

Cover
 Regio- and chemo-selective C–F activation at nickel provides new methodology for synthesis of fluorinated N-heterocycles.



Chemical biology articles published in this journal also appear in the *Chemical Biology Virtual Journal*:
www.rsc.org/chembiol

contents

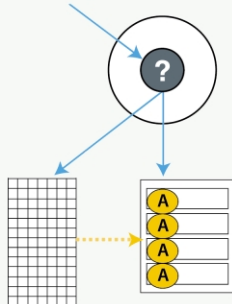
FOCUS ARTICLE

2745

Developing tools and standards in molecular informatics

Robert Glen

Molecular informatics can be used to manage the mountains of data and information associated with compounds and their structures.



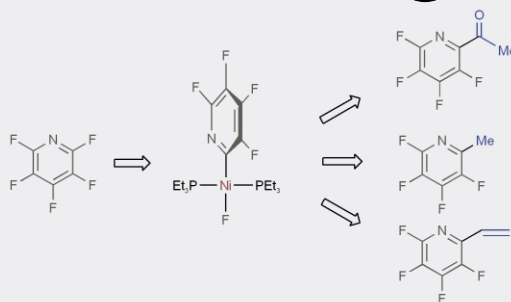
FEATURE ARTICLE

2749

Routes to fluorinated organic derivatives by nickel mediated C–F activation of heteroaromatics

Thomas Braun and Robin N. Perutz

New fluorinated azaheterocycles can be synthesised regio- and chemo-selectively *via* C–F activation of fluorinated precursors at nickel, with subsequent functionalisation and release from the coordination sphere of the metal; the requirements for productive C–F activation are significantly different from those for C–H bond activation.



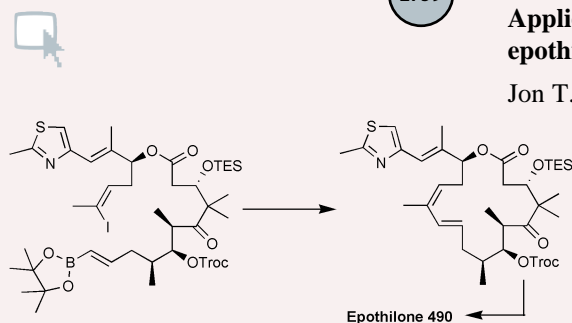
COMMUNICATIONS

2759

Application of hitherto unexplored macrocyclization strategies in the epothilone series: novel epothilone analogs by total synthesis

Jon T. Njardarson, Kaustav Biswas and Samuel J. Danishefsky*

Total synthesis of Epothilone 490 and 11-hydroxy desoxyepothilone B using Suzuki and Nozaki–Kishi macrocyclizations is presented.



2762

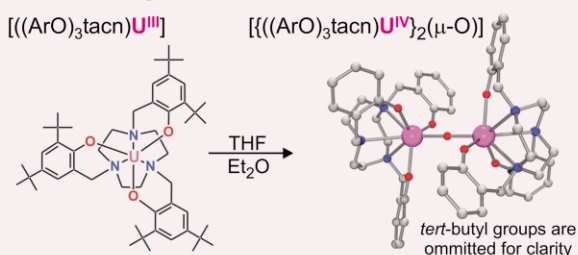


Combinatorial parallel synthesis and automated screening of a novel class of liquid crystalline materials

Oliver Deeg, Peer Kirsch, Detlef Pauluth and Peter Bäuerle*

Combinatorial parallel synthesis led to a library of novel liquid crystalline quaterphenyls. Subsequent screening and data analysis revealed structure–property relationships.

2764

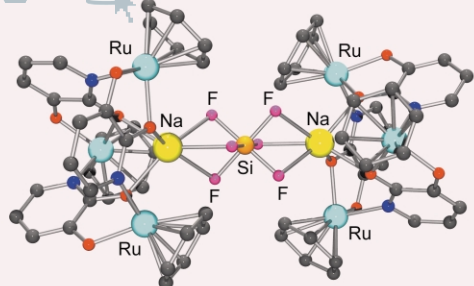


Uranium complexes supported by an aryloxy functionalised triazacyclononane macrocycle: synthesis and characterisation of a six-coordinate U(III) species and insights into its reactivity

Ingrid Castro-Rodriguez, Kristian Olsen, Peter Gantzel and Karsten Meyer*

A reactive low-valent uranium(III) complex supported by an aryloxy functionalised triazacyclononane has been synthesised. This complex provides a platform for enhanced uranium reactivity. The molecular and electronic structure is presented.

2766

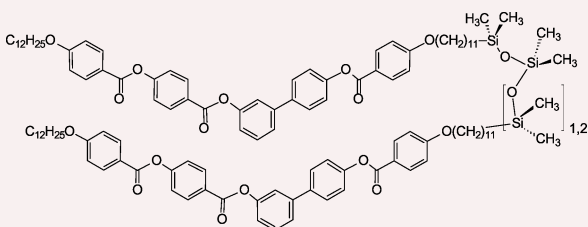


Encapsulation of molecular Na₂SiF₆ by two metallacrown complexes

Marie-Line Lehaire, Rosario Scopelliti and Kay Severin*

A complex of molecular Na₂SiF₆, stabilised by two 12-metallacrown-3 host complexes, has been synthesised and characterised by single crystal X-ray diffraction.

2768

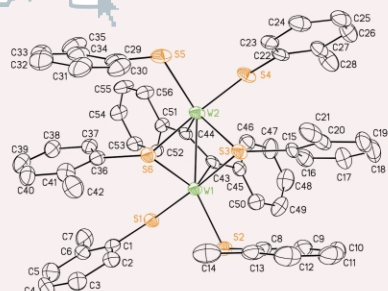


The first liquid crystalline dimers consisting of two banana-shaped mesogenic units: a new way for switching between ferroelectricity and antiferroelectricity with bent-core molecules

Gert Dantlgraber, Siegmund Diele and Carsten Tschierske*

The first dimesogens in which two banana-shaped molecules are connected by a flexible spacer unit are reported. Depending on the number of dimethylsiloxane units in the spacer either ferroelectric or antiferroelectric switchable polar smectic C phases were obtained.

2770

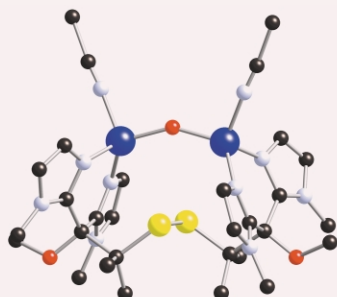
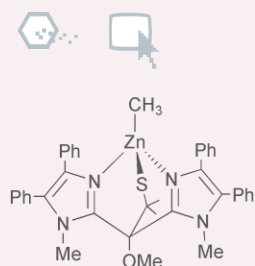


Insights into the Schrock ‘chop-chop’ reaction gained from density functional theory and preparation and structure of W₂(μ-PhCCPh)(SC₆H₄-2-Me)₆

Malcolm H. Chisholm,* Ernest R. Davidson,* Maren Pink and Kristine B. Quinlan

Density functional theory calculations predicted that the alkyne adduct of model complex, W₂(μ-HCCH)(SH)₆ was stable by 18 kcal mol⁻¹ relative to the alkyldiene species, which lead to the synthesis of W₂(μ-PhCCPh)(SC₆H₄-2-Me)₆ from W(CPh)(O^tBu)₃ and aryl thiol.

2772

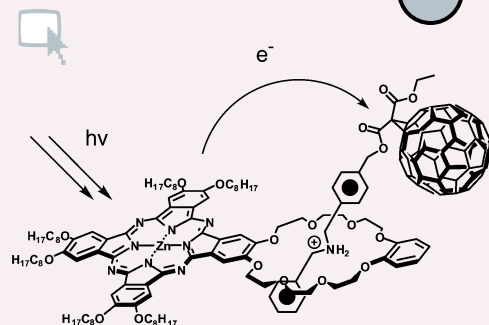


A new bis(imidazolyl)(alkylthiolate) tripodal ligand and the spontaneous formation of a disulfide-linked, hydroxo-bridged dinuclear zinc complex

Vivek V. Karambelkar, Divya Krishnamurthy, Charlotte L. Stern, Lev N. Zakharov, Arnold L. Rheingold and David P. Goldberg*

Protonolysis of a zinc alkyl complex, prepared from a new tripodal ligand L^{Im2SH} , has led to the formation of a novel disulfide-linked, dinucleating ligand and a $Zn_2(\mu-OH)(CH_3CN)_2$ complex.

