

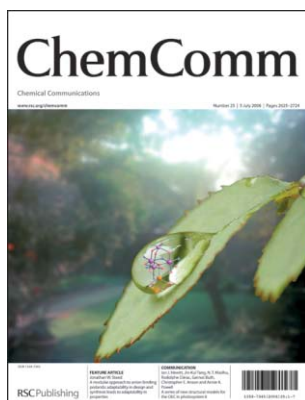
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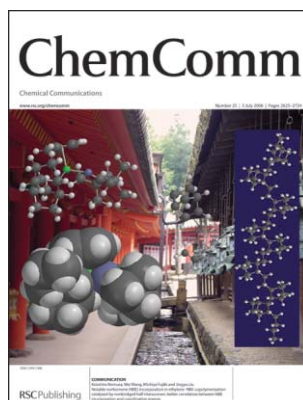
IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (25) 2625-2724 (2006)



Cover

See Annie K. Powell *et al.*, page 2650. New model compounds could shed light on the structural and electronic features of the Oxygen Evolving Centre responsible for splitting water in Photosynthesis. Image created from http://image02.webshots.com/2/0/88/26/80108826uLMlXy_fs.jpg and a photograph by Janet Pain. Reproduced by permission of Ian J. Hewitt, Jin-Kui Tang, N. T. Madhu, Rodolphe Clérac, Gernot Buth, Christopher E. Anson and Annie K. Powell from *Chem. Commun.*, 2006, 2650.



Inside cover

See Kotohiro Nomura *et al.*, page 2659. A schematic illustration of the copolymerisation of ethylene with norbornene by nonbridged half-titanocene over historic architecture (Kasuga Taisha Shrine, Nara, The World Heritage). Image reproduced by permission of Kotohiro Nomura, Wei Wang, Michiya Fujiki and Jingyu Liu from *Chem. Commun.*, 2006, 2659.

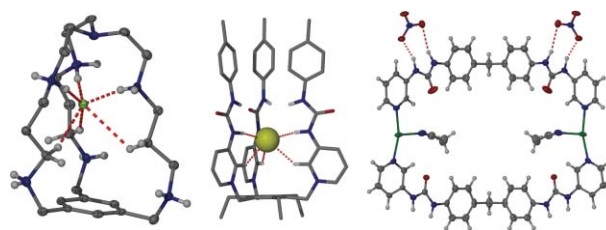
FEATURE ARTICLE

2637

A modular approach to anion binding podands: adaptability in design and synthesis leads to adaptability in properties

Jonathan W. Steed*

Adaptable anion binding systems have potential applications in sensing, extraction and nanostructured gel phase materials



COMMUNICATION

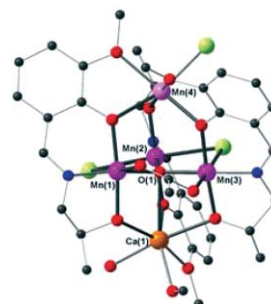
2650



A series of new structural models for the OEC in photosystem II

Ian J. Hewitt, Jin-Kui Tang, N. T. Madhu, Rodolphe Clérac, Gernot Buth, Christopher E. Anson and Annie K. Powell*

A new series of MMn^{II-III}_4 clusters ($M = Na, Ca$) has been structurally characterised and their relevance to understanding the oxygen evolving centre of photosystem II is discussed.



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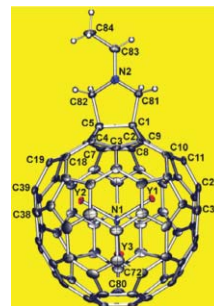
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X-Ray crystallographic and EPR spectroscopic characterization of a pyrrolidine adduct of $Y_3N@C_{80}$

Luis Echegoyen,* Christopher J. Chancellor, Claudia M. Cardona, Bevan Elliott, José Rivera, Marilyn M. Olmstead and Alan L. Balch*

Crystallographic data for the pyrrolidine adduct $Y_3N@C_{80}C_4H_9N \cdot 2.5CS_2$ reveals a slightly pyramidalized Y_3N unit with idealized mirror symmetry that avoids contact with the site of addition.

