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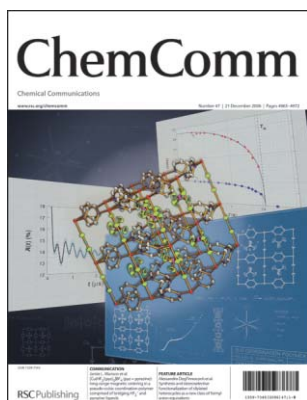
Chemical Communications

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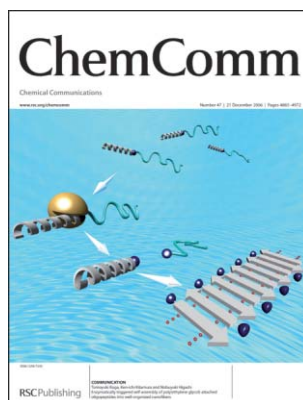
IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (47) 4865-4972 (2006)



Cover

See J. L. Manson *et al.*, page 4894.
[Cu(HF₂)(pyz)₂]BF₄ is a thermally robust coordination polymer comprised of bifluoride and pyrazine linkages that antiferromagnetically orders at low temperature. Image reproduced by permission of Jamie L. Manson, Marianne M. Conner, John A. Schlueter, Tom Lancaster, Stephen J. Blundell, Michael L. Brooks, Francis L. Pratt, Thomas Papageorgiou, Andreas D. Bianchi, Jochen Wosnitza and Myung-Hwan Whangbo from *Chem. Commun.*, 2006, 4894.



Inside cover

See N. Higashi *et al.*, page 4897. Enzymatically triggered self-assembly of poly(ethylene glycol)-attached oligopeptide into well-organized beta-sheet nanofibers. Image reproduced by permission of Tomoyuki Koga, Ken-ichi Kitamura and Nobuyuki Higashi from *Chem. Commun.*, 2006, 4897.

CHEMICAL SCIENCE

C89

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

December 2006/Volume 3/Issue 12

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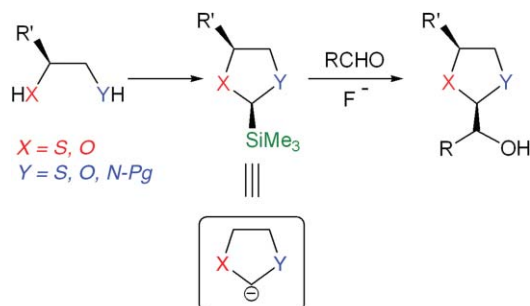
FEATURE ARTICLE

4881

Synthesis and stereoselective functionalization of silylated heterocycles as a new class of formyl anion equivalents

Alessandro Degl'Innocenti,* Salvatore Pollicino and Antonella Capperucci

Fluoride ion induced reactivity of silyl dithiolanes, oxathiolanes, dioxolanes, thiazolidines and oxazolidines, obtained through a novel general protocol, leads to their stereoselective functionalization, thus disclosing new classes of formyl and acyl anion synthons.



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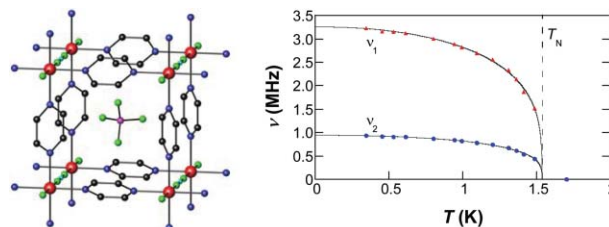
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4894

[Cu(HF₂)(pyz)₂]BF₄ (pyz = pyrazine): long-range magnetic ordering in a pseudo-cubic coordination polymer comprised of bridging HF₂⁻ and pyrazine ligands

Jamie L. Manson,* Marianne M. Conner, John A. Schlueter, Tom Lancaster, Stephen J. Blundell, Michael L. Brooks, Francis L. Pratt, Thomas Papageorgiou, Andreas D. Bianchi, Jochen Wosnitza and Myung-Hwan Whangbo

[Cu(HF₂)(pyz)₂]BF₄ is a pseudo-cubic antiferromagnet consisting of bridging pyrazine and HF₂⁻ which undergoes a transition to long-range magnetic ordering below $T_N = 1.54(1)$ K.

