

**Cover**

Recent introduction of ionically cross-linked LB films provides new opportunities for an old technology (pp. 2787–2791).



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Chemical Technology
in this issue

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T5

Chemical Technology

December 2004/Volume 1/Issue 2

www.rsc.org/chemicaltechnology

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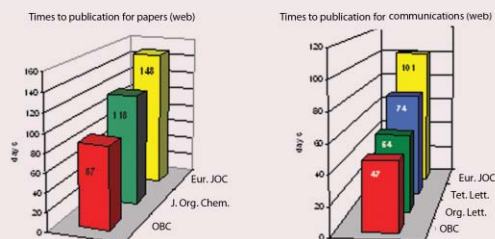
COMMENT

2781

Comment: 2004's fastest organic and biomolecular chemistry!

Caroline V. Potter,* Sarah Thomas, Janet L. Dean, Adrian P. Kybett, Richard Kidd, Melanie James and Helen Saxton

Comment: 2004's fastest organic and biomolecular chemistry!



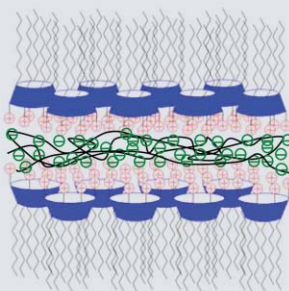
FEATURE ARTICLE

2787

Don't forget Langmuir–Blodgett films

Donald H. McCullough, III and Steven L. Regen*

Despite considerable efforts that have been aimed at exploiting the nonlinear optical, piezoelectric, pyroelectric, semiconducting, sensing and barrier properties of Langmuir–Blodgett (LB) films, problems associated with film quality and stability have hampered their practical development. The recent introduction of ionically cross-linked (*i.e.*, 'glued') LB films provides new opportunities for an old technology that has been waning in recent years.



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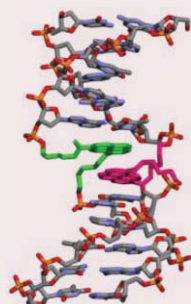
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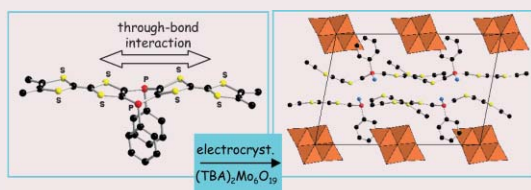


Excimer formation by interstrand stacked pyrenes

Simon M. Langenegger and Robert Häner*

Non-nucleosidic, pyrene-derived base surrogates form excimers *via* interstrand stacking in duplex DNA.

2794

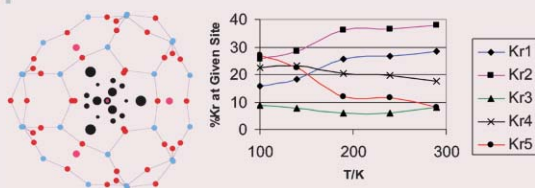


1,4-Dihydro-1,4-diphosphinine fused with two tetrathiafulvalenes

Narcis Avarvari* and Marc Fourmigué*

Electronic interactions between two TTF moieties fused to a rigid 1,4-dihydro-1,4-diphosphinine (single crystal X-ray structures of the *cis* isomer and a mixed-valent radical cation salt of the same isomer) are identified thanks to electrochemical and theoretical investigations.

2796

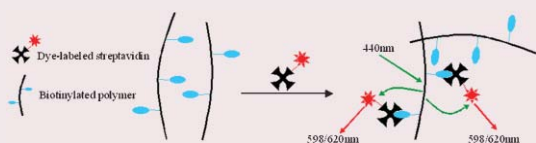


The dynamic desorption of krypton from the zeolite chabazite

S. P. Cork, G. Cressey, R. H. Jones,* S. J. Teat and V. L. Zholobenko

Single crystal diffraction studies of chabazite show that at high loading krypton atoms must occupy sites with unfavourable interatomic Kr–Kr separations. Upon desorption the remaining Kr atoms occupy sites with no such unfavourable separations.

2798

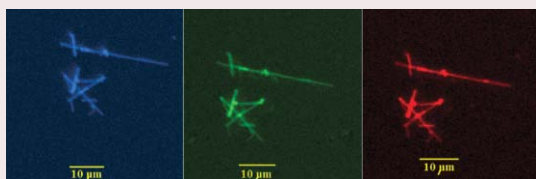


Biotinylated poly(*p*-phenylene ethynylene): unexpected energy transfer results in the detection of biological analytes

Juan Zheng and Timothy M. Swager*

A sensitive assay was designed based on the interaction between biotinylated conjugated polymer and dye-labeled streptavidin, using energy transfer as a transduction platform. Higher energy transfer was observed with decreased spectral overlap between the donor and the acceptor.