2774

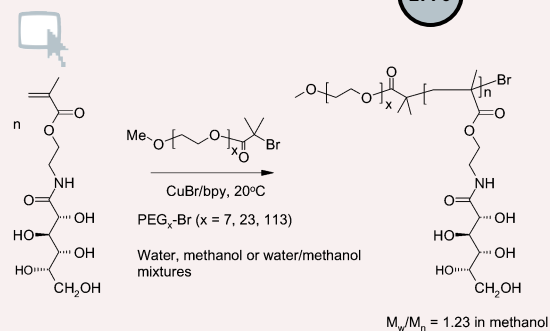


Reversible zinc phthalocyanine fullerene ensembles

Dirk M. Guldi,* Jeff Ramey, M. Victoria Martínez-Díaz, Andrés de la Escosura, Tomás Torres,* Tatiana Da Ros and Maurizio Prato*

Novel zinc phthalocyanine (ZnPc)/fullerene ligand (L) ensembles are assembled following simple supramolecular principles, which upon photoexcitation give rise to *intra* complex electron transfer quenching of the 1ZnPc fluorescence.

2776

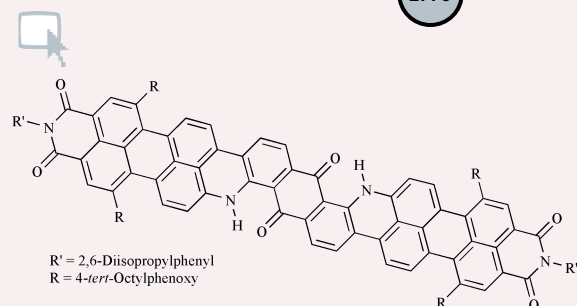


Synthesis of low polydispersity, controlled-structure sugar methacrylate polymers under mild conditions without protecting group chemistry

Ravin Narain and Steven P. Armes*

We report the synthesis of low polydispersity, controlled-structure sugar methacrylate polymers by the ring-opening reaction of 2-aminoethyl methacrylate with D-gluconolactone, followed by the atom transfer radical polymerisation of the resulting sugar methacrylate in methanol at 20 °C.

2778

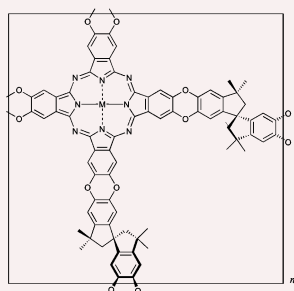


Bis(rylenedicarboximide)-a,d-1,5-diaminoanthraquinones as unique infrared absorbing dyes

Christopher Kohl, Stefan Becker and Klaus Müllen*

Design and synthesis of a new class of dyestuff compounds exhibiting three characteristics, namely absorption in the near (NIR) region, high photostability and good processability, is described.

2780

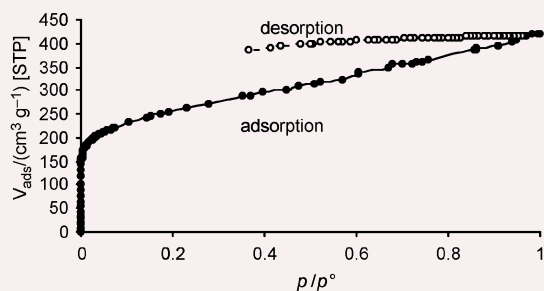


Phthalocyanine-based nanoporous network polymers

Neil B. McKeown,* Saad Makhseed and Peter M. Budd

Network polymers exhibiting large surface areas ($450\text{--}950\text{ m}^2\text{ g}^{-1}$) are prepared by the phthalocyanine-forming reaction of a bis(phthalonitrile) monomer containing a rigid spirocyclic linking group.

2782

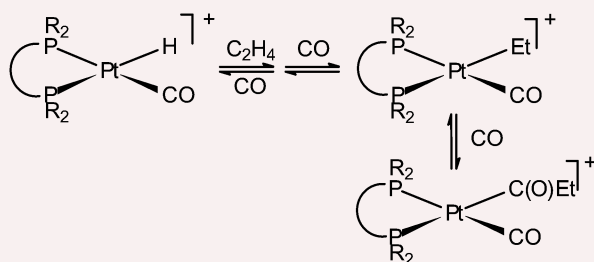


Porphyrin-based nanoporous network polymers

Neil B. McKeown,* Shabir Hanif, Kadhum Msayib, Carin E. Tattershall and Peter M. Budd

Network polymers exhibiting large surfaces areas ($900\text{--}1000\text{ m}^2\text{ g}^{-1}$) are prepared by the highly efficient dibenzodioxane-forming reaction between *meso*-tetrakis(pentafluorophenyl)porphyrin and a rigid bis(catechol) monomer.

2784

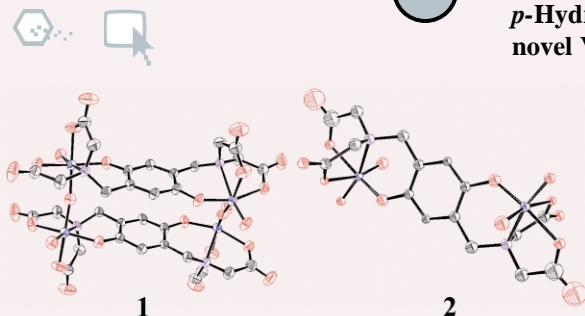


The effect of mechanistic pathway on activity in the Pd and Pt catalysed methoxycarbonylation of ethene

Joanna Wolowska, Graham R. Eastham, Brian T. Heaton,* Jonathan A. Iggo,* Chacko Jacob and Robin Whyman*

The low activity of platinum catalysts in the methoxycarbonylation of ethene is due to trapping of the active intermediates by CO at every step in the catalytic cycle and to the ready reversibility of the product forming reactions.

2786

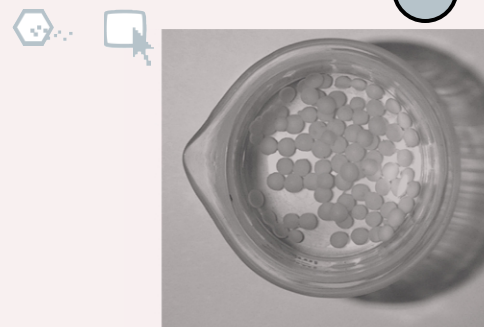


p-Hydroquinone–metal compounds: synthesis and crystal structure of two novel V^{IV}–*p*-hydroquinonate and V^{IV}–*p*-semiquinonate species

Chryssoula Drouza, Vagelis Tolis, Volker Gramlich, Cathrine Raptopoulou, Aris Terzis, Michael P. Sigalas,* Themistoklis A. Kabanos* and Anastasios D. Keramidas*

Reaction of the *p*-hydroquinone derivative $\text{H}_2\text{Na}_4\text{bicah}\cdot 4\text{H}_2\text{O}$ with either $\text{V}^{\text{IV}}\text{OSO}_4\cdot 3\text{H}_2\text{O}$ and $\text{NaV}^{\text{V}}\text{O}_3$ or with $\text{NaV}^{\text{V}}\text{O}_3$ yields the tetranuclear $\text{V}^{\text{IV}}\text{O}_2^+$ macrocycle–semiquinonate compound **1** and the dinuclear *cis*- $\text{V}^{\text{V}}\text{O}_2^+$ –hydroquinone species **2** respectively.

2788

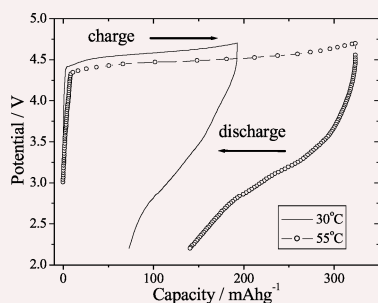


Shape fabrication of millimeter-sized metal-containing carboxymethyl cellulose hollow capsules

A. B. Bourlinos and D. Petridis*

The preparation and perspectives of uniform sized metal-derivatized carboxymethyl cellulose hollow capsules of different morphologies through a self-consistent route is the subject of the present communication.

2790



The origin of electrochemical activity in Li_2MnO_3

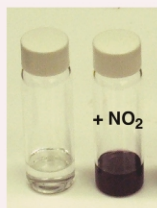
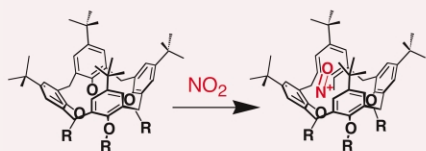
Alastair D. Robertson and Peter G. Bruce*

The layered intercalation compound Li_2MnO_3 , $\text{Li}[\text{Li}_{1/3}\text{Mn}_{2/3}]\text{O}_2$, is shown to be electrochemically active due to an unconventional mechanism involving the exchange of Li^+ by H^+ , the latter generated by oxidation of the non-aqueous electrolyte. There is no evidence that the activity of this material is associated with $\text{Mn}^{4+/5+}$ or loss of oxygen, as suggested previously for Mn^{4+} compounds.

