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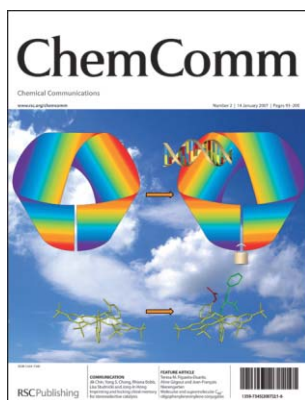
Chemical Communications

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IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (2) 93-200 (2007)



Cover

See J. Chin *et al.*, page 120. The image shows a right handed double helix used to imprint and then padlock a chiral Möbius strip. This is much like using an amino acid to imprint our diamine-based metal complex and then lock the chirality by acylation. Image reproduced by permission of Jik Chin, Yong S. Chong, Rhiana Bobb, Lisa Studnicki and Jong-In Hong from *Chem. Commun.*, 2007, 120.



Inside cover

See X. Duan *et al.*, page 123. Transparent self-supporting films may be fabricated from layered double hydroxide (LDH) crystallites, as long as the platelets all have comparable size, much as the Great Wall is constructed of a regular arrangement of uniform bricks. Image reproduced by permission of Lianying Wang, Cang Li, Miao Liu, David G. Evans and Xue Duan from *Chem. Commun.*, 2007, 123.

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T1

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January 2007/Volume 4/Issue 1

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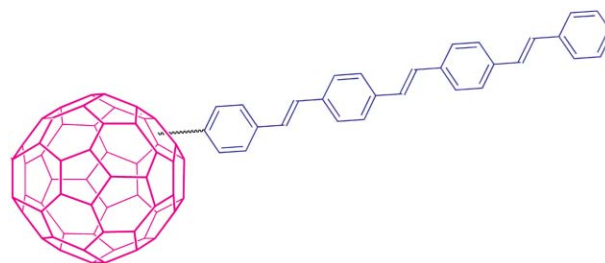
FEATURE ARTICLE

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Molecular and supramolecular C_{60} -oligophenylenevinylene conjugates

Teresa M. Figueira-Duarte, Aline Gégout and Jean-François Nierengarten*

Fullerene derivatives are attractive building blocks for the preparation of molecular and supramolecular photoactive devices. As a part of this research, combination of C_{60} with oligophenylenevinylene (OPV) subunits has generated significant research efforts, reviewed here, illustrating the current development of new photoactive materials.



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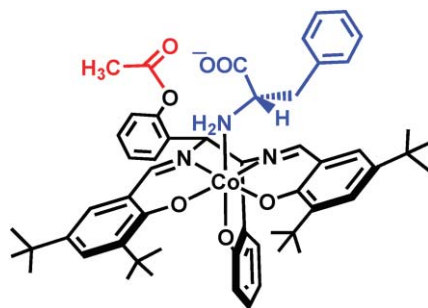
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Imprinting and locking chiral memory for stereoselective catalysis

Jik Chin,* Yong S. Chong, Rhiana Bobb, Lisa Studnicki and Jong-In Hong*

An achiral ligand-based cobalt–salen complex is imprinted with a chiral amino acid and locked with acetic anhydride to produce a stereoselective catalyst.



123

Large continuous, transparent and oriented self-supporting films of layered double hydroxides with tunable chemical composition

Lianying Wang, Cang Li, Miao Liu, David G. Evans and Xue Duan*

Films of functionalized layered double hydroxides (LDHs) have been obtained from an aqueous suspension of monodisperse LDH nanoparticles by a simple method, opening up new areas of applications of LDHs.

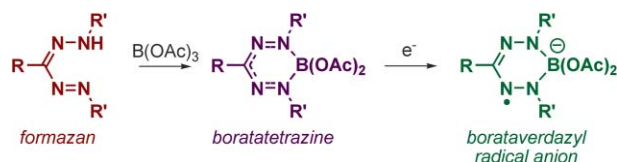


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Formazans as β -diketiminato analogues. Structural characterization of boratatetrazines and their reduction to borataverdazyl radical anions

Joe B. Gilroy, Michael J. Ferguson, Robert McDonald, Brian O. Patrick and Robin G. Hicks*

Formazans react with boron triacetate to produce boratatetrazines, which can be reduced to yield borataverdazyl radical anions—the first boron containing verdazyl radicals.