2800

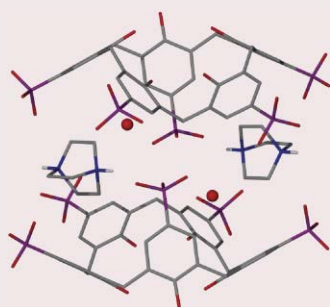


Crystalline oligopyrene nanowires with multicolored emission

Liangti Qu and Gaoquan Shi*

Highly crystalline oligopyrene nanowires have been prepared by template-assisted electropolymerization of pyrene, which can emit strong blue, green and red fluorescence as excited at 405, 488, 543 nm, respectively.

2802

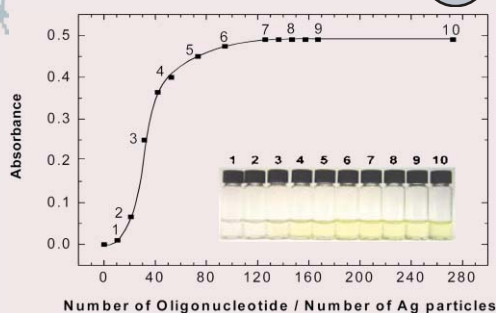


Conformation perturbation of *p*-sulfonatocalix[5]arene via complexation of 1,4-diazabicyclo[2.2.2]octane

Scott J. Dalgarno, Michaele J. Hardie and Colin L. Raston*

The conformation of bowl shaped *p*-sulfonatocalix[5]arene is dramatically altered through complexation of 1,4-diazabicyclo[2.2.2]octane, forming an unprecedented 'bis-molecular capsule' arrangement consisting of two di-protonated DABCO molecules and two water molecules shrouded by two *p*-sulfonatocalix[5]arenes.

2804

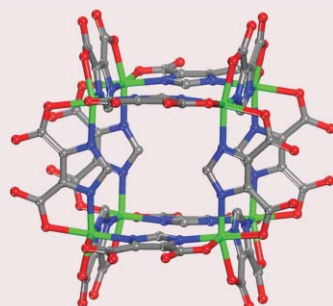


Gold and silver nanoparticles functionalized with known numbers of oligonucleotides per particle for DNA detection

Yang Chen, Jenny Aveyard and Robert Wilson*

The biospecificity of gold and silver nanoparticles, functionalized with known numbers of oligonucleotides linked to PDP-dextran, is demonstrated in colorimetric microbead assays for complementary and mismatch sequences.

2806



Directed assembly of metal-organic cubes from deliberately pre-designed molecular building blocks

Yunling Liu, Victor Kravtsov, Rosa D. Walsh, Pankaj Poddar, Hariharan Srikanth and Mohamed Eddaoudi*

A novel anionic metal-organic cube (MOC-1), $[\text{Ni}_8(\text{HImDC})_{12}]^{8-}$, has been synthesized by metal-ligand directed assembly of eight tri-connected Ni nodes and twelve doubly deprotonated bis(bidentate) imidazolecarboxylic acid ligands (HImDC).

2808

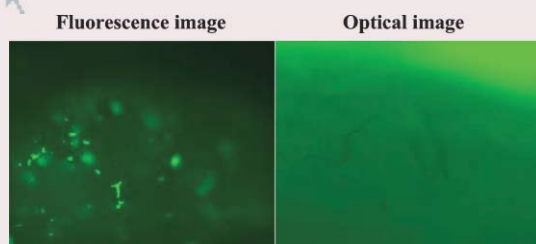


A discrete dimer of coordination clusters connected through additional bridging ligands

Jianyong Zhang, Mark Nieuwenhuyzen, Jonathan P. H. Charmant and Stuart L. James*

The self-assembly of a nanoscale 'cluster of clusters' has been achieved by using a directional cluster with unsaturated metal sites as a building block.

2810

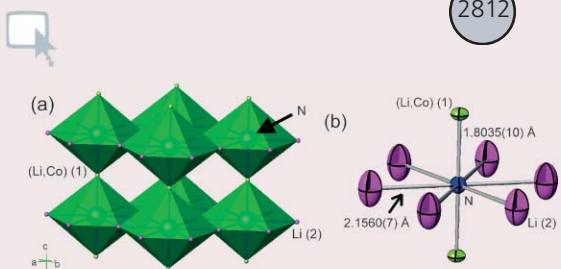


TAT conjugated, FITC doped silica nanoparticles for bioimaging applications

Swadeshmukul Santra,* Heesun Yang, Debamitra Dutta, Jessie T. Stanley, Paul H. Holloway, Weihong Tan, Brij M. Moudgil and Robert A. Mericle

Synthesis of TAT peptide conjugated 70 nm size FITC doped silica nanoparticles (TAT-FSNPs) is reported for the first time. Using TAT-FSNPs, human lung adenocarcinoma (A-549) cells (*in vitro*) and rat brain tissue (*in vivo*) were successfully labeled, which demonstrated the feasibility of using TAT mediated nanoparticle based bioimaging.