2792

Supramolecular fixation of NO₂ with calix[4]arenes

Grigory V. Zyryanov, Yanlong Kang, Stephen P. Stamp and Dmitry M. Rudkevich*

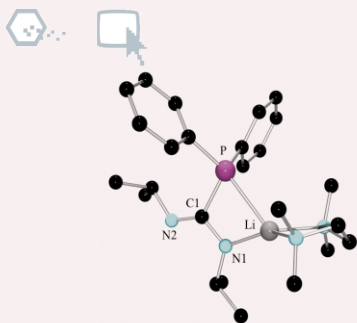


Detection and fixation of NO₂ by calix[4]arenes is demonstrated through encapsulation of nitrosonium NO⁺ cation. Calixarene–NO₂ interactions result in dramatic color changes and can be used for sensing. The reported chemistry also involves reactions of calixarene–NO⁺ complexes with H₂O, alcohols and amides.

2794

Variable coordination chemistry of the phospho(III)guanidinate anion; application as a metal-functionalised phosphine ligand

Martyn P. Coles* and Peter B. Hitchcock



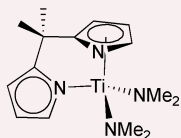
Retention of the lone-pair at phosphorus in the [Ph₂PC{NⁱPr}₂][−] anion leads to a number of possible coordination geometries, which has been exploited in the synthesis of a new class of metal-functionalised phosphine ligand.

2796

Titanium and zirconium complexes supported by dipyrroliide ligands

Andrew Novak, Alexander J. Blake, Claire Wilson and Jason B. Love*

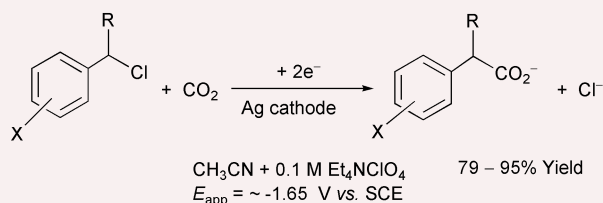
The reactions between *meso*-disubstituted dipyrromethanes and titanium and zirconium amides and alkyls have generated the first examples of dipyrroliide complexes of Group 4 metals.



2798

Electrocatalytic carboxylation of benzyl chlorides at silver cathodes in acetonitrile

Abdirisak A. Isse and Armando Gennaro*



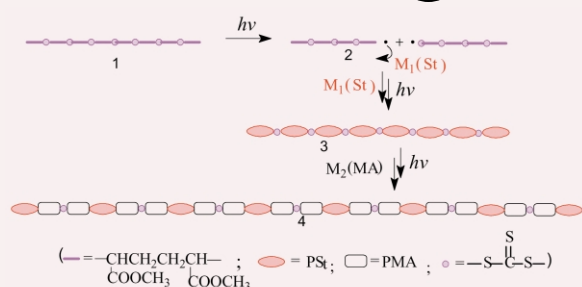
Benzyl chlorides are carboxylated by reduction at Ag, Hg and carbon cathodes in CO₂-saturated CH₃CN. The process at silver gives excellent results in terms both of the required reduction potential and current efficiency.

2800

A novel strategy for synthesis of multiblock copolymers

Ye-Zi You, Chun-Yan Hong and Cai-Yuan Pan*

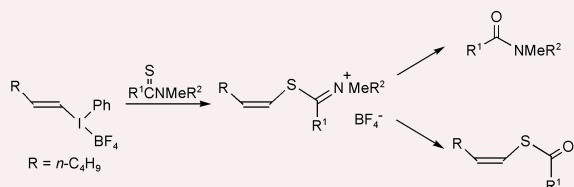
N-triblock copolymers with a well-controlled number of blocks and block chain length can be synthesized in two steps using a 'polyinitiator'.



2802

Vinyl- λ^3 -iodanes act as efficient sulfur atom acceptors: vinylic S_N2 -based strategy for conversion of tertiary thioamides to amides

Masahito Ochiai* and Shinji Yamamoto

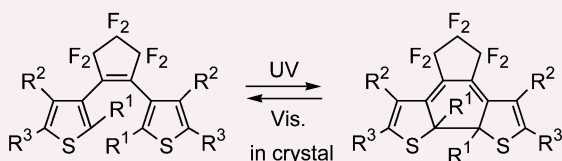


Exposure of tertiary thioamides to (*E*)-1-hexenyl(phenyl)- λ^3 -iodane results in vinylic S_N2 reaction to give inverted (*Z*)-*S*-vinylthioimidonium salts, which under alkaline hydrolysis afford amides, while (*Z*)-*S*-vinyl thioesters are obtained under acidic hydrolysis.

2804

Single-crystalline photochromism of diarylethenes: reactivity–structure relationship

Seiya Kobatake, Kingo Uchida, Eriko Tsuchida and Masahiro Irie*

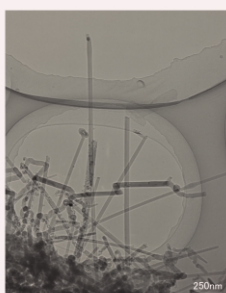


Photochromic reactivity of diarylethenes in the single-crystalline phase was controlled by the distance between the reactive carbon atoms in the antiparallel conformation.

2806

Synthesis of crystalline boron nanowires by laser ablation

Yingjiu Zhang,* Hiroki Ago, Motoo Yumura,* Toshiki Komatsu, Satoshi Ohshima, Kunio Uchida and Sumio Iijima

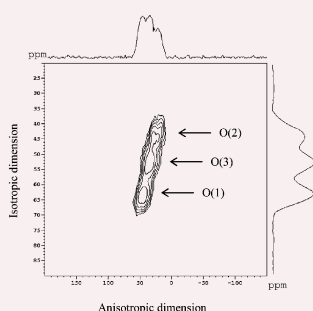


Boron nanowires with tetragonal structure are synthesized by laser ablation; the nanowires at the different positions of the surface of a B/NiCo target usually have different morphologies and sizes.

2808

 ^{17}O MQMAS NMR studies of Na-A and Ca-A

Jennifer E. Readman, Namjun Kim, Martine Ziliox and Clare P. Grey*

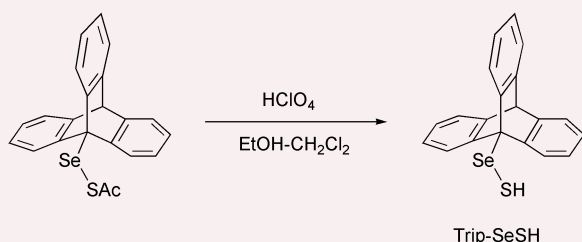


We report, for the first time, ^{17}O MQMAS and $^{17}\text{O}/^{23}\text{Na}$ double resonance NMR studies on calcium-exchanged zeolite sodium-A; the results show that the isotropic shifts of the framework sites are strongly affected by factors including the hydration level and nature of the charge-balancing cations.

2810

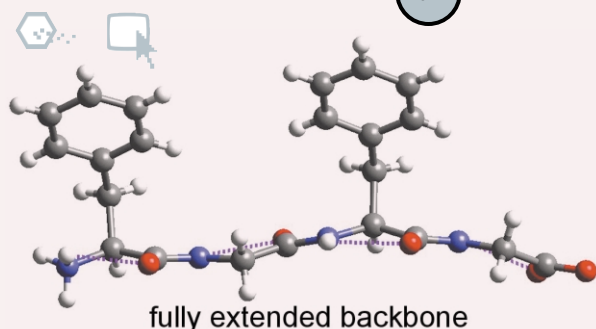
First synthesis and characterization of isolable thioselenenic acid, triptycene-9-thioselenenic acid

Akihiko Ishii,* Takeshi Takahashi, Akira Tawata, Aki Furukawa, Hideaki Oshida and Juzo Nakayama*



Hydrolysis of acetyl triptycene-9-thioselenenate under acidic conditions yielded the first isolable thioselenenic acid, triptycene-9-thioselenenic acid.

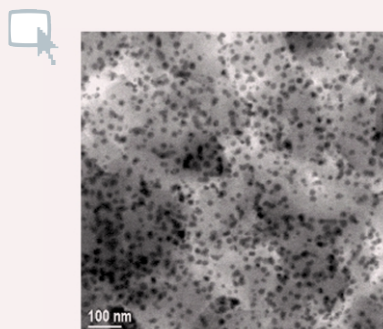
2812

**A fully extended tetrapeptide consisting of natural amino acids**

Henrik Birkedal,* Dieter Schwarzenbach and Philip Pattison

The crystal structure of the tetrapeptide FGFG presents the first example of a fully extended backbone, exempt of intermolecular backbone hydrogen bonding, in a peptide consisting of coded-for amino acids.