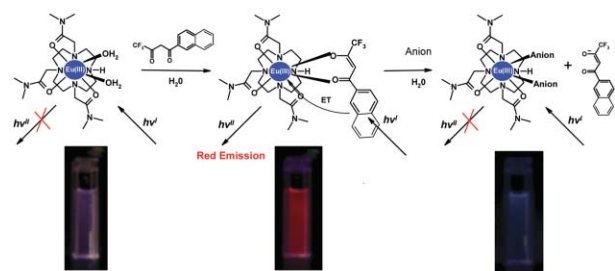


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pH driven self-assembly of a ternary lanthanide luminescence complex: the sensing of anions using a β -diketonate–Eu(III) displacement assay

Joseph P. Leonard,* Cidalia M. G. dos Santos, Sally E. Plush, Thomas McCabe and Thorfinnur Gunnlaugsson*

A new self-assembly Eu(III) based ternary complex **1**·Eu–**4** is shown to be formed as a function of pH. In pH 7.5 buffered solutions the complex can be dissociated by displacement of the antenna (**4**) using coordinating anions.





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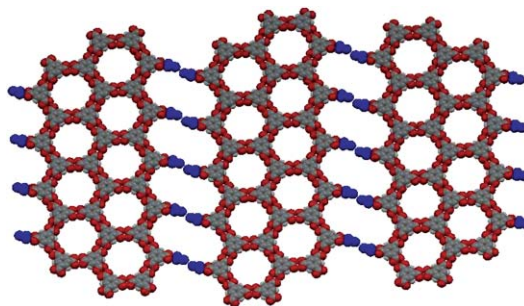
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Disruption of the hexagonal networks of trimesic acid (benzene-1,3,5-tricarboxylic acid, TMA) by acetic acid

Ilana Goldberg and Joel Bernstein*

The complete disruption of the hexagonal networks intrinsic to the structure of trimesic acid by acetic acid has been shown. This structure is composed of two sets of three parallel hexagonal networks, which are triply-catenated. One network is unary, as in the TMA structure itself. The second binary network is disrupted after every second ring formation.

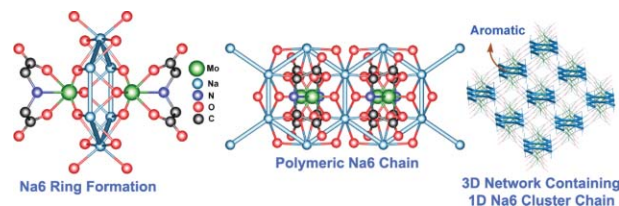


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Synthesis and structure of 1-D Na₆ cluster chain with short Na–Na distance: Organic like aromaticity in inorganic metal cluster

Snehadrinarayan Khatua, Debesh R. Roy, Pratim K. Chattaraj* and Manish Bhattacharjee*

A unique 1-D chain of sodium cluster containing (Na₆) rings stabilized by a molybdenum containing metalloligand has been synthesized and DFT calculations show that (Na₆) rings are aromatic in nature.

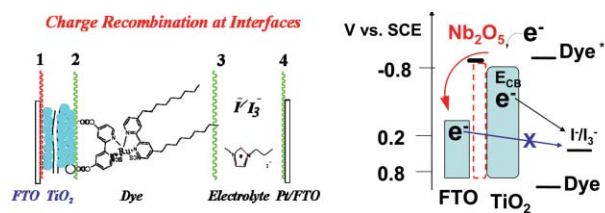


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Sputtered Nb₂O₅ as an effective blocking layer at conducting glass and TiO₂ interfaces in ionic liquid-based dye-sensitized solar cells

Jiangbin Xia, Naruhiko Masaki, Kejian Jiang and Shozo Yanagida*

Sputtered Nb₂O₅ works as a blocking layer at conducting glass and TiO₂ interfaces, improving V_{oc} and fill factor with power conversion efficiency over 5.5% at 1 sun irradiation in ionic liquid-based dye-sensitized solar cells.

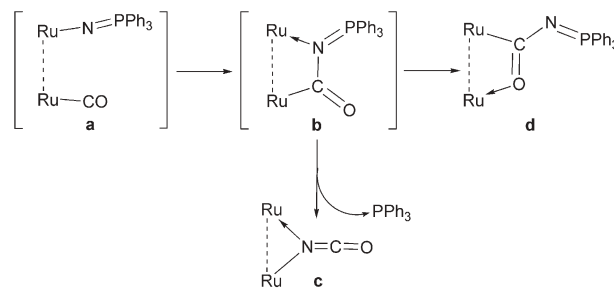


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Trapping a pseudo-Hofmann rearrangement on a ruthenium cluster

Daniele Belletti, Pierre Braunstein, Abdelatif Messaoudi, Roberto Pattacini,* Giovanni Predieri and Antonio Tiripicchio

Crossed theoretical, experimental and crystallographic studies confirmed a pseudo-Hofmann formation mechanism for the isocyanate ligand found on clusters [Ru₃(μ₃-NPPH₃)(μ₃-OSiMe₃)(μ-X)(μ_{C,O}-OC=NPPH₃)(μ-CO)(CO)₆] (X = NCO, Cl), bearing also the first capping silanolate on carbonyl clusters.