2812

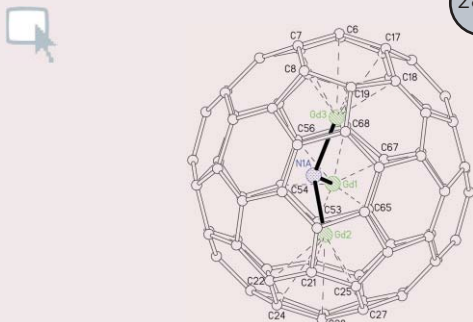


Crystal growth, defect structure and magnetism of new Li_3N -derived lithium nitridocobaltates

Alexandra G. Gordon, Ronald I. Smith, Claire Wilson, Zlatka Stoeva and Duncan H. Gregory*

New nitridocobaltates $\text{Li}_{3-x-y}\text{Co}_x\text{N}$ contain significant Li^+ vacancies ($y \approx 0.45$) disordered within lithium–nitrogen planes and exhibit increased covalency through infinite $-\text{N}-(\text{Li},\text{Co})-\text{N}-$ chains. These features could yield improved anodes for secondary lithium ion batteries.

2814

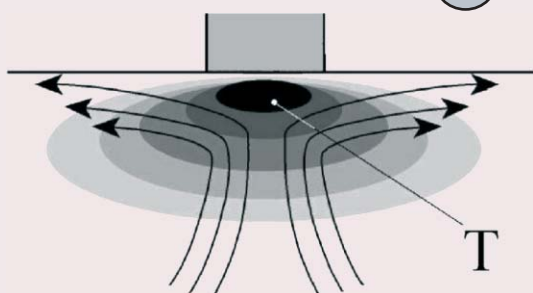


Pyramidalization of Gd_3N inside a C_{80} cage. The synthesis and structure of $\text{Gd}_3\text{N}@C_{80}$

Steven Stevenson,* J. Paige Phillips, Jon E. Reid, Marilyn M. Olmstead, Sankar Prasad Rath and Alan L. Balch*

The synthesis and X-ray crystal structure of $\text{Gd}_3\text{N}@C_{80}$ are reported.

2816

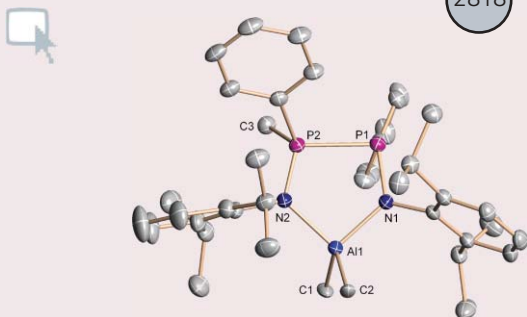


Microwave activation in ionic liquids induces high temperature–high speed electrochemical processes

Ujjal Kumar Sur, Frank Marken,* Barry A. Coles, Richard G. Compton and Jairton Dupont

Self-focusing of intense microwave radiation at microelectrodes immersed in ionic liquids dramatically enhances voltammetric current signals and temperatures to give extreme conditions sufficient for condensed phase pyrolysis processes to occur.

2818

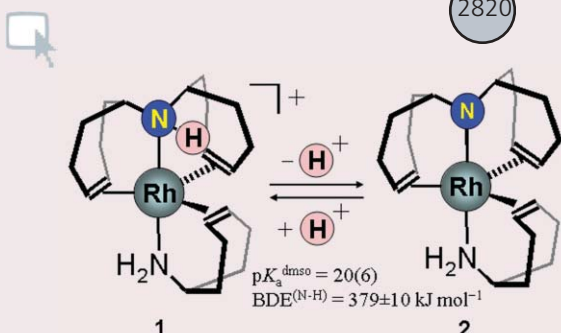


Formation of a chiral NPPN ligand *via* metallation of acyclic NPNCN systems

Tristram Chivers,* May C. Copsey and Masood Parvez

A new type of bidentate N,N' -chelating ligand containing a chiral phosphorus centre has been synthesized *via* the metallation of an acyclic NPNCN species. The zwitterionic ligand backbone contains a phosphonium centre stabilised by an imido phosphine fragment.

2820

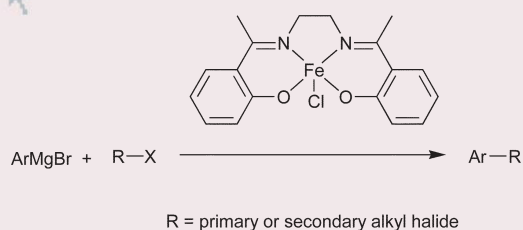


Amine olefin rhodium(i) complexes: $\text{p}K_a$ and NH bond strength

Torsten Büttner, Frank Breher and Hansjörg Grützmacher*

The rhodium amine olefin complex **1** is deprotonated to give the remarkably stable corresponding rhodium(i) amide **2**. Reversible oxidation at $E^\circ(\text{dmsO}) = -0.466 \text{ V}$ (vs. Fc/Fc^+) allows the determination of the NH bond dissociation energy (BDE).