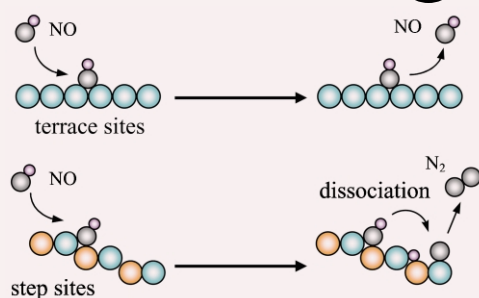
2814

**Synthesis of silver nanoparticles *via* electrochemical reduction on compact zeolite film modified electrodes**

Yahong Zhang, Fei Chen, Jihua Zhuang, Yi Tang,* Deju Wang, Yajun Wang, Angang Dong and Nan Ren

Using compact ultrathin faujasite zeolite film modified electrodes (CZFMEs-FAU) as a substrate, monodisperse silver nanoparticles with different sizes were synthesized by electrochemical reduction inside or outside zeolite crystals according to the silver exchange degree of CZFMEs-FAU.

2816

**Comprehensive study combining surface science and real catalyst for NO direct decomposition**

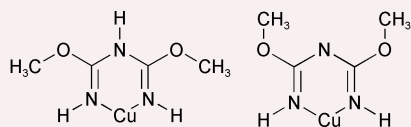
Masaaki Haneda,* Yoshiaki Kintaichi, Isao Nakamura, Tadahiyo Fujitani and Hideaki Hamada

The catalytic activity of Pd/Al₂O₃ prepared from various palladium precursors for direct NO decomposition is closely related to the fraction of surface step sites capable of dissociating NO, on the basis of a surface science study using single-crystal model catalyst.

2818

**A proton induced conformational change in metal complexes with potential hydrogen bonding triplet motifs**

Ian M. Atkinson, Michael M. Bishop, Leonard F. Lindoy,* Srihari Mahadev and Peter Turner

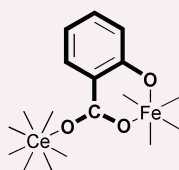


Biguanide-like bidentate ligands in a variety of transition metal complexes of different geometries exhibit conformational changes upon protonation/deprotonation that alter their capacity to recognise complementary hydrogen bonding motifs

2820

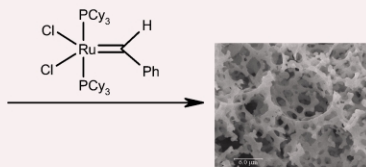
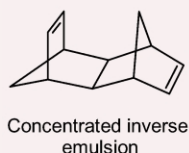
**Heterometallic Ce^{III}-Fe^{III}-salicylate networks: models for corrosion mitigation of steel surfaces by the 'Green' inhibitor, Ce(salicylate)₃**

Glen B. Deacon,* Craig M. Forsyth, Thomas Behrsing, Kristina Konstas and Maria Forsyth



Doubly deprotonated salicylic acid residues, chelating to Fe^{III} and bridging to Ce^{III} form the building blocks of novel heterometallic (Ce/Fe) networks and may constitute structural units in protective layers on Ce(salicylate)₃ treated steel surfaces.

2822

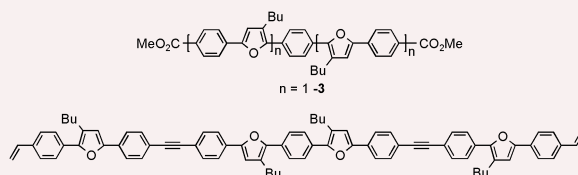


Preparation and functionalisation of emulsion-derived microcellular polymeric foams (polyHIPEs) by ring-opening metathesis polymerisation (ROMP)

Hervé Deleuze,* Romain Faivre and Valérie Herroguez

PolyHIPEs have been prepared by ROMP of a norbornene derivative using a Grubb's catalyst. The resulting material has been further functionalised using the active catalytic sites remaining on its structure.

2824

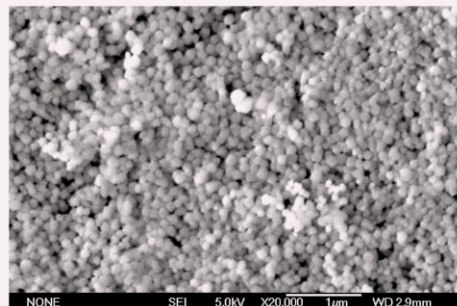


Bidirectional iterative synthesis of alternating benzene-furan oligomers towards molecular wires

Chin-Fa Lee, Ching-Yuan Liu, Hua-Can Song, Shr-Jie Luo, Jui-Chang Tseng, Hsi-Hua Tso and Tien-Yau Luh*

Treatment of propargylic dithioacetal **2a** with BuLi followed by reacting with a dialdehyde yields the corresponding alternating benzene-furan oligoaryls. A combination of this furan annulation, Heck and Sonogashira coupling leads to a variety of benzene-furan-alkene/alkyne conjugated oligomers.

2826

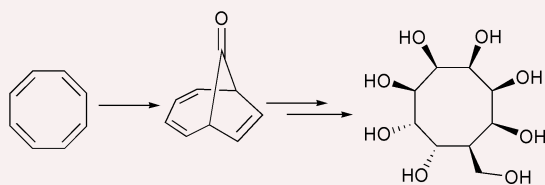


Large-scale synthesis and structure of boron nitride sub-micron spherical particles

Chengchun Tang,* Yoshio Bando* and Dmitri Golberg

A simple method to synthesize BN particles with a uniform diameter is reported.

2828

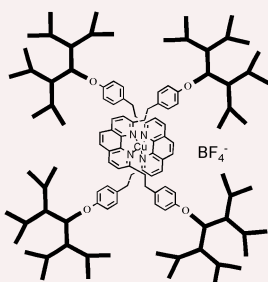


From hydrocarbons to polyols. Cyclooctatetraene to novel cyclooctitols

Goverdhan Mehta* and Kotapalli Pallavi

Cyclooctatetraene (COT) derived bicyclo[4.2.1]nona-2,4,7-trien-9-one has been elaborated to a range of novel cyclooctane polyols with variation in the level of oxygenation and stereochemical pattern.

2830

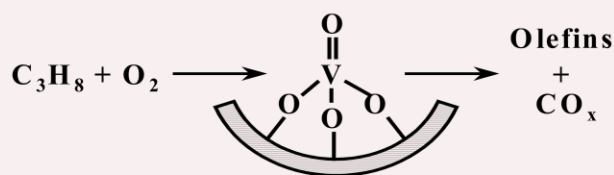


Thin layer cyclic voltammetry: an efficient tool to determine the redox characteristics of large dendrimers

Yannick Rio, Gianluca Accorsi, Nicola Armaroli,* Delphine Felder, Eric Levillain* and Jean-François Nierengarten*

Dendrimers with an electroactive bis(phenanthroline) copper(I) core have been prepared and thin layer cyclic voltammetry (TLCV) found to be an efficient tool to determine their redox characteristics in spite of the slow electron transfer kinetics observed for the largest compounds.

2832



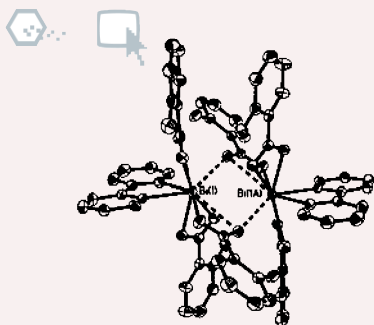
Olefins: propene + ethylene

Highly efficient VO_x/SBA-15 mesoporous catalysts for oxidative dehydrogenation of propane

Yong-Mie Liu, Yong Cao,* Ka-Ke Zhu, Shi-Run Yan, Wei-Lin Dai, He-Yong He and Kang-Nian Fan*

Highly dispersed vanadia species on SBA-15 mesoporous silica have been found to exhibit a highly efficient catalytic performance for the oxidative dehydrogenation (ODH) of propane to light olefins.

2834

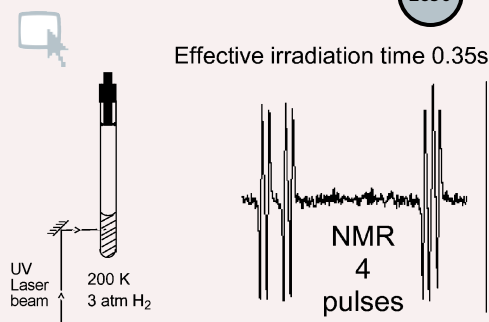


Towards a molecular model for bismuth(III) subsalicylate. Synthesis and solid-state structure of [Bi(Hsal)₃(bipy)(C₇H₈)₂] and [Bi(Hsal)(sal)(1,10-phenanthroline)(C₇H₈)₂]

John H. Thurston, Elodie M. Marlier and Kenton H. Whitmire*

The first homometallic bismuth salicylate complexes, related to biologically active bismuth subsalicylate, have been synthesized and characterized as their bipyridine and phenanthroline adducts that have surprisingly different structures.

