

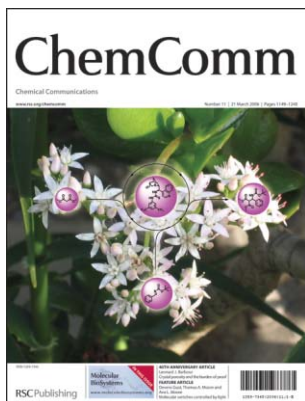
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IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (11) 1149–1240 (2006)



Cover

See Darren J. Dixon *et al.*, page 1191. A derivative of cinchonine, a compound found in the bark of the South American cinchona tree, can be used as an effective organocatalyst for the selective synthesis of β -amino acid derivatives. Image reproduced by permission of A. Louise Tillman, Jinxing Ye and Darren J. Dixon, from *Chem. Commun.*, 2006, 1191.



Inside cover

See Leroy Cronin *et al.*, page 1194. A five-step one-pot reaction leading to a new family of heterocyclic compounds with novel physical properties and the ability to bind to DNA has been discovered. Image reproduced by permission of Alexis D. C. Parenty, Kevin M. Guthrie, Yu-Fei Song, Louise V. Smith, Eric Burkholder and Leroy Cronin, from *Chem. Commun.*, 2006, 1194.

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.

Chemical Science

March 2006/Volume 3/Issue 3

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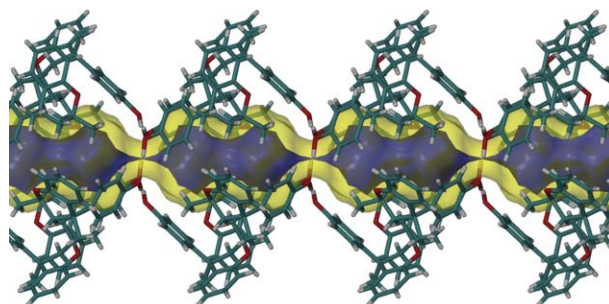
40TH ANNIVERSARY ARTICLE

1163

Crystal porosity and the burden of proof

Leonard J. Barbour

The study of porosity in the context of crystal engineering is rapidly growing in intensity. However, claims of porosity are often highly subjective and use of the term "porous" is susceptible to abuse. This contribution discusses some of the criteria to be considered when stating that a particular crystal structure is porous.



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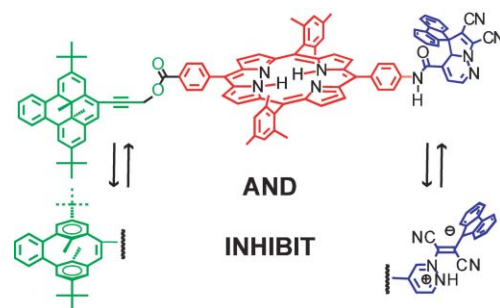
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Molecular switches controlled by light

Devens Gust, Thomas A. Moore and Ana L. Moore

Electron and energy transfer in covalently linked multichromophoric systems may be switched on or off by photoisomerization of attached photochromes, permitting the preparation of molecular switches and Boolean logic gates.



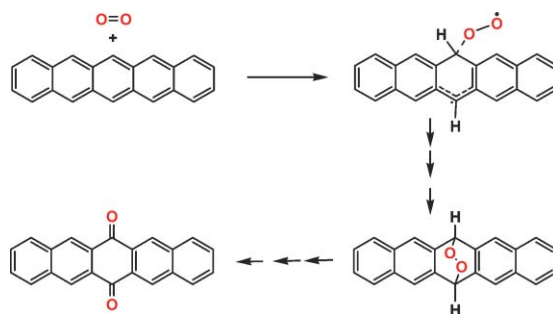
COMMUNICATIONS

1179

Diels–Alder reaction of acenes with singlet and triplet oxygen – theoretical study of two-state reactivity

A. Ravikumar Reddy and Michael Bendikov*

An interesting change in mechanism (from concerted to biradical) is described for the reaction of acenes (benzene through pentacene) with molecular oxygen (either singlet oxygen, $^1\Delta_g\text{-O}_2$, or triplet oxygen, $^3\Sigma_g^-\text{-O}_2$).

