoporous TiO₂ film between monomers and J-aggregates

Yusuke Fujii, Yasuchika Hasegawa, Shozo Yanagida and Yuji Wada*

The arrangement of TPPS₄ molecules fixed on mesoporous TiO₂ film as a monolayer can be changed reversibly depending on the pH value of the surrounding water.

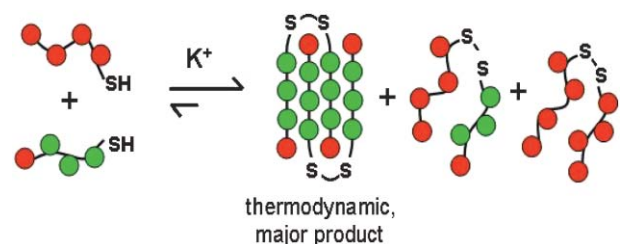


3068

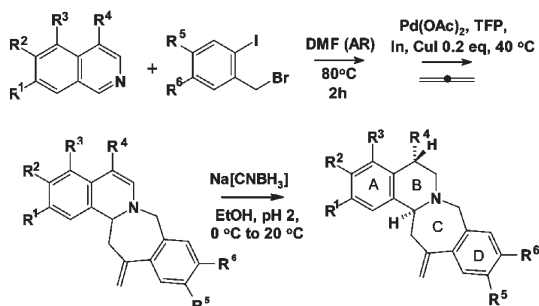
Dynamic covalent chemistry on self-templating PNA oligomers: formation of a bimolecular PNA quadruplex

Yamuna Krishnan-Ghosh, Andrew M. Whitney and Shankar Balasubramanian*

The tetramolecular PNA quadruplex motif has been probed using a dynamic covalent chemistry (DCC) approach to create and characterize a bimolecular PNA quadruplex.



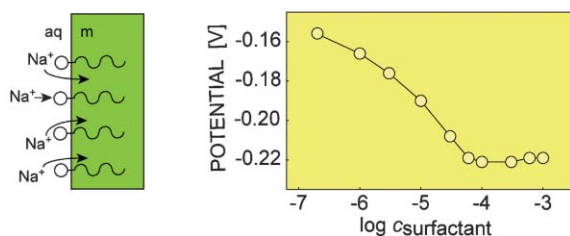
3071

**Bimetallic catalytic synthesis of annelated benzazepines**

Laura A. T. Cleghorn, Ronald Grigg,* Colin Kilner, William S. MacLachlan and Visvanthar Sridharan

A novel short synthetic route to annelated benzazepines tolerating a variety of substituents in the A, B and D rings has been developed using additive enhanced Pd/In catalytic three-component cascade methodology where isoquinolines, pyridines and β -carbolines can be utilised as the annelation partners.

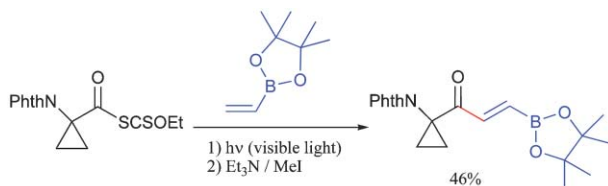
3074

ION DIFFUSION HINDRANCE**Reversible electrochemical monitoring of surface confined reactions at liquid–liquid interfaces by modulation of ion transfer fluxes**

Yida Xu, Roland De Marco, Alexey Shvarev and Eric Bakker*

The adsorption of the neutral surfactant Brij35 at a liquid–liquid interface is reversibly monitored *via* its disturbance of an electrochemically imposed ion flux across the interface, forming a promising experimental tool for the detection of surface confined reactions at such liquids and polymers.

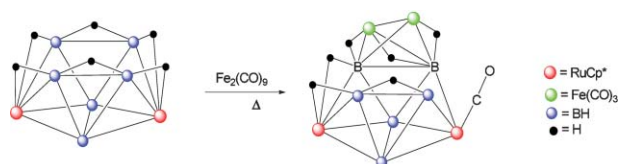
3077

**A convergent approach to γ -carbonyl vinyl boronates**

Markus R. Heinrich, Lisa A. Sharp and Samir Z. Zard*

γ -Carbonyl vinyl boronates can be prepared by a visible light induced radical chain addition of an *S*-acyl dithiocarbonate (xanthate) to the pinacol ester of vinyl boronic acid, followed by treatment with base.

3080

**Condensed metallaborane clusters: synthesis and structure of $\text{Fe}_2(\text{CO})_6(\eta^5\text{-C}_5\text{Me}_5\text{RuCO})(\eta^5\text{-C}_5\text{Me}_5\text{Ru})\text{B}_6\text{H}_{10}$**

Sundargopal Ghosh,* Thomas P. Fehlner and Bruce C. Noll

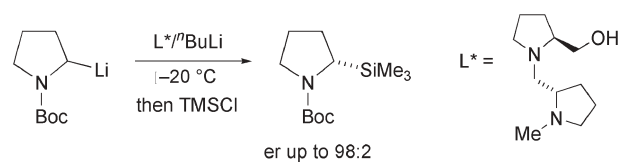
A novel class of hybrid multiple cluster $\text{Fe}_2(\text{CO})_6(\eta^5\text{-C}_5\text{Me}_5\text{RuCO})(\eta^5\text{-C}_5\text{Me}_5\text{Ru})\text{B}_6\text{H}_{10}$ is synthesized from an edge sharing condensation of $(\eta^5\text{-C}_5\text{Me}_5\text{Ru})_2\text{B}_6\text{H}_{12}$ and $\text{Fe}_2(\text{CO})_9$, in which a Fe_2B_2 tetrahedron has been fused to a ruthenaborane substrate.