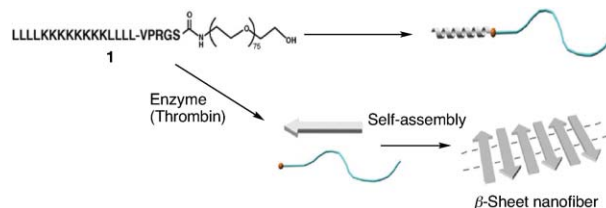


4897

Enzymatically triggered self-assembly of poly(ethylene glycol)-attached oligopeptides into well-organized nanofibers

Tomoyuki Koga, Ken-ichi Kitamura and Nobuyuki Higashi*

A unique and programmable peptide self-assembling system has been fabricated by using poly(ethylene glycol)-attached amphiphilic oligopeptide, which shows rapid self-assembly into well-organized β -sheet nanofibers in response to an enzymatic reaction.

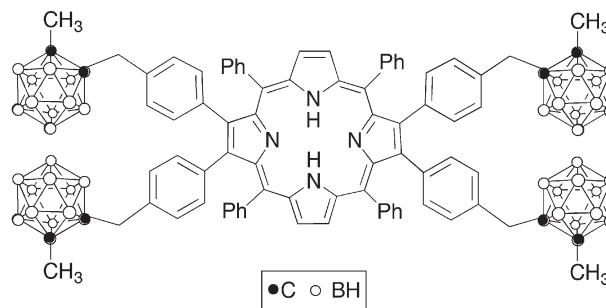


4900

Carborane functionalized pyrroles and porphyrins via the Suzuki cross-coupling reaction

Erhong Hao, Frank R. Fronczek and M. Graça H. Vicente*

The expeditious synthesis of carborane-substituted pyrroles and porphyrins from readily available starting materials is described.

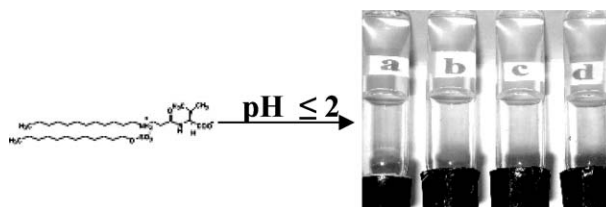


4903

A supramolecular hydrogel that responds to biologically relevant stimuli

Dibyendu Khatua, Rabindranath Maiti and Joykrishna Dey*

First demonstration of heat and pH-responsive hydrogel of SDS and a zwitterionic amphiphile, sodium *N*-(*n*-dodecyl-2-aminoethanoyl)-*L*-valinate with very low minimum gelation concentration.



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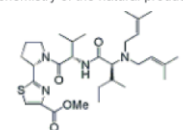
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Z. Chen; T. Ye*
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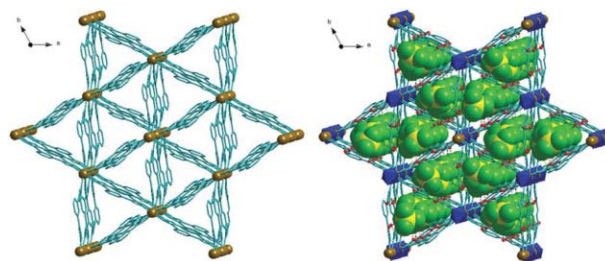
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4906

A novel 3D porous metal–organic framework based on trinuclear cadmium clusters as a promising luminescent material exhibiting tunable emissions between UV and visible wavelengths

Yong-Quan Huang, Bin Ding, Hai-Bin Song, Bin Zhao, Peng Ren, Peng Cheng,* Hong-Gen Wang, Dai-Zheng Liao and Shi-Ping Yan

The emission wavelength can be tuned by controlling the number of guest molecules.