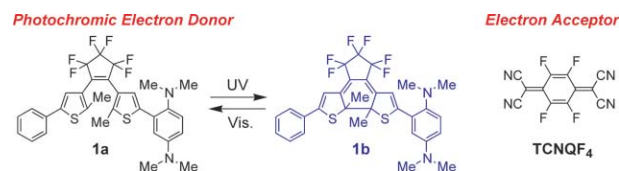


2656

Photochromism of a diarylethene charge-transfer complex: photochemical control of intermolecular charge-transfer interaction

Masakazu Morimoto, Seiya Kobatake and Masahiro Irie*

Photochromic diarylethene **1** formed radical ions upon mixing with $TCNQF_4$ in organic solvents. The absorption intensity of the radical ions was modulated by photochromic reactions of the diarylethene. This behavior is ascribed to the difference in the electron-donating character between open- and closed-ring isomers of the diarylethene.

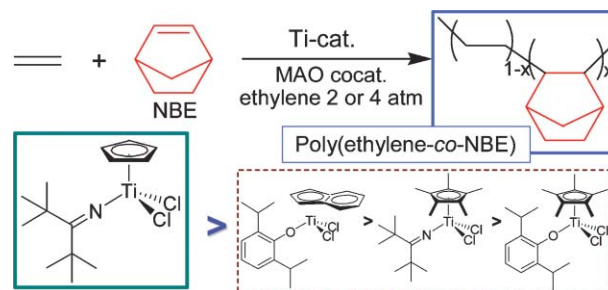


2659

Notable norbornene (NBE) incorporation in ethylene–NBE copolymerization catalysed by nonbridged half-titanocenes: better correlation between NBE incorporation and coordination energy

Kotohiro Nomura,* Wei Wang, Michiya Fujiki and Jingyu Liu

$CpTiCl_2(N=C^tBu_2)$ exhibited remarkable catalytic activity and efficient norbornene (NBE) incorporation in ethylene–NBE copolymerization; efficient synthesis of high molecular weight polymers with high NBE contents has been achieved.

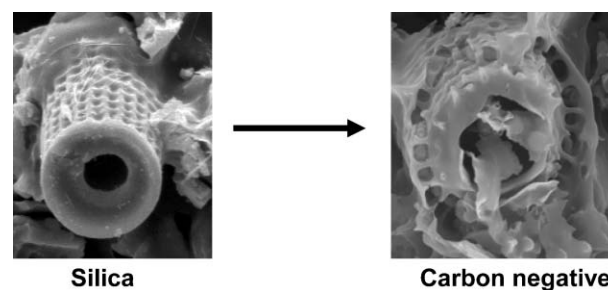


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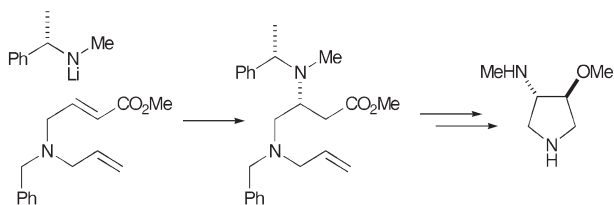
A novel porous carbon based on diatomaceous earth

S. M. Holmes,* B. E. Graniel-Garcia, P. Foran, P. Hill, E. P. L. Roberts, B. H. Sakakini and J. M. Newton

The impregnation of a sucrose solution into the structure of diatomaceous earth followed by carbonisation and dissolution of the silica leads to a novel intricate porous carbon which has potential as a support in a range of catalytic processes.



2664

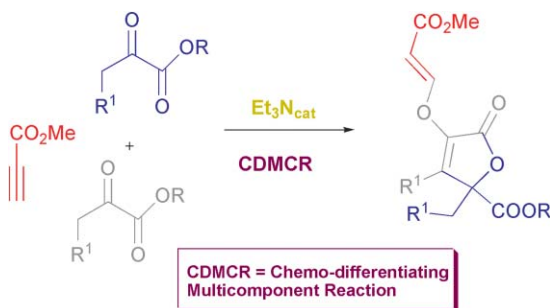


Lithium amide conjugate addition for the asymmetric synthesis of 3-aminopyrrolidines

Stephen G. Davies,* A. Christopher Garner, Euan C. Goddard, Dennis Kruchinin, Paul M. Roberts, Humberto Rodriguez-Solla and Andrew D. Smith

Conjugate addition of homochiral lithium amides to methyl 4-(*N*-benzyl-*N*-allylamino)but-2-enoate, followed by stereoselective enolate functionalisation and deprotection gives access to both *syn*- and *anti*-3,4-disubstituted aminopyrrolidines in high d.e. and e.e.