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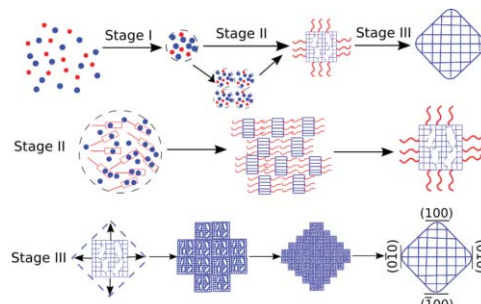
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Uniform NH_4TiOF_3 mesocrystals prepared by an ambient temperature self-assembly process and their topotaxial conversion to anatase

Lei Zhou, David Smyth Boyle and Paul O'Brien*

For the first time, we describe a simple, room-temperature surfactant-mediated route to inorganic mesocrystals of NH_4TiOF_3 . Washing or annealing achieves remarkable topotaxial conversion to technologically important TiO_2 as anatase mesocrystals.

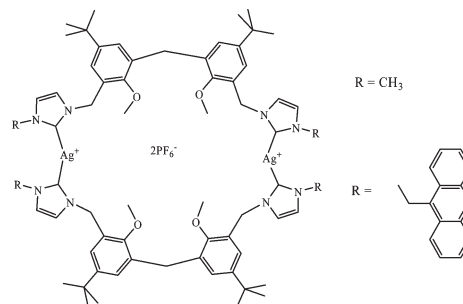


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Silver(I) N-heterocyclic carbene-bridged calix[4]arene analogues as efficient [60]fullerene receptors

Dabin Qin, Xianshun Zeng,* Qingshan Li, Fengbo Xu,* Haibin Song and Zheng-Zhi Zhang*

A fragment-coupling approach was used for the synthesis of silver(I) N-heterocyclic carbene bridged calix[4]arene analogues, a novel type of fluorescent receptor for [60]fullerene.

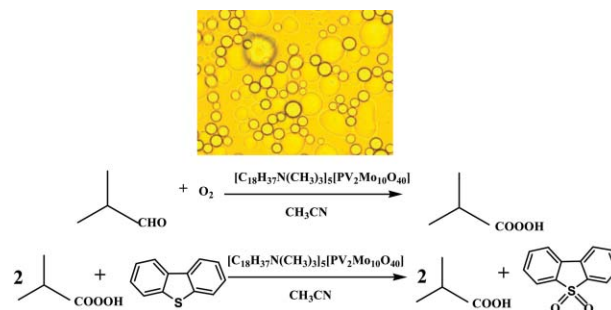


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Oxidative desulfurization of dibenzothiophene with molecular oxygen using emulsion catalysis

Hongying Lü, Jinbo Gao, Zongxuan Jiang, Yongxing Yang, Bo Song and Can Li*

Dibenzothiophene (DBT) is oxidized to the corresponding sulfoxide and sulfone in an emulsion system (W/O) composed of polyoxometalate anion $[\text{C}_{18}\text{H}_{37}\text{N}(\text{CH}_3)_3]_5[\text{PV}_2\text{Mo}_{10}\text{O}_{40}]$ as both the surfactant and catalyst, using molecular oxygen as the oxidant and aldehyde as the sacrificial agent under mild conditions.

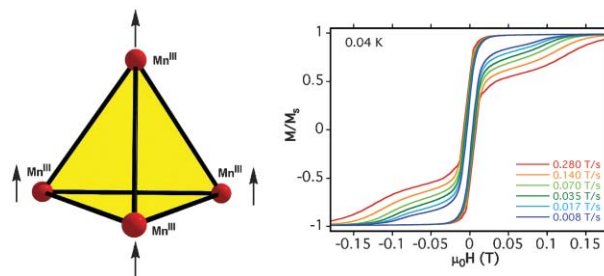


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A rare ferromagnetic manganese(III) 'cube'

Constantinos J. Milios, Alessandro Prescimone, Abhudaya Mishra, Simon Parsons, Wolfgang Wernsdorfer, George Christou, Spyros P. Perlepes and Euan K. Brechin*

An unusual $\{\text{Mn}^{\text{III}}_4\}$ distorted cube has been synthesized that possesses an $S = 8$ ground state and single-molecule magnetism behaviour.