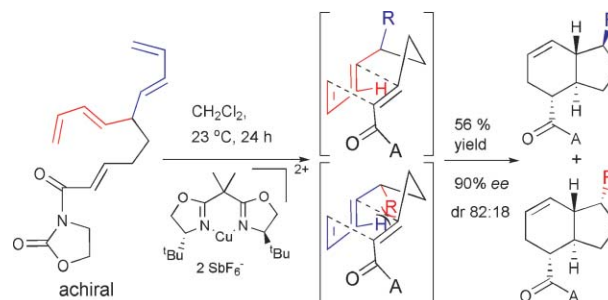


4909

An enantioselective desymmetrisation approach to C9-substituted *trans*-hydrindene rings based on a diastereotopic group-selective intramolecular Diels–Alder reaction

Nadia Azzi, Ed Griffen, Mark Light and Bruno Linclau*

An achiral skipped bis(1,3-diene) substrate was shown to undergo an enantioselective, diastereotopic group-selective, intramolecular Diels–Alder reaction to afford a substituted *trans*-hydrindene ring.

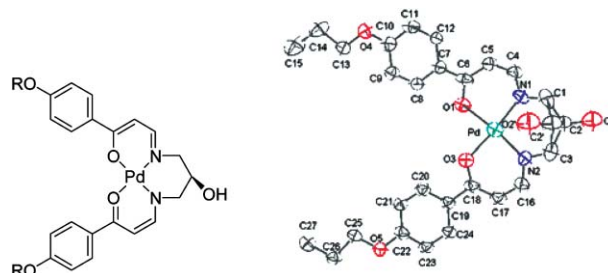


4912

Supramolecular metallomesogens. Self-organization of an H-bonded tetrameric assembly into columnar phase from single component

Yueh-Ju Wang, Jian-Hong Song, Yu-Siang Lin, Ching Lin, Hwo-Shuenn Sheu, Gene-Hsiang Lee and Chung K. Lai*

Supramolecular metallomesogens exhibiting columnar phases are generated by self-organization of a tetrameric H-bonded assembly from palladium complexes.

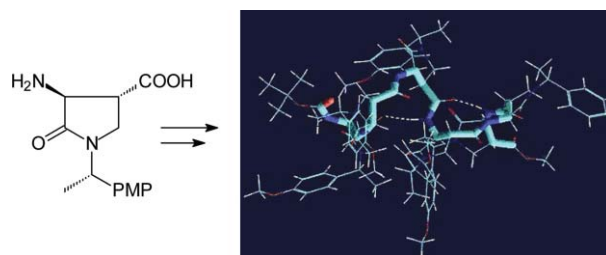


4915

Synthesis and structural characterisation as 12-helix of the hexamer of a β -amino acid tethered to a pyrrolidin-2-one ring

Ileana Menegazzo, Alexander Fries, Stefano Mammi,* Roberta Galeazzi, Gianluca Martelli, Mario Orena* and Samuele Rinaldi

Starting from (3*S*,4*R*,1'*S*)-3-amino-2-oxo-1-[1'-(4-methoxyphenylethyl)]pyrrolidinecarboxylic acid, a new β -foldamer containing pyrrolidin-2-one rings was obtained, having a 12-helix conformation.



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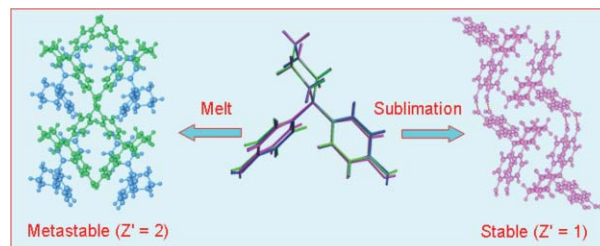
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4918

Polymorphs of 1,1-bis(4-hydroxyphenyl)cyclohexane and multiple Z' crystal structures by melt and sublimation crystallization

Bipul Sarma, Saikat Roy and Ashwini Nangia*

Solvent-free methods of melt and sublimation crystallization afforded polymorphs of the pure title host in which packing conflicts in the metastable $Z' = 2$ crystal structure are resolved in the stable $Z' = 1$ form.