2836

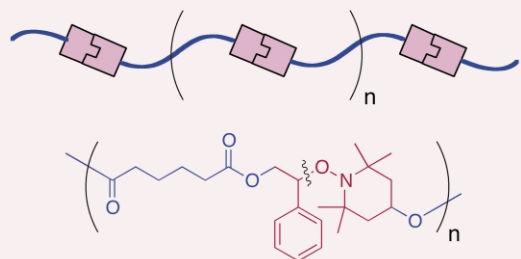


NMR characterisation of unstable solvent and dihydride complexes generated at low temperature by *in-situ* UV irradiation

Cyril Godard, Philip Callaghan, Jenny L. Cunningham, Simon B. Duckett,* Joost A. B. Lohman and Robin N. Perutz

In-situ laser irradiation at *ca.* 200 K is used to generate unstable complexes of the type (η⁵-C₅H₅)Rh(alkene)(η²-toluene) and (η⁵-C₅H₅)Rh(alkene)(H)₂; parahydrogen enhanced spectra can now be observed on photolysis before nuclear relaxation (inset spectrum).

2838

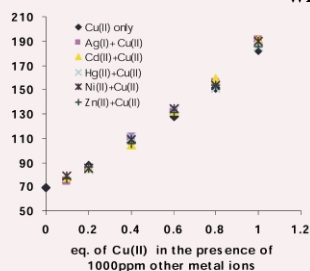
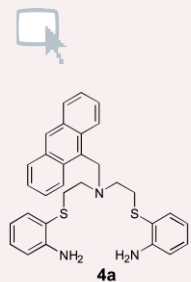


A dynamic (reversible) covalent polymer: radical crossover behaviour of TEMPO-containing poly(alkoxyamine ester)s

Hideyuki Otsuka,* Koichiro Aotani, Yuji Higaki and Atsushi Takahara*

A dynamic covalent polymer incorporating thermally alkoxyamine units in the main chain was synthesized. Due to a radical crossover reaction between the alkoxyamine units, an interchange of the main chains in poly(alkoxyamine ester) was observed on heating.

2840

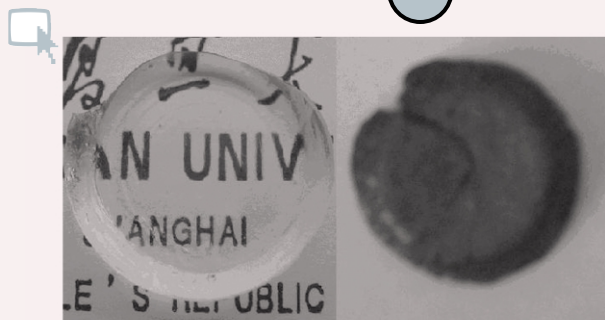


Photoactive chemosensors 3: a unique case of fluorescence enhancement with Cu(II)

Sukhdeep Kaur and Subodh Kumar*

Chemosensor (**4a**) shows fluorescence enhancement with Cu(II) and can estimate Cu(II) by using fluorescence (1–20 μM) spectroscopy.

2842



Synthesis of ordered mesoporous carbon monoliths with bicontinuous cubic pore structure of $Ia3d$ symmetry

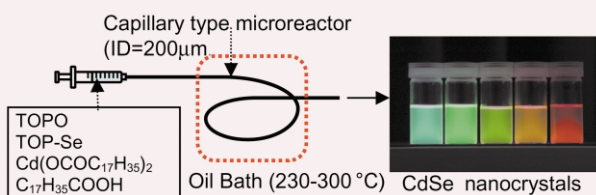
Haifeng Yang, Qihui Shi, Xiaoying Liu, Songhai Xie, Decheng Jiang, Fuqiang Zhang, Chengzhong Yu, Bo Tu and Dongyuan Zhao*

Mesoporous carbon monoliths with bicontinuous cubic structure of $Ia3d$ symmetry were synthesized by using mesoporous silica monoliths as hard templates; the material shows potential application of advanced electrodes and electrochemical double layer capacitors.

2844

Preparation of CdSe nanocrystals in a micro-flow-reactor

Hiroyuki Nakamura, Yoshiko Yamaguchi, Masaya Miyazaki, Hideaki Maeda,* Masato Uehara and Paul Mulvaney

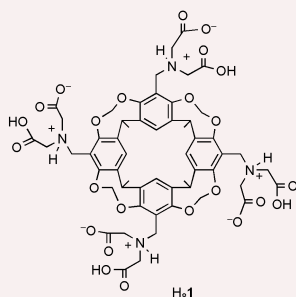


A micro-reactor was utilized for continuous and controlled CdSe nanocrystal preparation in hot surfactant; rapid and exact temperature control of the reactor was beneficial for exact and reproducible controlling of particle diameter.

2846

Novel resorcinarene-based pH-triggered gelator

Scott R. Haines and Roger G. Harrison*

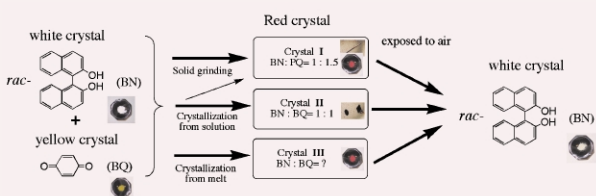


An iminodiacetate resorc[4]arene molecule, **1**, produces gels that are pH-reversible. When the pH of a solution of **1** (concentration >7.6 mM) is lowered to below 2.5 the dissolved molecules aggregate and cause gelation of water.

2848

Generation of a co-crystal phase with novel coloristic properties *via* solid state grinding procedures

Reiko Kuroda,* Yoshitane Imai and Nobuo Tajima

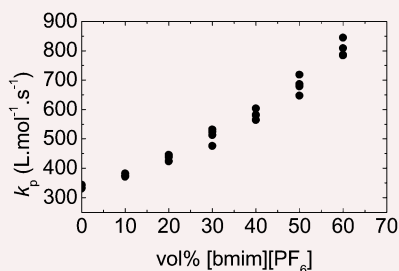


Mixing/grinding of *rac*-BN and BQ crystals produces a co-crystal phase **I** which is different from co-crystals obtained by crystallization from solution (**II**) or melt (**III**), through crystal shearing and molecular diffusion processes in the solid state.

2850

Unprecedented solvent-induced acceleration of free-radical propagation of methyl methacrylate in ionic liquids

Simon Harrison, Stuart R. Mackenzie and David M. Haddleton*

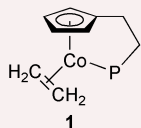


The rate of propagation in the free-radical polymerization of methyl methacrylate in an ionic liquid has been determined and shows unprecedented solvent-induced acceleration, partially explaining the surprising increase in overall rates of polymerization and molecular weights in these solvents.

2852

The first cobalt catalyzed [2 + 2 + 2] alkyne cyclotrimerization in aqueous medium at room temperature

Li Yong and Holger Butenschön*

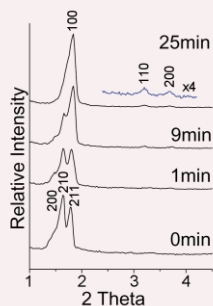


Cobalt(I) chelate complex **1** was found to catalyze the trimerization of terminal alkynes at room temperature in water/ethanol (80:20).

2854

Drying induced phase transformation of mesoporous silica

Ming-Chang Liu, Hwo-Shuenn Sheu and Soofin Cheng*

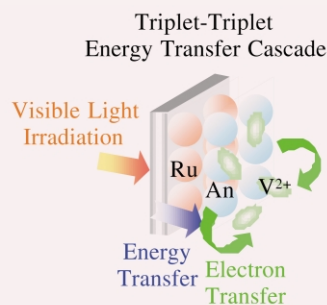


Solvent evaporation upon drying precipitates formed under acidic conditions was the key factor for the phase transformation of mesoporous silica from cubic SBA-1 to hexagonal SBA-3.

2856

Photocurrent amplification by an energy/electron transfer cascade in polymer Langmuir–Blodgett films

Jinfeng Chen, Masaya Mitsuishi, Atsushi Aoki and Tokuji Miyashita*

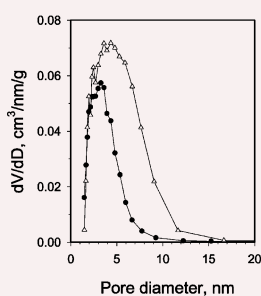


Effective photocurrent amplification was observed in a photoinduced energy/electron transfer cascade system containing hetero-deposited polymer Langmuir–Blodgett films.