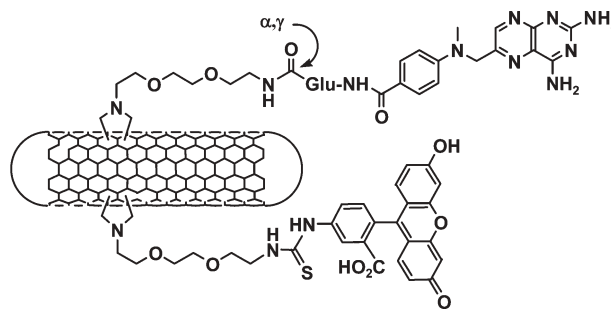


1182

Double functionalisation of carbon nanotubes for multimodal drug delivery

Giorgia Pastorin, Wei Wu, Sébastien Wieckowski, Jean-Paul Briand, Kostas Kostarelos, Maurizio Prato* and Alberto Bianco*

Carbon nanotubes can be doubly functionalised *via* 1,3-dipolar cycloaddition of azomethine ylides with orthogonally protected amino functions that can be selectively modified with different types of drugs and fluorescent probes.

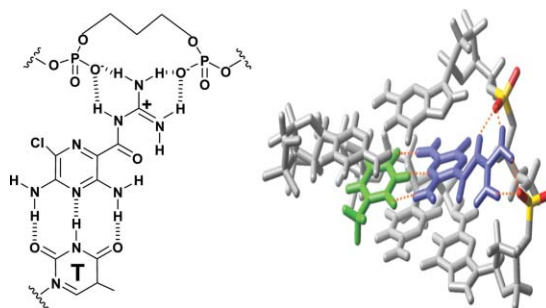


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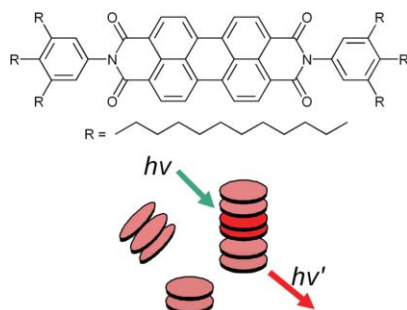
Strong and selective binding of amiloride to thymine base opposite AP sites in DNA duplexes: simultaneous binding to DNA phosphate backbone

Chunxia Zhao, Qing Dai, Takehiro Seino, Ying-Yu Cui, Seiichi Nishizawa and Norio Teramae*

Due to two sets of hydrogen-bond forming sites suitable for target nucleotides and the phosphodiester DNA backbone, amiloride can recognize a thymine opposite an abasic site in DNA duplexes with high selectivity and affinity.



1188

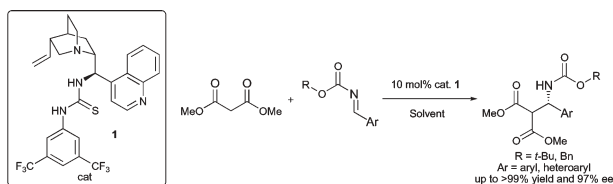


One-dimensional luminescent nanoaggregates of perylene bisimides

Frank Würthner,* Zhijian Chen, Volker Dehm and Vladimir Stepanenko

A new perylene bisimide dye has been synthesized which self-assembles into columnar nanoaggregates and liquid crystalline mesophases with striking photoluminescent properties.

1191

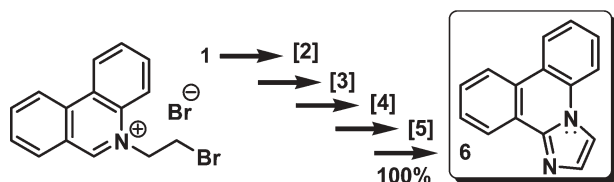


Direct enantio- and diastereoselective Mannich reactions of malonate and β -keto esters with *N*-Boc and *N*-Cbz aldimines catalysed by a bifunctional cinchonine derivative

A. Louise Tillman, Jinxing Ye and Darren J. Dixon*

A highly enantioselective Mannich reaction between malonate esters and *N*-Boc and *N*-Cbz aldimines, catalysed by a bifunctional cinchonine derivative, has been developed.