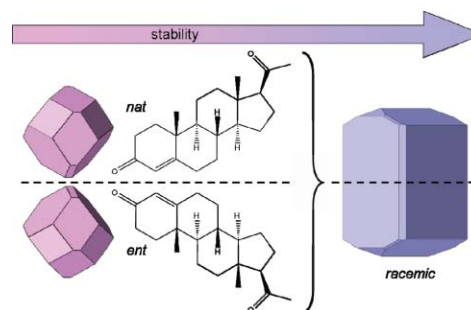


4921

Racemic progesterone: predicted *in silico* and produced in the solid state

Robert W. Lancaster, Panagiotis G. Karamertzanis, Ashley T. Hulme, Derek A. Tocher, Douglas F. Covey and Sarah L. Price*

A computational prediction that mixing the synthetic mirror image of progesterone with its natural form would produce a specific racemic crystal structure was validated.

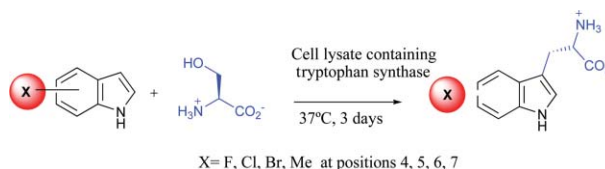


4924

A convenient enzymatic synthesis of L-halotryptophans

Rebecca J. M. Goss* and Philip L. A. Newill

A general, scalable, one-step synthesis of halo and methyl tryptophans, using a readily prepared cell-free extract.

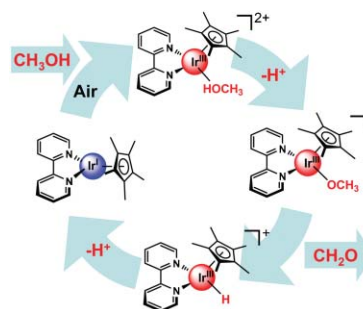


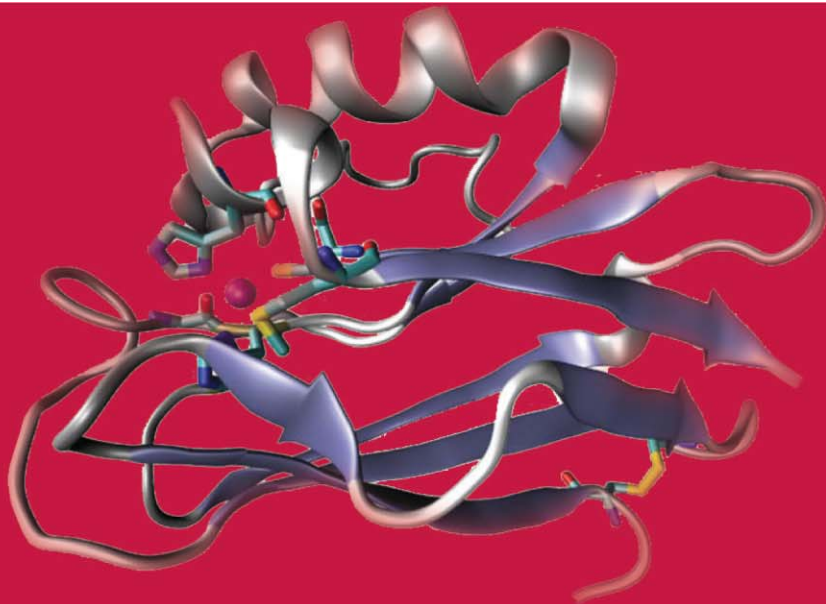
4926

Acidic iridium hydrides: Implications for aerobic and Oppenauer oxidation of alcohols

Anders Gabrielsson,* Piet van Leeuwen and Wolfgang Kaim

Two common iridium based transfer hydrogenation catalysts are also active towards the aerobic oxidation of alcohols under basic conditions. The catalytic cycle involves a highly oxygen sensitive iridium(I) complex obtained by deprotonation of an iridium hydride complex.