2667

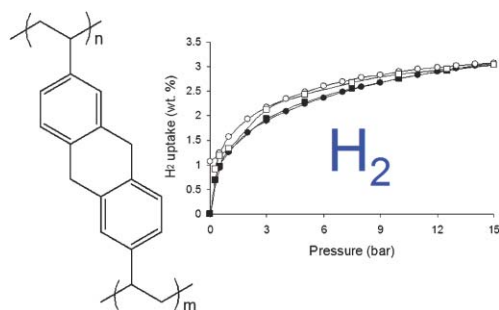


Chemo-differentiating MCRs based on α -ketoesters and terminal alkynoates. A homoaldol-based ABB' system

David Tejedor, Alicia Santos-Expósito and Fernando García-Tellado*

A novel chemo-differentiating ABB' 3-CR system based on the organocatalyzed homoaldolic condensation of α -ketoesters in the presence of terminal conjugated alkynoates is described. This 3-CR manifold generates polyfunctionalized isotetronic acid derivatives with atom-efficiency and easy chemical processing.

2670



Hydrogen adsorption in microporous hypercrosslinked polymers

Jun-Young Lee, Colin D. Wood, Darren Bradshaw, Matthew J. Rosseinsky and Andrew I. Cooper*

A microporous hypercrosslinked polymer resin was synthesized and shown to adsorb 3.04 wt.% hydrogen at 77 K and 15 bar.

2673



First C-3 lithiation of DMAP: a new entry into chemical tuning of acylation catalysts

Philippe C. Gros,* Abdelatif Doudouh and Christopher Woltermann

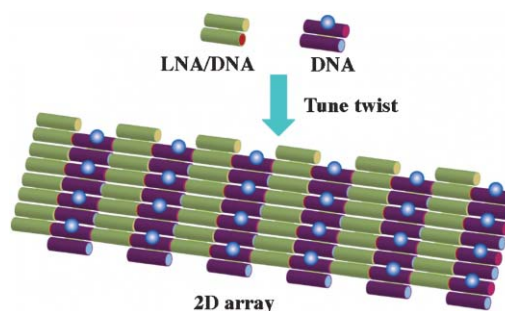
A TMSCH₂Li-based reagent promoted the first C-3 lithiation of DMAP opening a direct access to functional diversity in acylation catalysts.

2675

Two-dimensional LNA/DNA arrays: estimating the helicity of LNA/DNA hybrid duplex

Sherri Rinker, Yan Liu and Hao Yan*

The helical repeat of a LNA/DNA hetero-duplex was measured to be 13.2 ± 0.9 base pairs per turn by incorporating LNA oligos into self-assembled two-dimensional DNA tile arrays.

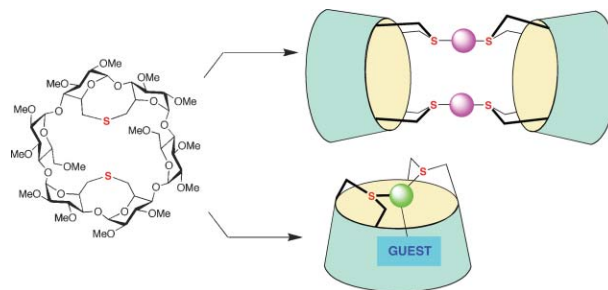


2678

Sulfur-capped cyclodextrins: a new class of cavitands with extroverted as well as introverted donor functionalities

Belkacem Benmerad, Pascaline Clair, Dominique Armpach,* Dominique Matt,* Fadila Balegroune and Loic Toupet

Ansa-cyclodextrins were obtained in high yields by reaction of sodium sulfide with *A,B*-di- or *A,B,D,E*-tetramesylylated α -CD precursors; the resulting thiocavitands are suitable for forming nanotubular molecules, as well as for hosting metal-organic fragments.