2858

Porous nanocomposites of zirconium dioxide and silicate

H. Y. Zhu,* Z. P. Hao and J. C. Barry

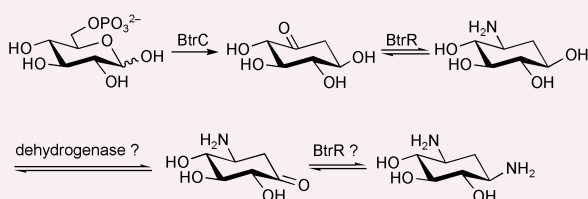


Highly porous nanocomposites of zirconium dioxide and silicate are synthesised in an aqueous system from an inorganic salt of zirconium; the nanocomposites, with tailorable pore structures, exhibit superior performance as catalyst supports.

2860

Biosynthesis of aminoglycoside antibiotics: cloning, expression and characterisation of an aminotransferase involved in the pathway to 2-deoxystreptamine

Fanglu Huang, Yanyan Li, Jinqian Yu and Jonathan B. Spencer*

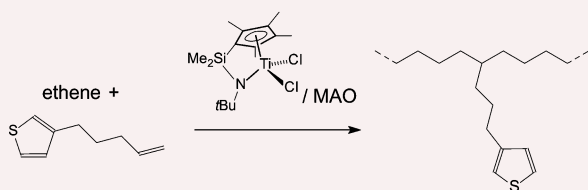


L-Glutamine:2-deoxy-*scyllo*-inosose aminotransferase (BtrR) is shown to catalyses the transamination of 2-deoxy-*scyllo*-inosose to give 2-deoxy-*scyllo*-inosamine, an intermediate in the biosynthesis of 2-deoxystreptamine.

2862

Polyethene with pendant 3-thienyl functionalities

Xiaochun Zhang and Bart Hessen*

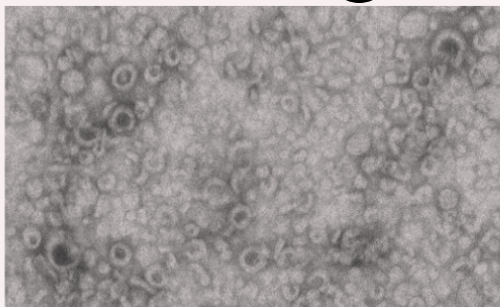


Polyethene with 3-thienyl functionalities pendant on short-chain branches was prepared by catalytic random copolymerisation of ethene and 3-(penten-1-yl)thiophene; the functionalities can be used to graft poly(3-hexylthiophene) onto the polyethene surface.

2864

Cationic β -cyclodextrin bilayer vesicles

Ruth Donohue, Antonino Mazzaglia, Bart Jan Ravoo and Raphael Darcy*

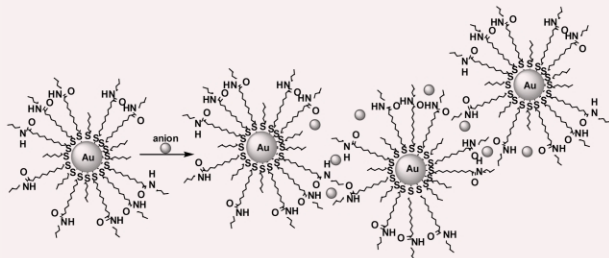


β -Cyclodextrins substituted with hydrophobic *n*-alkylthio chains at the primary hydroxyl side and hydrophilic ω -amino-oligo(ethylene glycol) units at the secondary side are cationic amphiphilic macrocycles that form bilayer vesicles in water.

2866

Enhanced optical sensing of anions with amide-functionalized gold nanoparticles

Shigeru Watanabe,* Miyoko Sonobe, Mari Arai, Yuki Tazume, Takeshi Matsuo, Takashi Nakamura and Katsuhira Yoshida

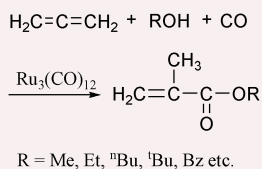


A gold nanoparticle surface-modified with amide ligands shows enhanced optical sensing of anions: the detection limit is increased by about three orders of magnitude higher than that originally expected from the anion binding ability of neutral amide ligands.

2868

Ruthenium-catalyzed carbonylation of allene: direct synthesis of methacrylates and methacrylamides

Da-Yang Zhou, Eiji Yoneda, Kiyotaka Onitsuka and Shigetoshi Takahashi*

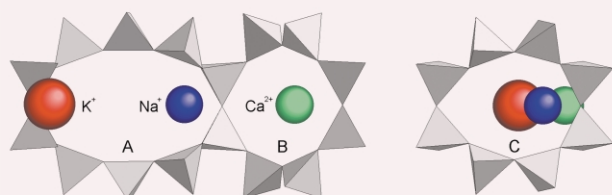


Allene undergoes alkoxy- and amino-carbonylations in alcohols and amines in the presence of a ruthenium carbonyl catalyst under mild conditions to give methacrylates and methacrylamides, respectively, in good yields with an atom economy of 100%.

2870

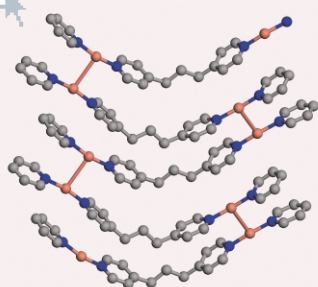
Efficient methane/nitrogen separation with low-sodium clinoptilolite

Jodie E. Guest* and Craig D. Williams



The presence of sodium is shown to have a highly detrimental effect on the methane/nitrogen separation ability of the zeolite clinoptilolite.

2872



[Cu(I)(bpp)]BF₄: the first extended coordination network prepared solvothermally in an ionic liquid solvent

Kun Jin, Xiaoying Huang, Long Pang, Jing Li,* Aaron Appel and Scot Wherland

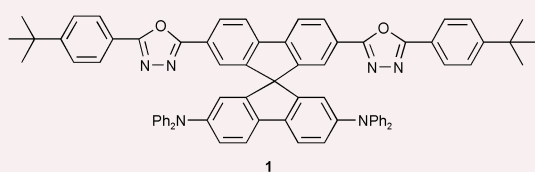
Use of an ionic liquid [bmim][BF₄] (bmim = 1-butyl-3-methylimidazolium) as solvent has resulted in the first extended coordination structure, the two-dimensional network [Cu(bpp)]BF₄ [bpp = 1,3-bis(4-pyridyl)propane] produced *via* a solvothermal route.

2874



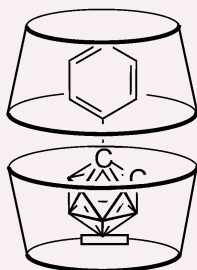
Syntheses and spectroscopic studies of spirobifluorene-bridged bipolar systems; photoinduced electron transfer reactions

Yuh-Yih Chien, Ken-Tsung Wong,* Pi-Tai Chou* and Yi-Ming Cheng



Some 9,9'-spirobifluorene-bridged bipolar systems **1–3** have been synthesized, in which **1** exhibits remarkable solvent-polarity dependent fluorescence properties due to a highly efficient photoinduced electron transfer reaction.

2876

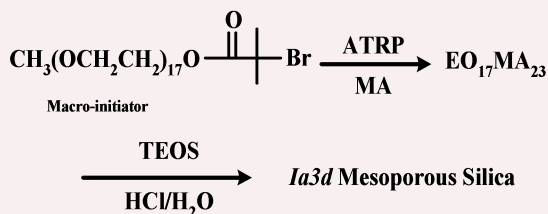


Formation of a remarkably robust 2:1 complex between β -cyclodextrin and a phenyl-substituted icosahedral carborane

Christophe Frixia, Martin Scobie, Steven J. Black, Andrew S. Thompson and Michael D. Threadgill*

The structure of the 2:1 complex between β -cyclodextrin and 1-phenyl-1,2-dicarba-*closo*-dodecaborane(12) is demonstrated by NOE and NOESY spectroscopy; this complex is remarkably refractory.

2878

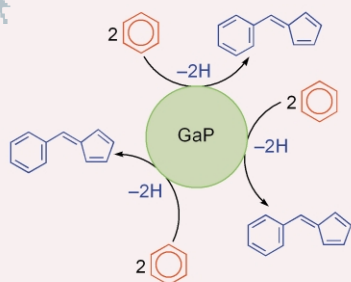


Ia3d Cubic mesoporous silicas using EO₁₇MA₂₃ diblock copolymers made from ATRP

Yi-Tsu Chan, Hong-Ping Lin, Chung-Yuan Mou and Shih-Tzung Liu*

Poly(ethylene oxide)-*b*-poly(methyl acrylate) diblock copolymer (EO_{*m*}MA_{*n*}) prepared *via* an atom transfer radical polymerization (ATRP) approach was used as a template to synthesize Ia3d mesostructured silica with thick walls under acidic conditions.