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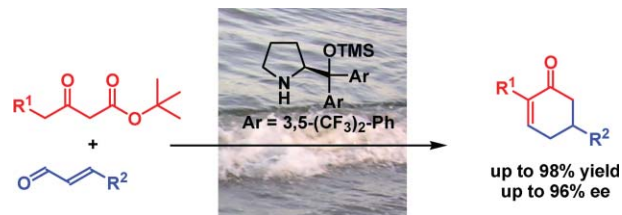
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4928

A simple asymmetric organocatalytic approach to optically active cyclohexenones

Armando Carlone, Mauro Marigo, Chris North, Aitor Landa and Karl Anker Jørgensen*

Optically active 2,5-disubstituted-cyclohexen-2-one derivatives have been prepared in a one-pot process consisting of five reaction steps.

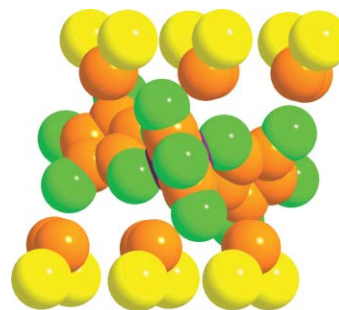


4931

A chirality-induced α phase and a novel molecular magnetic metal in the BEDT-TTF/tris(croconate)ferrate(III) hybrid molecular system

Carlos J. Gómez-García,* Eugenio Coronado, Simona Curreli, Carlos Giménez-Saiz, Paola Deplano, Maria Laura Mercuri,* Luca Pilia, Angela Serpe, Christophe Faulmann and Enric Canadell

The first chirality-induced α phase (also the first pentamerized one) and a novel molecular paramagnetic metal, both with the same 5 : 1 stoichiometry, have been prepared from BEDT-TTF and the novel chiral anion $[\text{Fe}^{\text{III}}(\text{C}_5\text{O}_5)_3]^{3-}$.

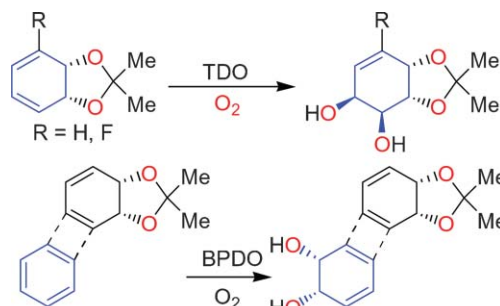


4934

Dioxygenase-catalysed dihydroxylation of arene *cis*-dihydrodiols and acetonide derivatives: a new approach to the synthesis of enantiopure tetraoxygenated bioproducts from arenes

Derek R. Boyd,* Narain D. Sharma, Tayeb Belhocine, John F. Malone, Stuart McGregor and Christopher C. R. Allen

Dioxygenase-catalysed *cis*-dihydroxylation of arene *cis*-diols and arene diol acetonides yields enantiopure bis(*cis*-diol)s and *cis*-diol acetonides respectively.

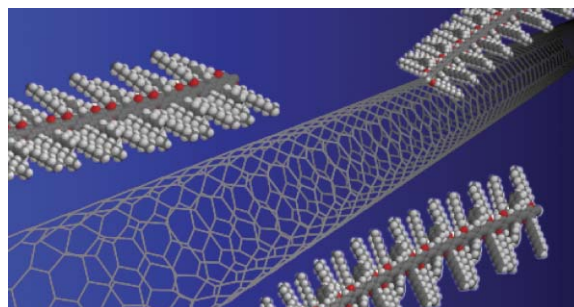


4937

Dispersing as-prepared single-walled carbon nanotube powders with linear conjugated polymers

Nicole A. Rice, Katie Soper, Ningzhang Zhou, Erika Merschrod* and Yuming Zhao*

Suitably modified linear conjugated poly(arylene ethynylene)s are able to assist effective debundling and dispersion of crude as-prepared single-walled carbon nanotube powders in organic solvents.