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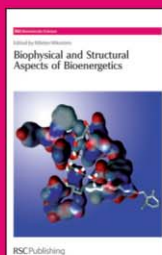
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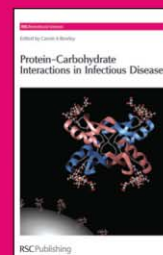


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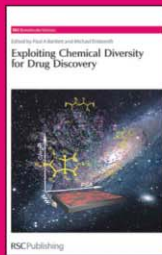


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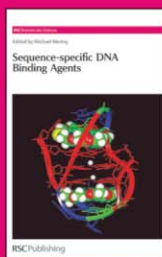


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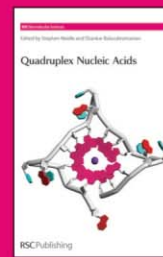


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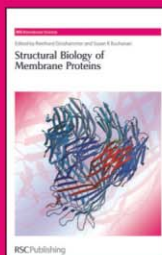


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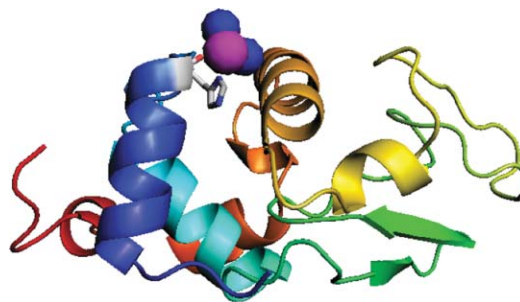
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ESI mass spectrometry and X-ray diffraction studies of adducts between anticancer platinum drugs and hen egg white lysozyme

Angela Casini, Guido Mastrobuoni, Claudia Temperini, Chiara Gabbiani, Simona Francese, Gloriano Moneti, Claudiu T. Supuran, Andrea Scozzafava and Luigi Messori*

The reactivities of various platinum anticancer drugs with hen egg white lysozyme were comparatively investigated through ESI mass spectrometry and X-ray diffraction analysis.

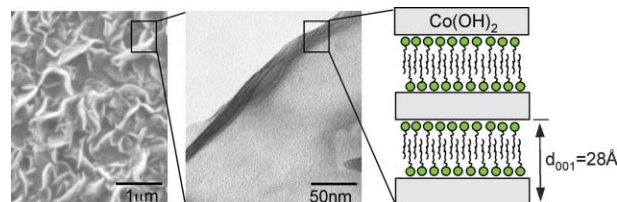


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Electrochemical synthesis of cobalt hydroxide films with tunable interlayer spacings

Matthew S. Yarger, Ellen M. P. Steinmiller and Kyoung-Shin Choi*

Cobalt hydroxide films with significantly increased basal spacings ($d_{001} \geq 25.0 \text{ \AA}$) were prepared by incorporating anionic surfactants (sodium dodecyl sulfate and 1-hexadecanesulfonate) into the interlayer regions during the electrochemical synthesis of the cobalt hydroxide framework.

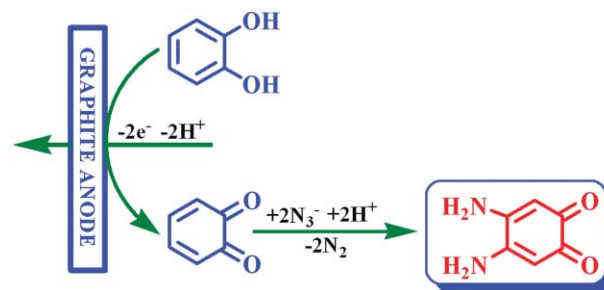


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An efficient electrochemical synthesis of diamino-*o*-benzoquinone: Mechanistic and kinetic evaluation of the reaction of azide ion with *o*-benzoquinone

Davood Nematollahi,* Abbas Afkhami, Esmail Tammari, Tahere Shariatmanesh, Mahdi Hesari and Maryam Shojaeifard

An efficient electrochemical method for the synthesis of diamino-*o*-benzoquinone is described, as well as an estimation of the homogeneous rate constant (k_{obs}) by the digital-simulation method.