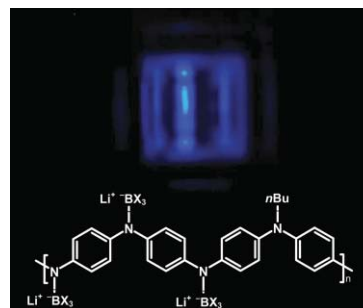


2681

Blue emitting polyaniline

Debanghsu Chaudhuri and D. D. Sarma*

A novel functionalization of polyaniline (PANI) leads to materials exhibiting a bright, deep blue photoluminescence. The synthetic strategy provides a general route for functionalizing PANI.

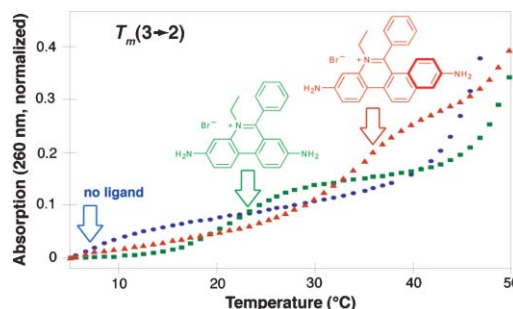


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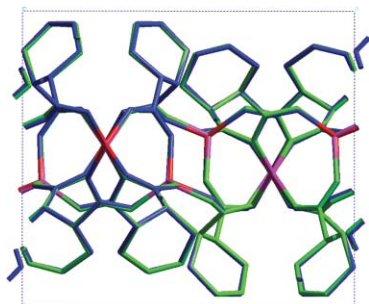
Extended ethidium bromide analogue as a triple helix intercalator: synthesis, photophysical properties and nucleic acids binding

Victor K. Tam, Qi Liu and Yitzhak Tor*

Ethidium bromide has been extended by fusing an additional aromatic ring resulting in a larger intercalator with increased affinity for poly r(A)·r(U), poly d(A)·d(T) and triple helices when compared to the parent heterocycle.



2687

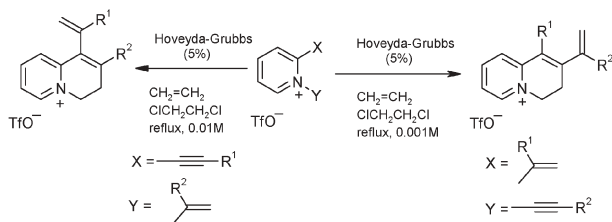


Thermodynamic and kinetic factors in the hydrothermal synthesis of hybrid frameworks: zinc 4-cyclohexene-1,2-dicarboxylates

Clare Lee, Caroline Mellot-Draznieks, Ben Slater, G. Wu, William T. A. Harrison, C. N. R. Rao and Anthony K. Cheetham*

Experimental and computational observations indicate that the formation of zinc 4-cyclohexene-1,2-dicarboxylates proceeds largely under thermodynamic control.

2690

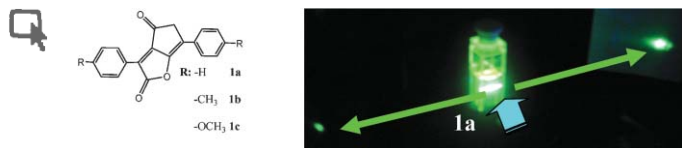


Enyne ring-closing metathesis on heteroaromatic cations

Ana Núñez, Ana M. Cuadro,* Julio Alvarez-Builla and Juan J. Vaquero*

The first use of cationic heteroaromatic enynes as suitable substrates in enyne ring-closing metathesis is described. The metathesis reaction affords new 1-vinyl- and 2-vinyl-substituted 3,4-dihydroquinolinium salts, useful precursors for biologically relevant cations.

2693

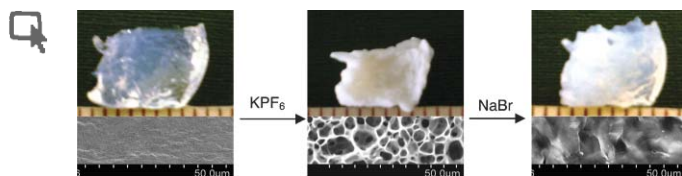


A new class of laser dyes, 2-oxa-bicyclo[3.3.0]octa-4,8-diene-3,6-diones, with unity fluorescence yield

Chao-Yu Wang, Yu-Shan Yeh, Elise Y. Li, Yi-Hong Liu, Shih-Ming Peng, Shih-Tzung Liu* and Pi-Tai Chou*

A new class of dyes, **1a–c**, have been synthesized. **1a–c** all exhibit unity fluorescence quantum yield in common organic solvents and have demonstrated remarkable amplified spontaneous emission with a gain efficiency of > 10 .