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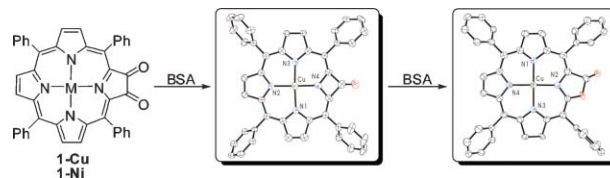
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Elucidation of the extraordinary 4-membered pyrrole ring-contracted azeteporphyrinoid as an intermediate in chlorin oxidation

Tillmann Köpke, Maren Pink and Jeffrey M. Zaleski*

Reaction of 2,3-dioxochlorins with benzeneselenenic anhydride (BSA) results in the formation of unusual ring-contracted azetine derivatives that further react with BSA to afford porpholactones.

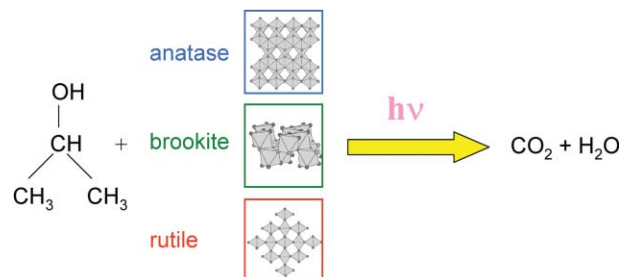


4943

Preparation and photoactivity of nanostructured anatase, rutile and brookite TiO₂ thin films

Maurizio Addamo, Marianna Bellardita, Agatino Di Paola and Leonardo Palmisano*

Pure anatase, brookite and rutile films have been prepared. Their photoactivity has been tested in a gas–solid system by using degradation of 2-propanol as a probe reaction.

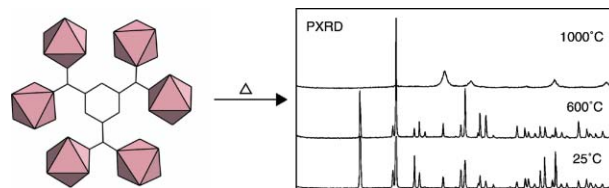


4946

An unusually high thermal stability within a novel lanthanide 1,3,5-cyclohexanetricarboxylate framework: synthesis, structure, and thermal data

Daniel T. de Lill and Christopher L. Cahill*

A novel three-dimensional lanthanide–organic framework has been synthesized. This material has an exceptionally high thermal stability (600 °C) and an unusually low coordination number for a lanthanide ion (CN = 6).

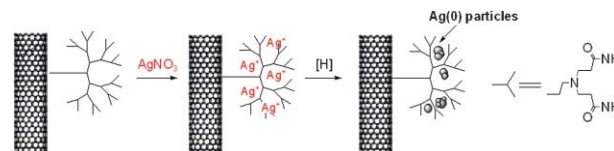


4949

Modification of multi-wall carbon nanotube surfaces with poly(amidoamine) dendrons: Synthesis and metal templating

Lei Tao, Gaojian Chen, Giuseppe Mantovani, Steve York and David M. Haddleton*

Hydroxyl functional poly(amidoamine) dendron wedges have been reacted with the surface of multi-walled carbon nanotubes and used for templating silver nanoparticles.



4952

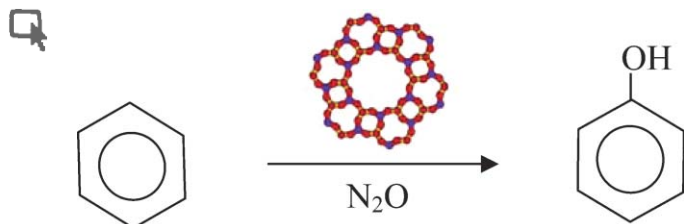


Iodine catalyzed one-pot diamination of glycols with chloramine-T: a new approach to 2-amino- β -glycosylamines for applications in *N*-glycopeptide synthesis

Vipin Kumar and Namakkal G. Ramesh*

Iodine catalyzes a facile one-pot direct diamination of glycols with chloramine-T to afford stereoselectively 2-amino- β -glycosylamine derivatives that serve as convenient precursors for the synthesis of *N*-linked glycopeptides.