2880



Thermal conversion of benzene into 6-phenylfulvene with high yield mediated by GaP nanocrystals

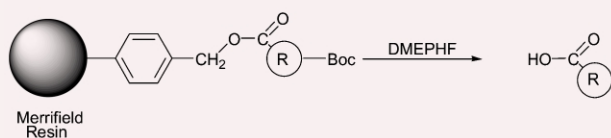
Shanmin Gao, Jun Lu, Yan Zhao, Nan Chen and Yi Xie*

With GaP nanocrystals being used in a closed reaction system, 6-phenylfulvene is successfully obtained *via* a high yield thermal conversion from benzene, which provides the possibility of applying nanocrystals to mediate organic reactions.

2882

Deprotection and cleavage of peptides bound to Merrifield resin by stable dimethyl ether–poly(hydrogen fluoride) (DMEPHF) complex. a new and convenient reagent for peptide chemistry

Béla Török, Imre Bucsi, G. K. Surya Prakash* and George A. Olah*

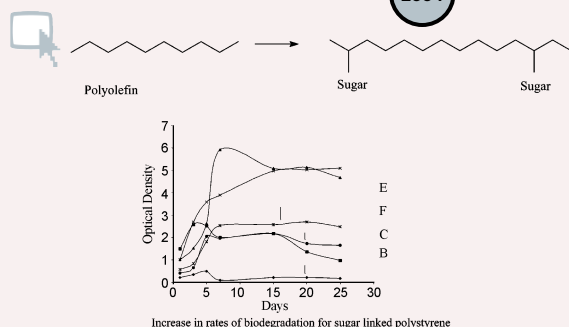


The newly developed stable DMEPHF (1/15) complex was found to be a highly effective reagent for the cleavage of peptides from Merrifield resins; ease of handling and its simple, complete removal from the reaction mixture make the reagent system a very useful HF equivalent for applications in solid-phase peptide synthesis.

2884

Towards biodegradable polyolefins: strategy of anchoring minute quantities of monosaccharides and disaccharides onto functionalized polystyrene, and their effect on facilitating polymer biodegradation

Padmaja Galgali, Anjani J. Varma,* Ulka S. Puntambekar and Digambar V. Gokhale*

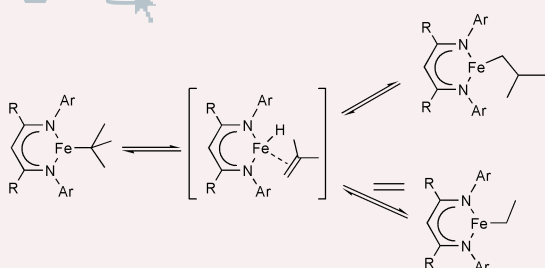


Rates of biodegradation of polystyrenes were greatly enhanced by anchoring minute quantities (1–3.7%) of glucose, sucrose or lactose, onto functionalized polystyrene.

2886

Alkyl isomerisation in three-coordinate iron(II) complexes

Javier Vela, Jeremy M. Smith, Rene J. Lachicotte and Patrick L. Holland*

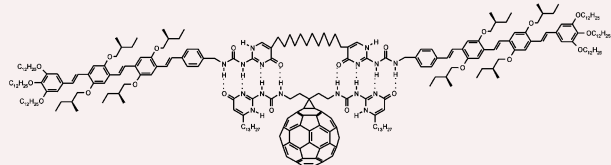


The *tertiary* to *iso*-butyl isomerisation of three-coordinate iron(II) diketiminate complexes is reported and a hydride intermediate is proposed on the basis of exchange experiments.

2888

Preferential hetero-dimer formation and equilibrium dynamics of self-complementary bifunctional oligo(*p*-phenylenevinylene) and C₆₀ ureido-pyrimidinone derivatives in solution

Edwin H. A. Beckers, Albertus P. H. J. Schenning, Paul A. van Hal, Abdelkrim El-ghayoury, Luis Sánchez, J. C. Hummelen, E. W. Meijer and René A. J. Janssen*

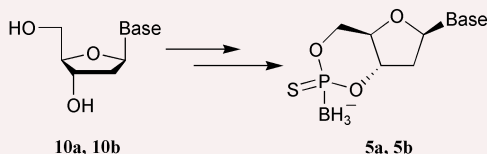


Hetero-dimers of bifunctional oligo (*p*-phenylenevinylene) and C₆₀ ureido-pyrimidinones was observed by ¹H-NMR and fluorescence techniques.

2890

Synthesis of nucleoside 3',5'-cyclic boranophosphorothioate, a new type of cyclic nucleotide

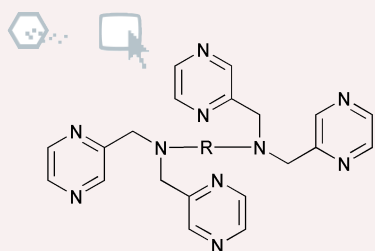
Ping Li and Barbara Ramsay Shaw*



a: Base = Thymine
b: Base = 5-Fluorouracil

The first examples of a borane-containing doubly *P*-modified chiral cyclic nucleoside monophosphate (cNMP), *e.g.*, thymidine and 5-fluoro-2'-deoxyuridine 3',5'-cyclic boranophosphorothioates **5**, have been synthesized; these cNMP analogues with increased lipophilicity could be potential anticancer prodrugs and useful probes for mechanistic studies.

2892



R = (CH₂)₂ tpzen FS_{Am/Eu} = 70
 R = (CH₂)₃ tpztn FS_{Am/Eu} = 2
 R = *trans*-1,2-*c*-C₆H₁₀ tpzcn FS_{Am/Eu} = 2

The important effect of ligand architecture on the selectivity of metal ion recognition in An(III)/Ln(III) separation with N-donor extractants

Lydia Karmazin, Marinella Mazzanti,* Christelle Gateau, Clément Hill and Jacques Pécaut

Small variations of the ligand architecture yield drastic differences in selectivity in the preferential extraction of Am(III) with respect to Eu(III). The tetrapodal ligand tpzen, is found to have one of the largest separation efficiencies so far reported for aza-aromatic extractants, while tpztn and tpzcn show no selectivity at all.

2894

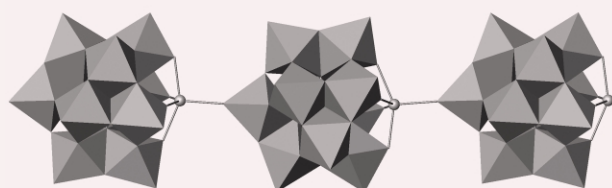


Silver nanowires: inclusion in and extrusion from a mesoporous template

Liam M. Worboys, Peter P. Edwards* and Paul A. Anderson*

Polycrystalline and single-crystal silver nanowires can be extruded under an electron beam from SBA-15 crystallites that also contain silver nanowires within their channels, prepared through the thermal decomposition of occluded silver nitrate.

2896

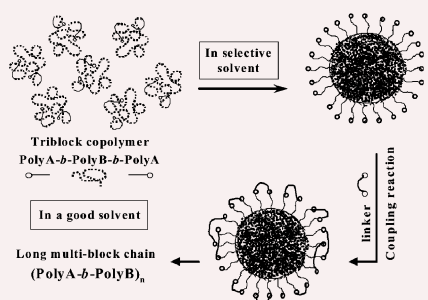


Self-assembly of a lacunary α -Keggin undecatungstophosphate into a three-dimensional network linked by *s*-block cations

Noritaka Honma, Katsuhiko Kusaka and Tomoji Ozeki*

In [(CH₃)₄N]₄Na₂H[PW₁₁O₃₉]·8H₂O, the sodium cation embedded into the lacuna of [PW₁₁O₃₉]⁷⁻ links the oxometalate building blocks into a 1-D chain and the other Na⁺ cation connects the chains into a 3-D network.

2898

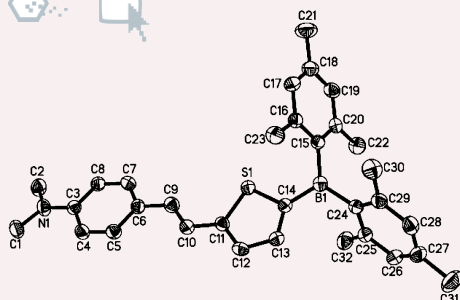


Self-assembly assisted polymerization (SAAP): approaching long multi-block copolymers with an ordered chain sequence and controllable block length

Chi Wu, Zuwei Xie, Guangzhao Zhang, Guofu Zi, Yingfeng Tu, Yali Yang, Ping Cai and Ting Nie

A combination of polymer physics and synthetic chemistry has enabled us to develop self-assembly assisted polymerization (SAAP), leading to the preparation of long multi-block copolymers with an ordered chain sequence and controllable block lengths.