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Geometric self-sorting in DNA self-assembly

Yu He, Ye Tian, Yi Chen, Alexander E. Ribbe and Chengde Mao*

Two types of DNA star motifs (tiles) can recognize and associate with like tiles to form 2D arrays but exclude unlike tiles even though the local interactions between any two tiles are exactly the same.





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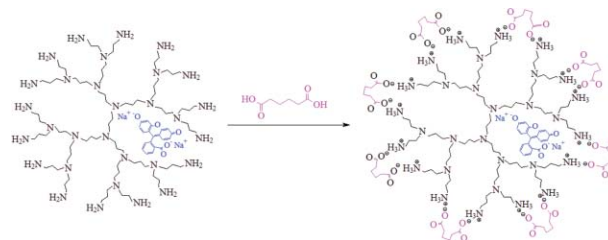


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Encapsulating fluorescein using adipic acid self-assembly on the surface of PPI-3 dendrimer

Minghui Chai,* Aaron K. Holley and Michael Kruskamp

A water-soluble self-assembly has been formed by associating adipic acid molecules onto the surface of the third generation poly(propyleneimine) dendrimer and this system has been used to encapsulate fluorescein.

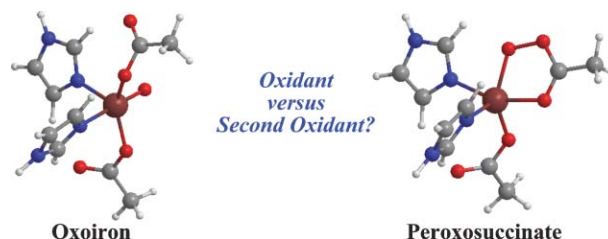


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Can the peroxosuccinate complex in the catalytic cycle of taurine/ α -ketoglutarate dioxygenase (TauD) act as an alternative oxidant?

Sam P. de Visser*

Density functional theoretical studies on the catalytic properties of the peroxosuccinate intermediate in the catalytic cycle of taurine/ α -ketoglutarate dioxygenase suggest that it cannot act as a second oxidant.

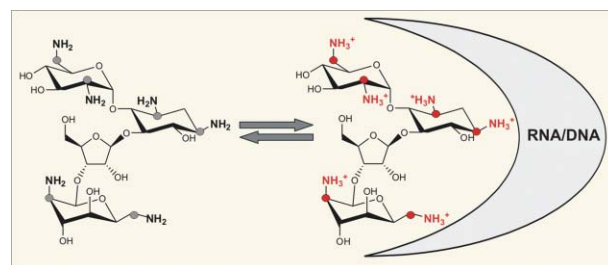


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A simple NMR analysis of the protonation equilibrium that accompanies aminoglycoside recognition: Dramatic alterations in the neomycin-B protonation state upon binding to a 23-mer RNA aptamer

Felix Freire, Igor Cuesta, Francisco Corzana, Julia Revuelta, Carlos González, Milos Hricovini, Agatha Bastida, Jesús Jiménez-Barbero and Juan Luis Asensio*

A complete characterisation of the protonation equilibrium that accompanies the molecular recognition of neomycin-B by a specific RNA receptor has been achieved by employing simple NMR measurements.

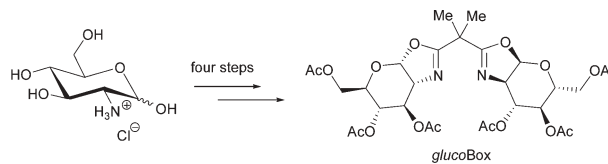


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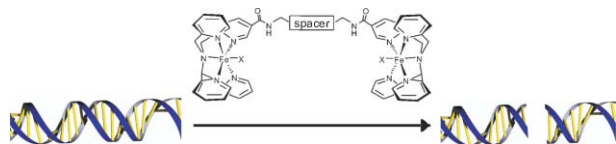
glucoBox—a new carbohydrate-based bis(oxazoline) ligand. Synthesis and first application

Mustafa Irmak, Annika Groschner and Mike M. K. Boysen*

The efficient and brief synthesis of a new carbohydrate-based bis(oxazoline) ligand from inexpensive D-glucosamine is described as well as its first successful application in asymmetric cyclopropanation reactions.



180

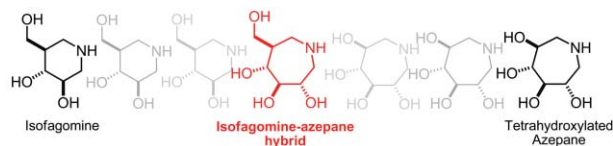


Double strand DNA cleavage with a binuclear iron complex

Tieme A. van den Berg, Ben L. Feringa* and Gerard Roelfes*

Covalently linking two single strand DNA cleaving agents resulted in a new biomimetic binuclear iron complex capable of effecting oxidative double strand DNA cleavage.