4955

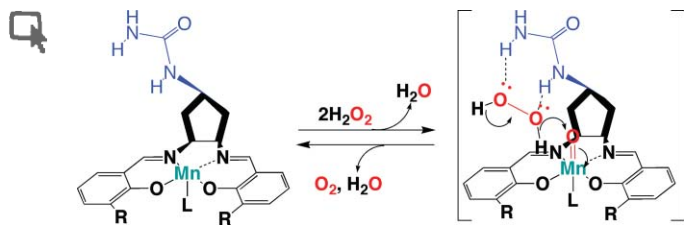


Selective oxidation of benzene to phenol over FeAlPO catalysts using nitrous oxide as oxidant

N. Raveendran Shiju, Steven Fiddy, Olivier Sonntag, Michael Stockenhuber and Gopinathan Sankar*

Framework substituted microporous FeAlPO-5 materials are shown to be active and selective for the hydroxylation of benzene to phenol, using nitrous oxide as the oxidant.

4958



Enhanced catalase-like activity of manganese salen complexes in water: effect of a three-dimensionally fixed auxiliary

Yoritada Watanabe, Azusa Namba, Naoki Umezawa, Masatoshi Kawahata, Kentaro Yamaguchi and Tsunehiko Higuchi*

A new Mn(Salen) complex bearing an ureido group as an auxiliary that is three-dimensionally fixed by a cyclopentane ring fused to the Salen exhibited considerably higher catalase-like activity than the original Mn(Salen).

4961



Guest-dependent inversion rate of a tetranuclear single metallohelicate

Shigehisa Akine, Takanori Taniguchi, Takashi Matsumoto and Tatsuya Nabeshima*

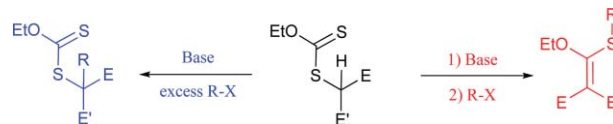
Complexation of linear hexaoxime ligand H_6L with Zn^{2+} and M^{n+} ($= La^{3+}$, Ba^{2+}) afforded a tetranuclear single metallohelicate $[LZn_3M]^{n+}$, whose inversion rate can be modulated by the central metal M^{n+} .

4964

An unexpected synthesis of ketene monothioacetals

Stéphanie Fabre, Xavier Vila* and Samir Z. Zard*

Some dithiocarbonates (xanthates) can be converted into ketene monothioacetals through extrusion of sulfur upon treatment with base and an alkylating agent.

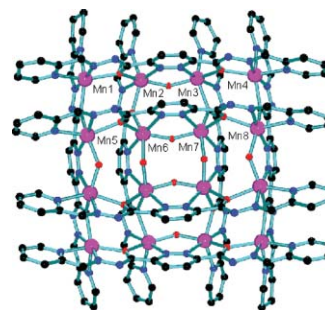


4967

A self-assembled hexadecanuclear $4 \times [2 \times 2]$ Mn(II)₁₆ square grid from a pyridazine bis(hydrazone) ligand: synthesis, structure and magnetism

Subrata K. Dey, Laurence K. Thompson* and Louise N. Dawe

A $\{4 \times [2 \times 2]\}$ Mn(II)₁₆ square grid results from the self-assembly reaction of a tetratopic pyridazine bis(hydrazone) ligand and Mn(II). The [Mn₄(μ₂-O)₄] subunits are bridged by μ₂-N₂ (pyridazine) and μ₂-(OH) connectors, leading to antiferromagnetic intra-grid spin exchange.



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