1194

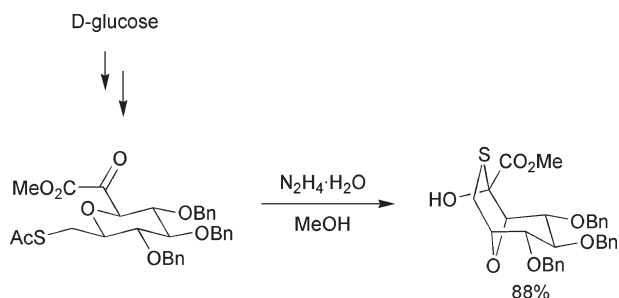


Discovery of an imidazo-phenanthridine synthon produced in a 'five-step one-pot reaction' leading to a new family of heterocycles with novel physical properties

Alexis D. C. Parenty, Kevin M. Guthrie, Yu-Fei Song, Louise V. Smith, Eric Burkholder and Leroy Cronin*

A new class of heterocyclic aromatic cation with novel physical properties has been constructed by an unprecedented reaction pathway that proceeds *via* five spontaneous steps to yield a 'synthon' that can be further derivatised by a final nucleophilic substitution step.

1197



Synthesis of the bicyclic core of tagetitoxin

Julien R. H. Plet and Michael J. Porter*

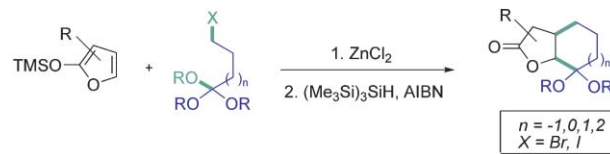
Synthesis of the core bicyclic skeleton of the RNA polymerase III inhibitor tagetitoxin has been achieved in an efficient manner from D-glucose; the unmasking of a primary thiol in the presence of an electrophilic α -ketoester, resulting in spontaneous cyclisation, is the final step.

1200

Stereoselective synthesis of bicyclic lactones by annelation with functionalised orthoesters

Nuno Maulide and István E. Markó*

Clipping molecules together: a highly stereoselective two-step annelation of functionalised orthoesters with trimethylsilyloxyfuran derivatives, which delivers suitably decorated bicyclo[3.n.0]lactones in high overall yields, is reported.

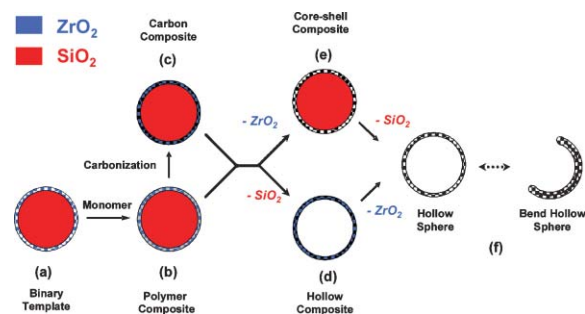


1203

A versatile method for the production of monodisperse spherical particles and hollow particles: Templating from binary core-shell structures

Pablo Maximiliano Arnal, Ferdi Schüth and Freddy Kleitz

Using the porosity of a binary exotemplate opens a new pathway to produce hybrid core-shell spheres, composite hollow spheres, and porous hollow spheres.

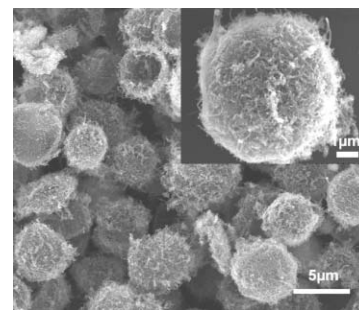


1206

Porous hollow carbon nanotube composite cages

Lijun Ji, Jin Ma, Chungui Zhao, Wei Wei, Lijun Ji, Xiaocong Wang, Mingshu Yang, Yunfeng Lu* and Zhenzhong Yang*

Mechanically robust, hollow carbon nanotube composite spheres that are permeable to large chemical species were prepared by a layer-by-layer assembly and templating technique.

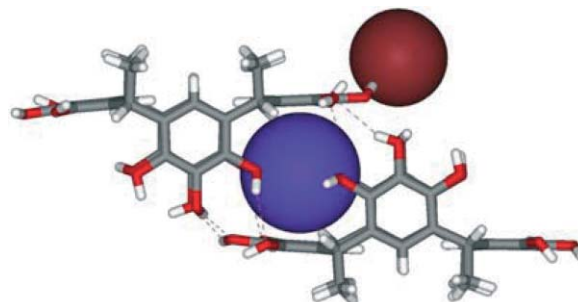


1209

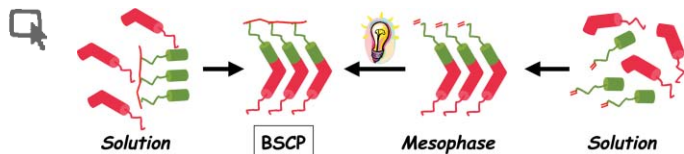
Pyrogallarenes as alkali metal receptors: the role of cation- π interactions in complexation

Antti Åhman and Maija Nissinen*

Crystallization of *C*-methyl pyrogallarene with alkali metal halides resulted in complexes in which alkali metal cations are η^6 coordinated to aromatic rings *via* strong cation- π interactions, showing pyrogallarenes to be novel receptors for alkali metals.