2822

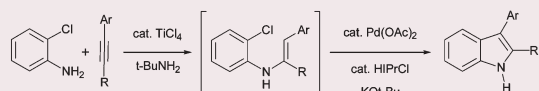


Iron(III) salen-type catalysts for the cross-coupling of aryl Grignards with alkyl halides bearing β -hydrogens

Robin B. Bedford,* Duncan W. Bruce, Robert M. Frost, John W. Goodby and Michael Hird

Salen-type complexes of iron(III) prove to be highly active catalysts in the coupling of aryl Grignard reagents with primary and secondary alkyl halides.

2824

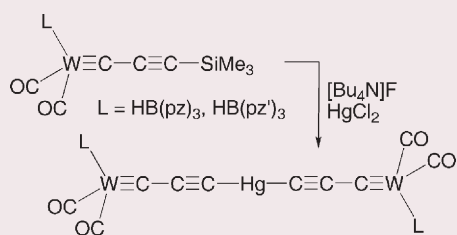


Hydroamination/Heck reaction sequence for a highly regioselective one-pot synthesis of indoles using 2-chloroaniline

Lutz Ackermann,* Ludwig T. Kaspar and Christian J. Gschrei

A one-pot protocol consisting of a highly regioselective TiCl_4 -catalyzed hydroamination and a 5-*endo* Heck cyclization starting from 2-chloroaniline allows a concise and efficient indole synthesis.

2826

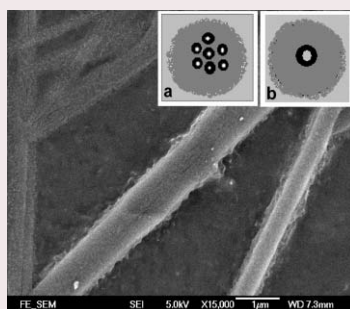


A mercury bis(tricarbido) complex: $[\text{Hg}\{\text{C}\equiv\text{C}-\text{C}\equiv\text{W}(\text{CO})_2\text{Tp}\}_2(\text{dmsO})_4(\text{dmsO})_2]$ (Tp = hydrotrispyrazolylborate)

Rian D. Dewhurst, Anthony F. Hill* and Anthony C. Willis

The first example of a structurally characterised octahedral diorganomercurial complex with unidentate ligands.

2828

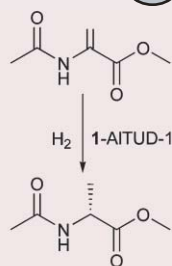
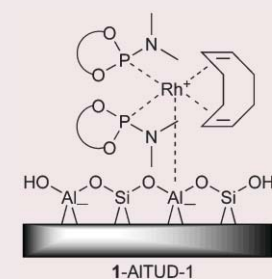


Fabrication of nanowires with polymer shells using treated carbon nanotube bundles as macro-initiators

Yuyang Liu,* Jing Tang and J. H. Xin

Nanowires with polymer shells were produced *via* radical grafting polymerization of methyl methacrylate using treated carbon nanotube bundles as macro-initiators, thereby providing an efficient way to produce high grafting ratio nanocomposites.

2830

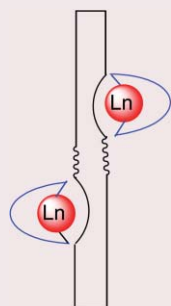


Efficient immobilisation of Rh-MonoPhos on the aluminosilicate AITUD-1

Chrétien Simons, Ulf Hanefeld, Isabel W. C. E. Arends, Adriaan J. Minnaard, Thomas Maschmeyer* and Roger A. Sheldon*

Rhodium-MonoPhos was successfully immobilised by ionic interactions on aluminosilicate AITUD-1. The resulting new heterogeneous catalyst can be used in water and showed excellent enantioselectivity and activity in the asymmetric hydrogenation of methyl-2-acetamidocrylate.

2832

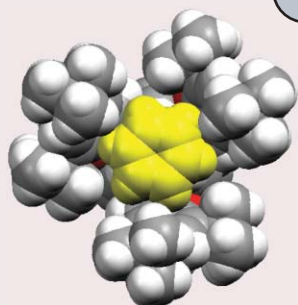


Controlled assembly of luminescent racks based on heteroleptic dinuclear lanthanide complexes

M. Margarita Castaño-Briones, Andrew P. Bassett, Linette L. Meason, Peter R. Ashton and Zoe Pikramenou*

Dinuclear luminescent lanthanide racks are formed in solution through controlled supramolecular assembly of different ligands around the lanthanide. This represents a powerful strategy for solution assembly of polynuclear lanthanide complexes.

2834

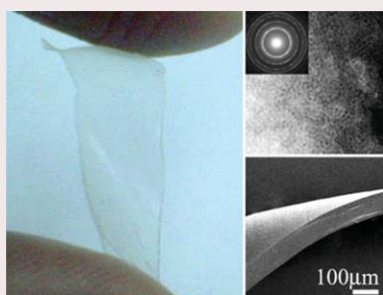


Boron–nitrogen macrocycles: a new generation of calix[3]arenes

Victor Barba,* Herbert Höpfl, Norberto Farfán, Rosa Santillan, Hiram I. Beltran and Luis S. Zamudio-Rivera

An air-stable boron–nitrogen macrocycle having a cone-like conformation and two possible sites for guest inclusion has been prepared in a simple one-pot synthesis.