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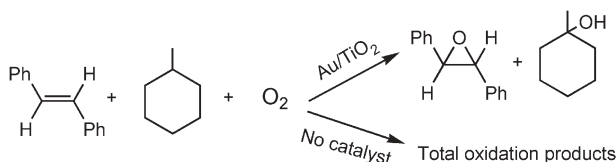


Tandem Staudinger–azaWittig mediated ring expansion: rapid access to new isofagomine-tetrahydroxyazepane hybrids

Hongqing Li, Yongmin Zhang, Pierre Vogel, Pierre Sinay and Yves Blériot*

New seven-membered iminosugars with potent and selective inhibition towards glycosidases have been prepared as 1-*N*-iminosugar homologues *via* a tandem Staudinger–azaWittig mediated ring expansion.

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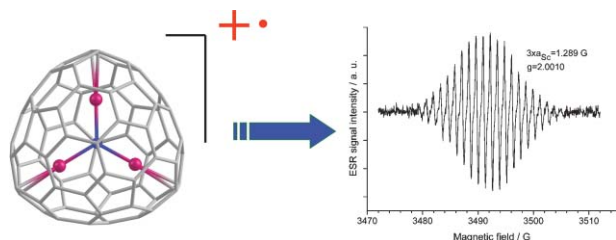


Stereoselective stilbene epoxidation over supported gold-based catalysts

Pascal Lignier, Franck Morfin, Stéphane Mangematin, Laurence Massin, Jean-Luc Rousset and Valérie Caps*

The gold reference catalyst Au/TiO₂ exhibits high activity in the stereoselective epoxidation of *trans*-stilbene in methylcyclohexane using catalytic amounts of TBHP, by activating molecular oxygen *via* a free-radical chain reaction.

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The spin state of a charged non-IPR fullerene: the stable radical cation of Sc₃N@C₆₈

Shangfeng Yang,* Peter Rapta and Lothar Dunsch*

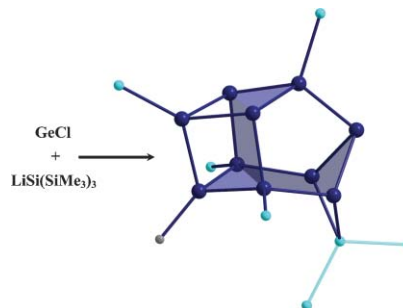
For the first time the stable paramagnetic radical cation of the non-IPR diamagnetic cluster fullerene Sc₃N@C₆₈ (left) is detected by the *in-situ* ESR/UV-Vis-NIR spectroelectrochemistry, indicating that a large part of the unpaired spin is symmetrically delocalised on the C₆₈ cage according to the ESR pattern with 22 narrow lines (right).

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{Ge₁₀Si[Si(SiMe₃)₃]₄(SiMe₃)₂Me}⁻: A Ge₁₀Si framework reveals a structural transition onto elemental germanium

Andreas Schnepf*

The new metalloid cluster {Ge₁₀Si[Si(SiMe₃)₃]₄(SiMe₃)₂Me}⁻ was synthesized and characterized, being the first mixed Ge–Si compound, showing a structural transition onto the solid state structure of elemental germanium.

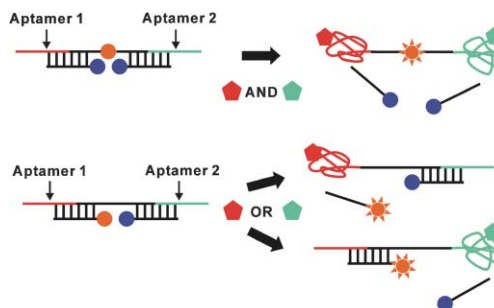


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Photonic boolean logic gates based on DNA aptamers

Wataru Yoshida and Yohei Yokobayashi*

We designed a pair of DNA-based logic gates that sense single-stranded DNAs and aptamer ligands to produce fluorescence outputs according to Boolean logic functions AND and OR.



ADDITION AND CORRECTION

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AlCl₃/ICl-mediated iodo-carbocyclization of α-iodo cycloalkanones: a new entry to spirocyclic ketones


Chin-Kang Sha, Fong-Cheng Lee and Hsien-Hsun Lin

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