2696



Surfactant ionic liquid-based microemulsions for polymerization

Feng Yan and John Texter*

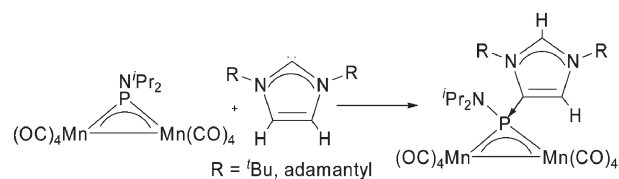
Surfactants based on imidazolium ionic liquids (ILs), including polymerizable surfactant ILs, have been synthesized and used to stabilize polymerizable microemulsions useful for producing polymeric nanoparticles, gels, and open-cell porous materials that exhibit semireversible poration with counter-ion exchange.

2699

Reactivity of electrophilic μ -phosphinidene complexes with N-heterocyclic carbenes: formation of the first main group element adducts of 'abnormal' carbene ligands

Todd W. Graham, Konstantin A. Udachin and Arthur J. Carty*

The phosphinidene complexes $[\text{Mn}_2(\text{CO})_8\{\mu\text{-P}(\text{N}^i\text{Pr}_2)\}]$ and $[\text{Co}_2(\text{CO})_4(\mu\text{-dppm})\{\mu\text{-P}(\text{N}^i\text{Pr}_2)\}]$ react with N-heterocyclic carbenes 1,3-bis(R)imidazol-2-ylidene (R = *t*Bu, adamantyl) to form 'abnormal' carbene adducts, where the carbene is bound to the phosphinidene fragment *via* C-4 instead of the expected C-2.

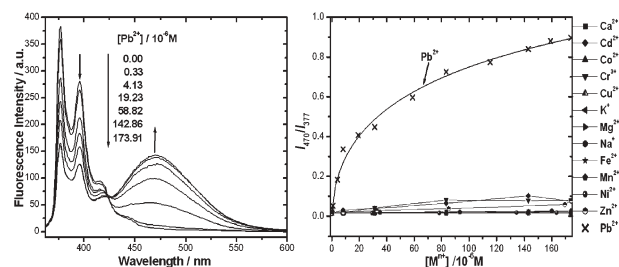


2702

A tryptophan-containing fluoroionophore sensor with high sensitivity to and selectivity for lead ion in water

Li-Jun Ma, Yi-Fu Liu and Yuqing Wu*

We report a fluoroionophore sensor, PLT, that shows high sensitivity to (detection limit up to 0.15 μM) and selectivity for lead ion over Ca^{2+} , Cd^{2+} , Co^{2+} , Cr^{3+} , Cu^{2+} , K^+ , Mg^{2+} , Na^+ , Fe^{2+} , Mn^{2+} , Ni^{2+} and Zn^{2+} in aqueous solution.

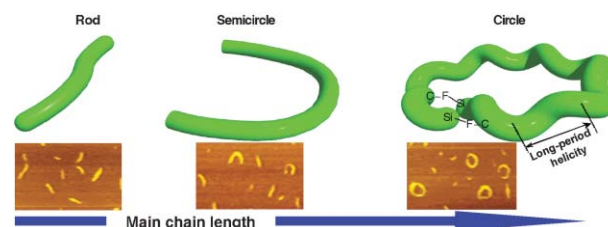


2705

Switching in molecular shapes: main chain length driven rod-circle transition of isolated helical polysilanes

Akihiro Ohira,* Sun-Young Kim, Michiya Fujiki,* Yusuke Kawakami, Masanobu Naito, Giseop Kwak and Anubhav Saxena

Unique conformations such as rod, semicircle, and circle structures of isolated semi-flexible helical polysilanes were observed by AFM and the chain topologies could be significantly related to the chain length on the surfaces.