2836

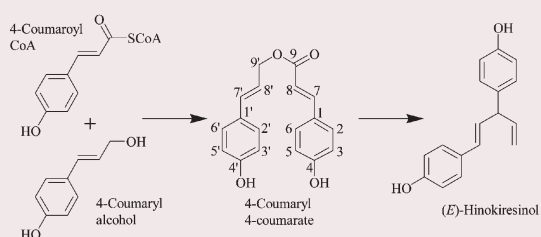


Synthesis of self-standing mesoporous nanocrystalline titania–phosphorus oxide composite films

Hui-suk Yun, Haoshen Zhou and Itaru Honma*

Self-standing, transparent, thick (~90 μm) mesoporous titania–phosphorus oxide films containing anatase nanocrystallites were synthesized by the evaporation-induced co-assembly of a triblock copolymer template, titanium tetraethoxide, and phosphorus chloride.

2838

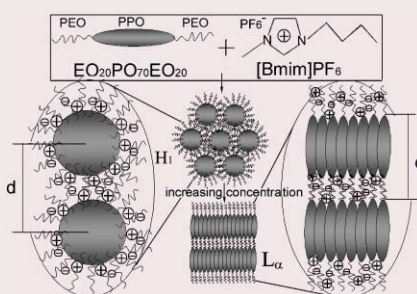


A heartwood norlignan, (*E*)-hinokiresinol, is formed from 4-coumaryl 4-coumarate by a *Cryptomeria japonica* enzyme preparation

Shiro Suzuki, Masaomi Yamamura, Mikio Shimada and Toshiaki Umezawa*

An enzyme preparation from *Cryptomeria japonica* catalyses the formation of (*E*)-hinokiresinol, but not via the (*Z*)-isomer, from 4-coumaroyl CoA and 4-coumaryl alcohol, and from 4-coumaryl 4-coumarate.

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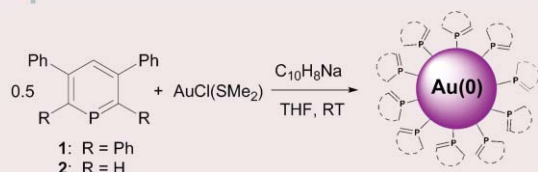


Lyotropic liquid crystalline phases formed in an ionic liquid

Luyan Wang, Xiao Chen,* Yongcun Chai, Jingcheng Hao, Zhenming Sui, Wenchang Zhuang and Zhenwen Sun

Block copolymer EO₂₀PO₇₀EO₂₀ can self-assemble in IL [Bmim]PF₆ to form hexagonal (H₁) and lamellar phases (L_α), including IL polar domains containing PEO blocks and solvophobic PPO domains, due to interactions between EO moieties and the IL.

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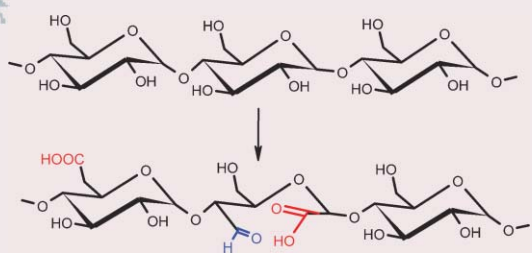


Phosphinine stabilised gold nanoparticles; synthesis and immobilisation on mesoporous materials

Audrey Moores, Frédéric Goettmann, Clément Sanchez* and Pascal Le Floch*

The first gold nanoparticles stabilised by sp^2 -hybridised P ligands were synthesised. The strong affinity of sp^2 -hybridised P atoms toward Au(0) centres allows sub-stoichiometric quantities of ligand to be used. These phosphinine-based nanoparticles were also immobilised on mesostructured materials.

2844

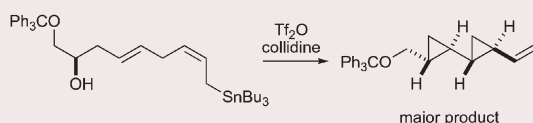


A novel clean catalytic method for waste-free modification of polysaccharides by oxidation

Svetlana L. Kachkarova-Sorokina, Pierre Gallezot and Alexander B. Sorokin*

A single step, tailor made modification of polysaccharides by oxidation exemplified with starch has been achieved using only a small amount of iron phthalocyanine catalyst (0.0078 mol%), benign H_2O_2 oxidant and water.

2846

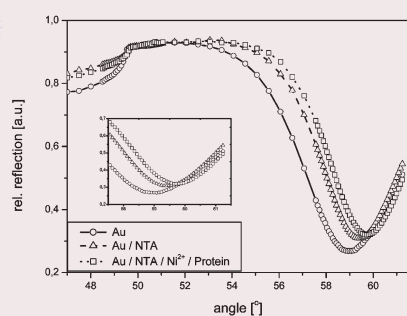


Stereochemistry of contiguous cyclopropane formation from cascade cyclization of a skipped dienylyl triflate

Christopher M. Lincoln, James D. White* and Alexandre F. T. Yokochi

Solvolysis of asymmetric homoallylic triflates bearing a terminal stannyl substituent gives disubstituted cyclopropanes and bicyclopropanes bearing differentiated termini in high enantiomeric purity.