2900



Trivalent boron as acceptor in D- π -A chromophores: synthesis, structure and fluorescence following single- and two-photon excitation

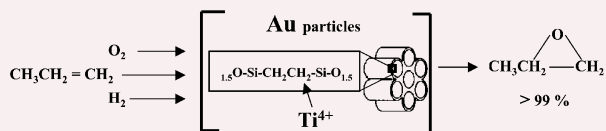
Zhi-qiang Liu, Qi Fang,* Dong Wang, Gang Xue, Wen-tao Yu, Zong-shu Shao and Min-hua Jiang

A series of new stable D- π -A type compounds with trivalent boron as acceptor have been synthesized and one crystal structure described. These compounds show strong two-photon excited up-conversion fluorescence.

2902

Hydrophobicity induced vapor-phase oxidation of propene over gold supported on titanium incorporated hybrid mesoporous silsesquioxane

M. P. Kapoor, A. K. Sinha, S. Seelan, S. Inagaki,* S. Tsubota, H. Yoshida and M. Haruta



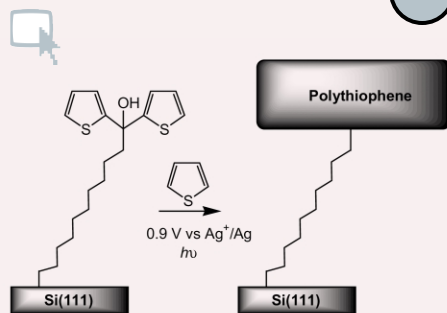
Gold nanoparticles supported on highly hydrophobic ethane bridged Ti incorporated mesoporous organosilica are reported for enhanced vapor phase epoxidation of propene using H₂ and O₂.

2904

Functionalization of Si(111) surfaces with alkyl chains terminated by electrochemically polymerizable thienyl units

Bruno Fabre, Greg P. Lopinski and Danial D. M. Wayner*

Novel polythiophene/semiconductor junctions have been achieved from Si(111) functionalized with a thiophene-terminated alkyl monolayer.

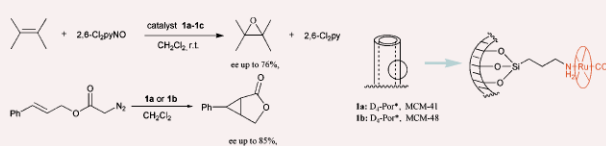


2906

Chiral ruthenium porphyrin encapsulated in ordered mesoporous molecular sieves (MCM-41 and MCM-48) as catalysts for asymmetric alkene epoxidation and cyclopropanation

Jun-Long Zhang, Yun-Ling Liu and Chi-Ming Che*

Encapsulation of chiral ruthenium porphyrin [Ru^{II}(D₄-Por*)CO] in modified mesoporous silica supports such as MCM-41 and MCM-48 achieves active catalysts for asymmetric epoxidation of alkenes by 2,6-dichloropyridine *N*-oxide and intramolecular cyclopropanation.

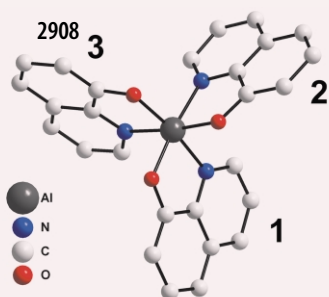


The

structure of the blue luminescent δ -phase of tris(8-hydroxyquinoline)aluminium(III) (Alq₃)

Michael Cölle,* Robert E. Dinnebier and Wolfgang Brütting

The first clear proof of the existence of the facial isomer in the δ -phase of Alq₃ is given. Both the higher symmetry of the molecule compared to the meridional isomer as well as the reduced interligand π -orbital overlap in the crystalline state are the reasons for the significantly different optical properties of δ -Alq₃ as compared to all other known phases.

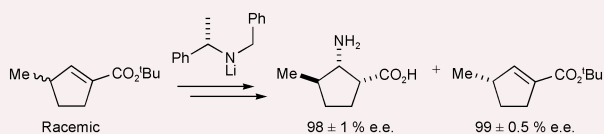


2910

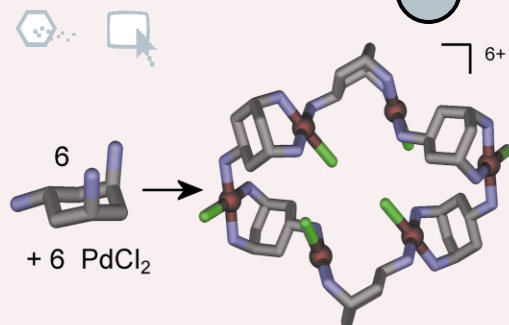
Asymmetric synthesis of (1*R*,2*S*,3*R*)- γ -methyl-*cis*-pentacin by a kinetic resolution protocol

Simon Bailey, Stephen G. Davies,* Andrew D. Smith and Jonathan M. Withey

The asymmetric synthesis of (1*R*,2*S*,3*R*)-3-methyl-2-aminocyclopentane carboxylic acid has been achieved *via* kinetic resolution of racemic *tert*-butyl 3-methylcyclopentene-1-carboxylate with homochiral lithium (*S*)-*N*-benzyl-*N*- α -methylbenzylamide.



2912

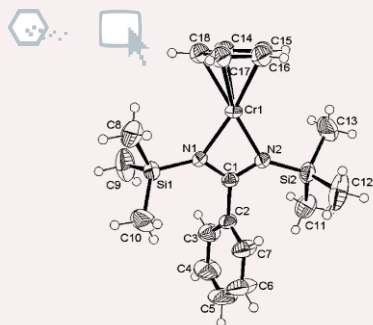


Self-assembly of a twelve-component hexanuclear metallomacrocycle constructed with a novel tri-amino ligand

Georg Seeber, Benson Kariuki and Leroy Cronin*

Reaction of the novel ligand *cis,trans*-1,3,5-triaminocyclohexane with palladium(II) chloride results in the self assembly of a hexanuclear ring cluster that has been characterised both in the solid state and in solution.

2914

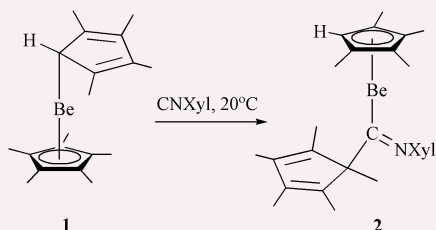


Cyclopentadienyl benzamidinato chromium complexes as models for alkyl halide activation by chromium reagents

Amanda J. Gallant, Kevin M. Smith* and Brian O. Patrick

The use of bulky, monoanionic, bidentate nitrogen-donor ligands permit the synthesis of the illustrated CpCr(II) complex, as well as the corresponding Cr(III) chloro and Cr(III) benzyl compounds.

2916



Synthesis and structural characterization of Be(η^5 -C₅Me₅)(η^1 -C₅Me₄H). Evidence for ring-inversion leading to Be(η^5 -C₅Me₄H)(η^1 -C₅Me₅)

M. M. Conejo, R. Fernández, D. del Río, E. Carmona,* A. Monge and C. Ruiz

Nonamethylberyllocene, characterized by X-ray methods as Be(η^5 -C₅Me₅)(η^1 -C₅Me₄H), reacts at room temperature with CNXyl (Xyl = C₆H₃-2,6-Me₂) to give the iminoacyl product derived from the inverted structure, Be(η^5 -C₅Me₄H)(η^1 -C₅Me₅).

ADDITIONS AND CORRECTIONS

2918

Haruhiko Taguchi, Hiroko Miyashita, Akira Tsubouchi, Takeshi Takeda

First anionic silyl migration from sp² carbon to carbonyl oxygen. Stereospecific allylation of (*Z*)- β -trimethylsilyl- α,β -unsaturated ketones

2919

Yasunari Maekawa, Tomonori Inaba, Hiroki Hobo, Tadashi Narita, Hiroshi Koshikawa, Seongyun Moon, Jun Kato, Masaru Yoshida

Radiation-induced reactions *via* the lowest excited states in cinnamic acid crystals

2919

Nathalie Guillou, Sybille Pastre, Carine Livage and Gérard Férey

The first 3-D ferrimagnetic nickel fumarate with an open framework: [Ni₃(OH)₂(O₂C-C₂H₂-CO₂)(H₂O)₄] \cdot 2H₂O

Dates, venues and contact details of forthcoming events.

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