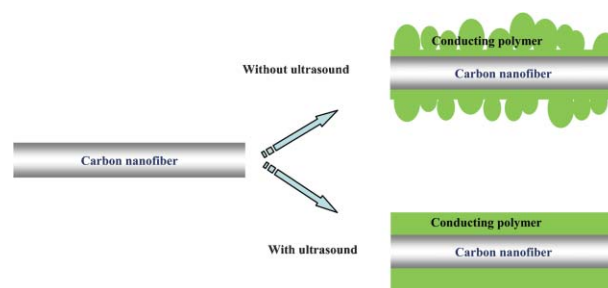


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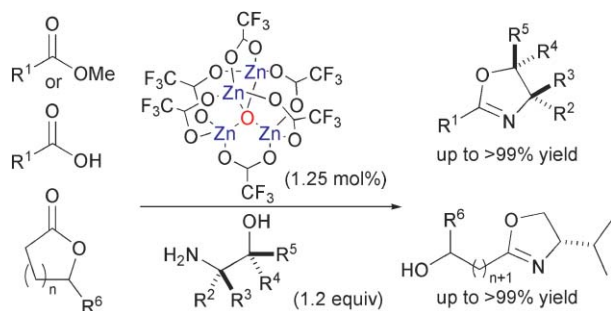
Highly-regulated nanocoatings of polymer films on carbon nanofibers using ultrasonic irradiation

Jong-Eun Park, Miyuki Saikawa, Mahito Atobe* and Toshio Fuchigami

It was demonstrated that the nanoprecise coating of a uniform and densely packed polymer layer on nanomaterials and the uniform polymer coating of individual nano-objects is possible using ultrasonic effects.



2711

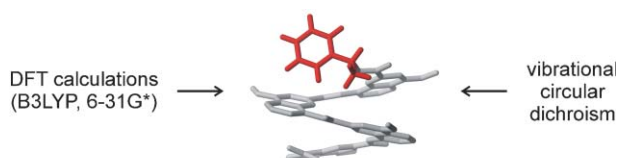


Direct conversion of esters, lactones, and carboxylic acids to oxazolines catalyzed by a tetranuclear zinc cluster

Takashi Ohshima,* Takanori Iwasaki and Kazushi Mashima*

A new efficient synthesis oxazoline from esters, lactones, and carboxylic acids catalyzed by a novel tetranuclear zinc cluster was developed.

2714

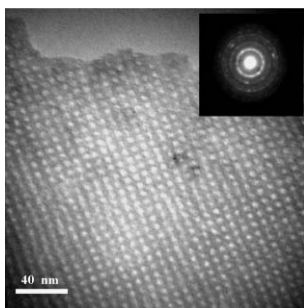


Vibrational circular dichroism and *ab initio* structure elucidation of an aromatic foldamer

Thierry Buffeteau, Laurent Ducasse, Legiso Poniman, Nicolas Delsuc and Ivan Huc*

Ab initio calculations together with vibrational circular dichroism (VCD) are validated as very accurate tools for studying conformations and estimating conformational energies and helical handedness preferences of an entire, large (112 atoms) abiotic foldamer.

2717

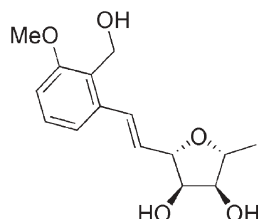


An ordered cubic *Im3m* mesoporous Cr–TiO₂ visible light photocatalyst

Jimmy C. Yu,* Guisheng Li, Xinchun Wang, Xianluo Hu, Cheuk Wan Leung and Zhendong Zhang

An ordered and well-crystallized cubic *Im3m* mesoporous Cr–TiO₂ photocatalyst with superb performance under visible light has been fabricated.

2720



An efficient total synthesis and absolute configuration determination of varitriol

Ryan T. Clemens and Michael P. Jennings*

The first total synthesis of the cytotoxic natural product varitriol is described. The key feature of the synthetic strategy included a convergent cross-metathesis reaction between the β -C-furanoside and substituted styrene subunits.

2722

Unusual variations in the incidence of $Z' > 1$ in oxo-anion structures

Kirsty M. Anderson, Andres E. Goeta,
Kirsty S. B. Hancock and Jonathan W. Steed

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