2848

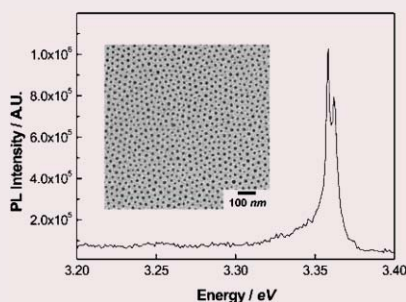


Monitoring the formation of biosilica catalysed by histidine-tagged silicatein

Muhammad Nawaz Tahir, Patrick Théato, Werner E. G. Müller, Heinz C. Schröder, Andreas Janshoff, Jian Zhang, Joachim Huth and Wolfgang Tremel*

Surface bound silicatein retains its biocatalytic activity, which was demonstrated by monitoring the immobilisation of silicatein using a histidine-tag chelating anchor and the subsequent biosilicification of SiO_2 on surfaces.

2850

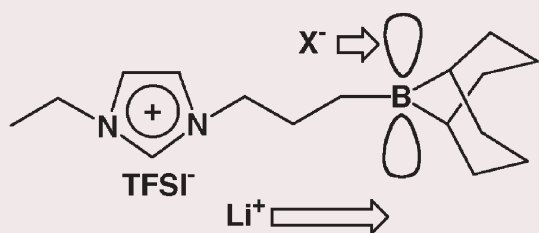


Self-assembled arrays of zinc oxide nanoparticles from monolayer films of diblock copolymer micelles

Seong Il Yoo, Byeong-Hyeok Sohn,* Wang-Cheol Zin, Sung-Jin An and Gyu-Chul Yi

A hexagonal array of optically active ZnO nanoparticles was synthesised *in situ* on the solid substrate by utilizing a single-layered film of diblock copolymer micelles as a nanostructured template.

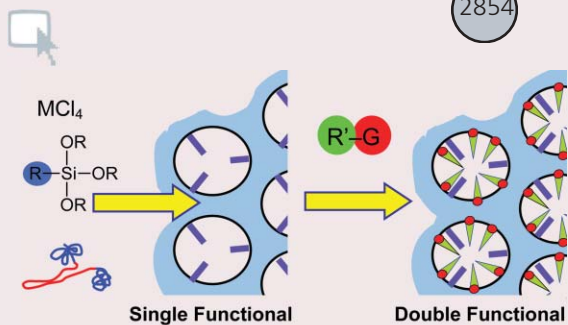
2852

**Molten salts bearing anion receptor**

Noriyoshi Matsumi, Masafumi Miyake and Hiroyuki Ohno*

Novel imidazolium type molten salts having anion receptors were prepared. Alkylborane type molten salts show a lithium transference number of 0.71–0.53 at 303 K due to a strong anion trapping effect.

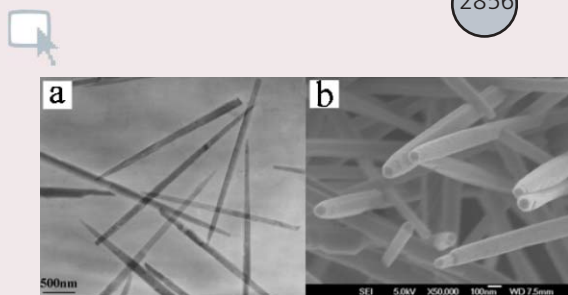
2854

**Highly ordered hybrid mesoporous bifunctional thin films**

Galo J. A. A. Soler-Illia,* Paula C. Angelomé and Patricia Bozzano

Mesoporous hybrid thin oxide films with two organic functions are produced by a two-step strategy: co-condensation of organosilica and M(IV) precursors in the presence of amphiphiles followed by pore post-functionalisation *via* complexation of M(IV) centres.

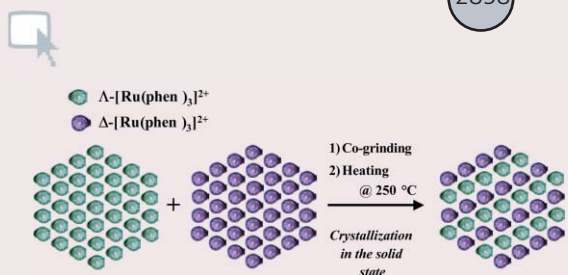
2856

**A simple low-temperature growth of ZnO nanowhiskers directly from aqueous solution containing $Zn(OH)_4^{2-}$ ions**

Ping Li, Yu Wei,* Hui Liu and Xinkui Wang

One-dimensional (1D) needle-like ZnO nanowhiskers have been grown directly from aqueous solution containing $Zn(OH)_4^{2-}$ ions produced by zinc chloride and sodium hydroxide, in the presence of sodium dodecyl sulfate (SDS).