1212

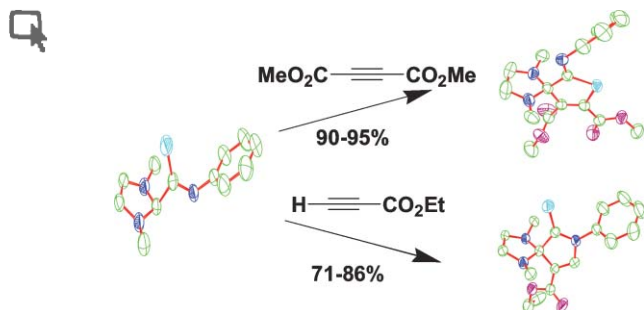


Self-assembled bent-core side-chain liquid crystalline polymers

Joaquín Barberá, Nélica Gimeno, Inmaculada Pintre, M. Blanca Ros* and José Luis Serrano

The versatility of non-covalent polymers could be extended to bent-core mesogenic materials. The synthesis of H-bonded side-chain liquid crystal polymers carried out by two alternative synthetic routes and their properties are reported.

1215

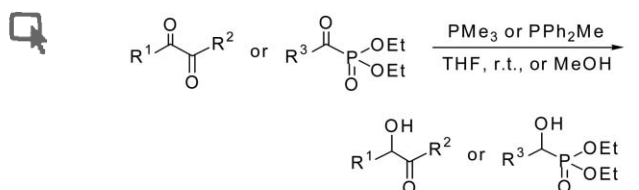


A *N*-heterocyclic carbene derived highly regioselective ambident C–C–S and C–C–N 1,3-dipolar system

Mei-Fang Liu, Bo Wang and Ying Cheng*

2-Thiocarbamoyl benzimidazolium and imidazolium inner salts are a unique ambident C–C–S and C–C–N 1,3-dipolar system able to undergo highly efficient and regioselective cycloaddition with dimethyl acetylenedicarboxylate and ethyl propiolate to furnish, respectively, spiro[imidazole-2,3'-thiophene] and spiro[imidazole-2,3'-pyrrole] derivatives in good to excellent yields.

1218



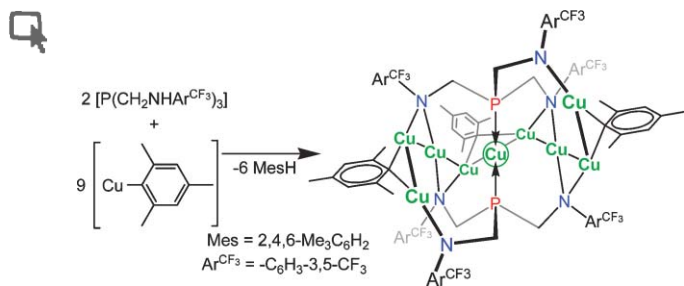
R¹ = aryl, alkyl, alkenyl, COOEt; R² = OMe, OEt, phenyl
R³ = phenyl, cinnamonyl

Reduction of activated carbonyl groups by alkyl phosphines: formation of α -hydroxy esters and ketones

Wen Zhang and Min Shi*

Reduction of activated carbonyl groups such as α -keto esters, benzils, 1,2-cyclohexanedione, and α -ketophosphonates by alkyl phosphines afforded the corresponding α -hydroxy esters or ketones in good to excellent yields in THF at room temperature. The mechanism of the proton transfer and intramolecular hydrolysis has been studied on the basis of deuterium and ¹⁸O labeling experiments.