3083

Dynamic kinetic resolution of *N*-Boc-2-lithiopyrrolidine

Iain Coldham,* Jignesh J. Patel and Graciela Sanchez-Jimenez

The two interconverting diastereomeric complexes of the chiral organolithium derived from *N*-Boc-pyrrolidine and a chiral ligand react at different rates, allowing a dynamic kinetic resolution.

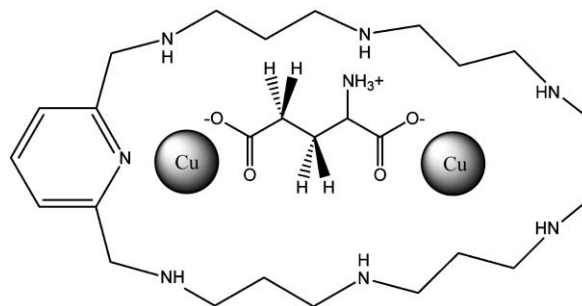


3086

Binuclear Cu^{2+} complex mediated discrimination between L-glutamate and L-aspartate in water

Begoña Verdejo, Juan Aguilar, Antonio Doménech, Carlos Miranda, Pilar Navarro, Hermás R. Jiménez, Conxa Soriano and Enrique García-España*

L-Glutamate and L-aspartate selectivity is achieved by the action of two Cu^{2+} metal ions rightly disposed in a cyclophane-type macrocyclic framework.

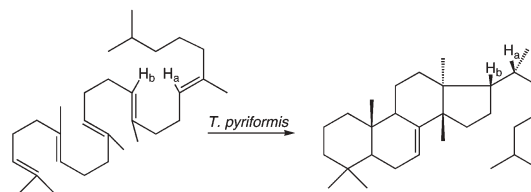


3089

Detection of 1,2-hydride shifts in the formation of euph-7-ene by the squalene–tetrahymanol cyclase of *Tetrahymena pyriformis*

José-Luis Giner, Stefano Rocchetti, Serge Neunlist, Michel Rohmer and Duilio Arigoni*

Incubation of samples of 2,3-dihydrosqualene, specifically labeled with deuterium at either carbon position 7 or 11, with an enzyme extract from *Tetrahymena pyriformis*, containing a squalene–tetrahymanol cyclase, provided specimens of euph-7-ene displaying deuterium patterns consistent with the biosynthetic operation of two consecutive 1,2-hydride shifts.

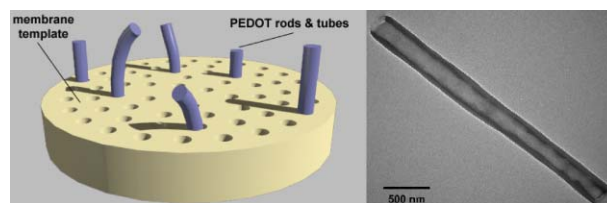


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1-Dimensional structures of poly(3,4-ethylenedioxythiophene) (PEDOT): a chemical route to tubes, rods, thimbles, and belts

Moon Gyu Han and Stephen H. Foulger*

The chemical synthesis of 1-dimensional (1-D) PEDOT nanostructures in the form of tubes, rods, thimbles, and belts has been successfully accomplished through the use of a “hard template”. The synthesis of these structures occurred in an aqueous solution using an Al_2O_3 membrane as a template and FeCl_3 as an oxidant–dopant for the system.




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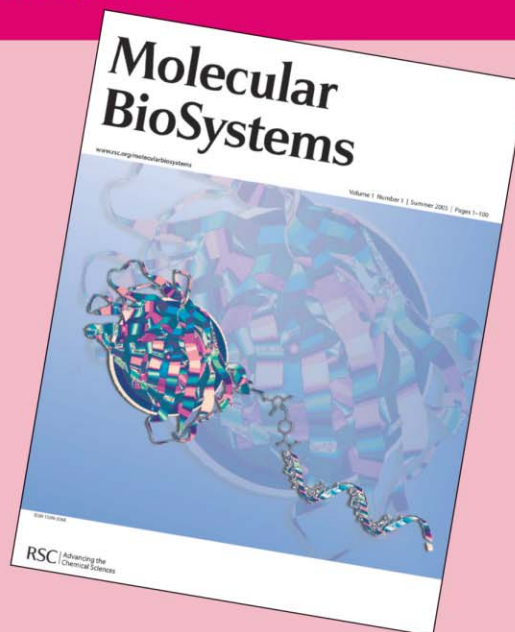
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