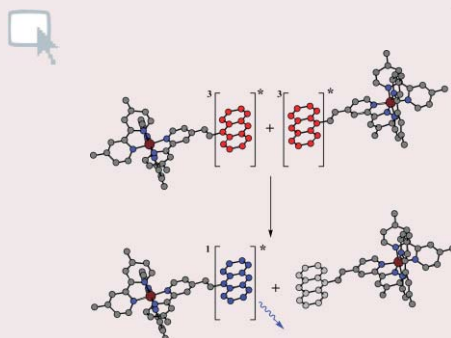
2858

**Formation of racemic crystals of transition metal complexes by grinding 1 : 1 mixtures of enantiomeric crystals**

Asao Nakamura,* Tomohiro Sato and Reiko Kuroda*

Grinding a 1 : 1 enantiomeric mixture of chiral transition metal complex crystals and subsequent annealing afforded crystals of a racemic compound by diffusion and rearrangement of component molecules, without melting and without racemization of each enantiomeric species.

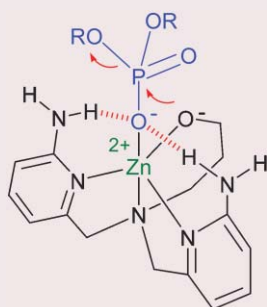
2860

**Anti-Stokes delayed fluorescence from metal–organic bichromophores**

Denis V. Kozlov and Felix N. Castellano*

Long wavelength excitation of $[Ru(dmb)_2(bpy-An)]^{2+}$ (dmb is 4,4'-dimethyl-2,2'-bipyridine and bpy-An is 4-methyl-4'-(9-anthrylethyl)-2,2'-bipyridine) in CH_3CN solution at room temperature produces upconverted delayed singlet anthracene fluorescence *via* bimolecular triplet annihilation.

2862

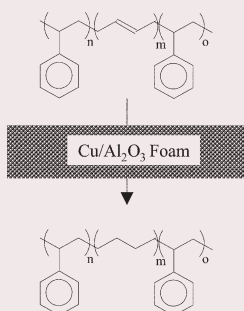


Multiple functional group cooperation in phosphate diester cleavage promoted by Zn(II) complexes

Monica Livieri, Fabrizio Mancin,* Umberto Tonellato and Jik Chin*

Zn(II) complexes bearing multiple auxiliary organic groups greatly accelerate the cleavage of bis-*p*-nitrophenyl phosphate.

2864

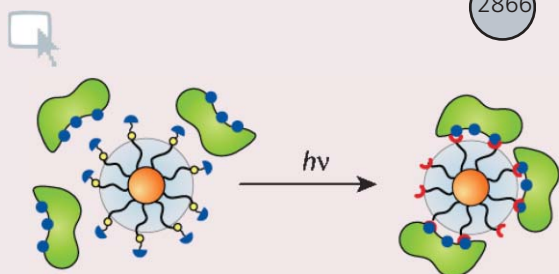


Monolithic catalysts for the fixed-bed hydrogenation of polymers

Jean-Paul Lange,* Lodewijk Schoon, Alan Villena and Wouter de Jong

Monolithic catalysts were successfully applied in a true fixed-bed hydrogenation of polymers such as SBS rubbers and polystyrene.

2866

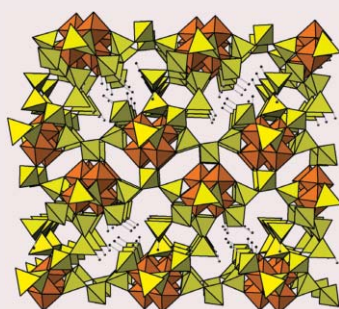


Light-induced inhibition of chymotrypsin using photocleavable monolayers on gold nanoparticles

Nicholas O. Fischer, Ralph Paulini, Ulf Drechsler and Vincent M. Rotello*

Positively charged gold nanoparticles featuring photocleavable units within their surrounding monolayer are switched from non-interacting species to inhibitors of chymotrypsin through UV irradiation.

2868



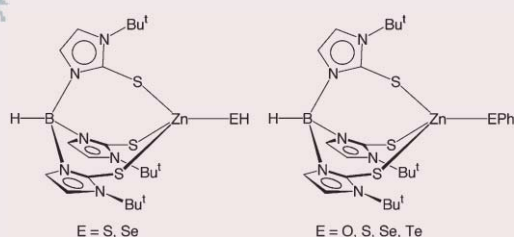
A germanium zeotype with a three-dimensional net of interconnected 14-, 12- and 12-ring channels.

$\text{Ge}_{13}\text{O}_{26}(\text{OH})_4[\text{C}_6\text{N}_2\text{H}_{16}]_2(\text{H}_2\text{O})_{1.5}$

Manuela E. Medina, Enrique Gutiérrez-Puebla,* M. Angeles Monge* and Natalia Snejko

$\text{Ge}_{13}\text{O}_{26}(\text{OH})_4[\text{C}_6\text{N}_2\text{H}_{16}]_2(\text{H}_2\text{O})_{1.5}$ is a new germanium zeotype, built up from SBU-13, formed by polyhedra distributed in three shells. Its open 3D structure has a three-dimensional system of intersecting channels, where the 14-ring channels are lined with OH^- anions.