1221



Facile assembly of a Cu₉ amido complex: a new tripodal ligand design that promotes transition metal cluster formation

Alana L. Keen, Meghan Doster, Hua Han and Samuel A. Johnson*

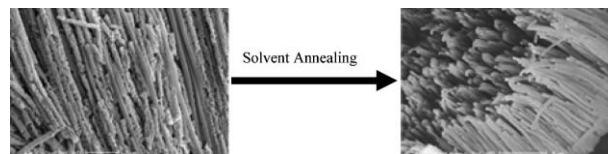
A tripodal amido ligand with a central non-chelating phosphorus donor allows for the facile assembly of a pentane soluble organometallic copper cluster with a central copper atom surrounded by a nonplanar chain of eight copper atoms and two terminal amido-copper bonds.

1224

General method for the synthesis of crystalline organic nanorods using porous alumina templates

Rabih O. Al-Kaysi and Christopher J. Bardeen*

Crystalline nanorods composed of a variety of conjugated organic molecules were synthesized using an anodized alumina template and solvent annealing.

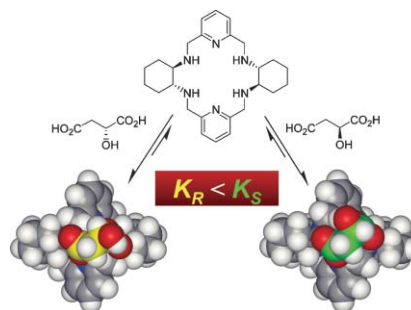


1227

A highly enantioselective abiotic receptor for malate dianion in aqueous solution

Almudena González-Álvarez, Ignacio Alfonso,* Pilar Díaz, Enrique García-España and Vicente Gotor*

The highly enantioselective molecular recognition of the malate dianion by a synthetic receptor in aqueous solution has been studied by potentiometric titrations, mass spectrometry (ESI-MS), diffusion measurements (PGSE NMR) and molecular modeling.

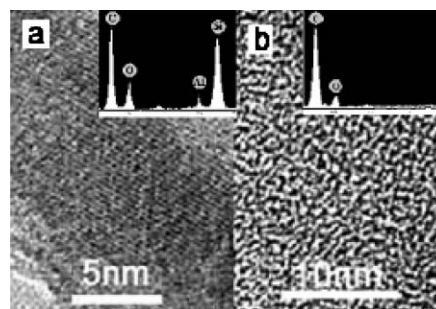


1230

A novel carbon/ZSM-5 nanocomposite membrane with high performance for oxygen/nitrogen separation

Qingling Liu, Tonghua Wang,* Jieshan Qiu* and Yiming Cao

A novel carbon/ZSM-5 nanocomposite membrane is successfully prepared by incorporating nano-sized ZSM-5 into polymeric precursor (polyimide), which shows excellent permselectivities for separation of oxygen/nitrogen gas pairs.

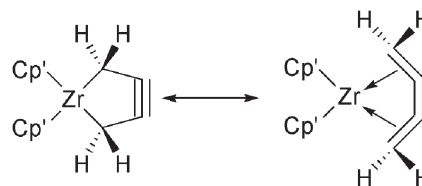


1233

An experimental electron density study on “1-zirconacyclopent-3-yne”

Daisuke Hashizume,* Noriyuki Suzuki and Teiji Chihara

The bonding nature of the cyclopentyne moiety in 1-zirconacyclopent-3-yne, the smallest cycloalkyne ring ever isolated, is clarified as a resonance hybrid between η^2 - σ , σ -coordination, the major contributor, and η^4 - π , π -coordination.



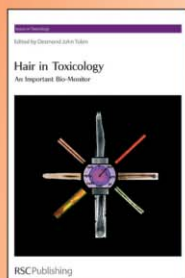
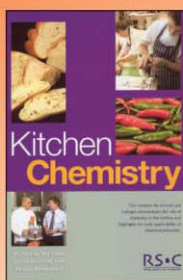
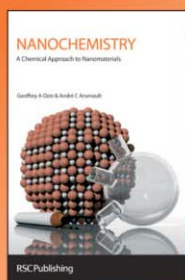
1236



GaCl₃-assisted [2 + 3] cycloaddition: A route to tetrazaphospholes

Alexander Villinger, Peter Mayer and Axel Schulz*

The GaCl₃-stabilized tetrazaphosphole 1-(2,4,6-tri-*tert*-butylphenyl)tetrazaphosphole was prepared in a simple, high yielding synthetic procedure, fully characterized and shown to be unstable at ambient temperature; a formal GaCl₃-assisted [2 + 3] cycloaddition mechanism is discussed.



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