2870

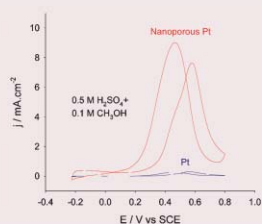
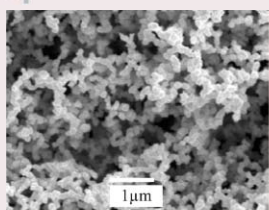


Methyl, hydrochalcogenido, and phenylchalcogenolate complexes of zinc in a sulfur rich coordination environment: syntheses and structural characterization of the tris(2-mercapto-1-tert-butylimidazolyl)hydroboratozinc complexes $[\text{Tm}^{\text{Bu}^t}]\text{ZnMe}$, $[\text{Tm}^{\text{Bu}^t}]\text{ZnEH}$ (E = S, Se) and $[\text{Tm}^{\text{Bu}^t}]\text{ZnEPh}$ (E = O, S, Se, Te)

Jonathan G. Melnick, Arefa Docrat and Gerard Parkin*

A series of hydrochalcogenido and phenylchalcogenolate complexes of zinc supported by tris(2-mercapto-1-tert-butylimidazolyl)hydroborato ligation, $[\text{Tm}^{\text{Bu}^t}]\text{ZnEH}$ (E = S, Se) and $[\text{Tm}^{\text{Bu}^t}]\text{ZnEPh}$ (E = O, S, Se, Te) have been synthesized from $[\text{Tm}^{\text{Bu}^t}]\text{ZnMe}$.

2872

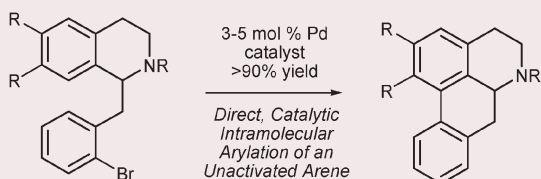


Fabrication and electrochemical properties of novel nanoporous platinum network electrodes

Xinsheng Peng, Kallum Koczkur, Stephanie Nigro and Aicheng Chen*

Three-dimensional nanoporous Pt networks were directly grown on a Ti substrate *via* a simple hydrothermal-assisted seed method. The formed nanoporous Pt network electrodes exhibit a large surface area and high activity, which supports the potential usefulness of these materials in novel electrochemical sensor design and catalyst development.

2874

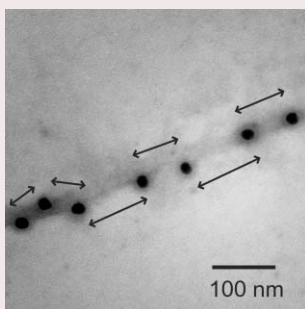


Direct intramolecular arylation of unactivated arenes: application to the synthesis of aporphine alkaloids

Marc Lafrance, Nicole Blaqui re and Keith Fagnou*

The direct intramolecular C–H arylation of unactivated arenes is a viable strategy for the synthesis of aporphine alkaloids. These reactions occur with 3 to 5 mol% catalyst and generate the aporphine skeleton in up to 99% yield.

2876

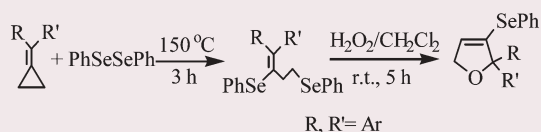


Construction of a protein array on amyloid-like fibrils using co-assembly of designed peptides

Hiroyuki Kodama, Sachiko Matsumura, Taro Yamashita and Hisakazu Mihara*

Streptavidin (labelled with colloidal gold) periodically bound onto cofibrils containing biotinylated peptides. The protein arrangement at every 50, 100, 150 nm intervals on the nanoscale construct was achieved.

2878

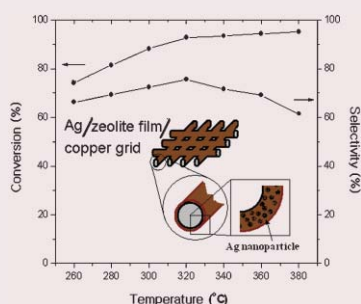


Ring-opening reactions of methylenecyclopropanes with diphenyl diselenide upon heating; formation of 3-phenylselenenyl-2,5-dihydrofuran derivatives

Le-Ping Liu and Min Shi*

The reactions of methylenecyclopropanes **1** with diphenyl diselenide give ring-opened products **2** in good yields at 150 °C under nitrogen atmosphere for 3 h. The products **2** can further undergo oxidative cyclization with hydrogen peroxide to furnish 3-phenylselenenyl-2,5-dihydrofurans **3** in moderate yields (three steps) at room temperature in CH₂Cl₂ for 5 h. A plausible reaction mechanism has been proposed.

2880

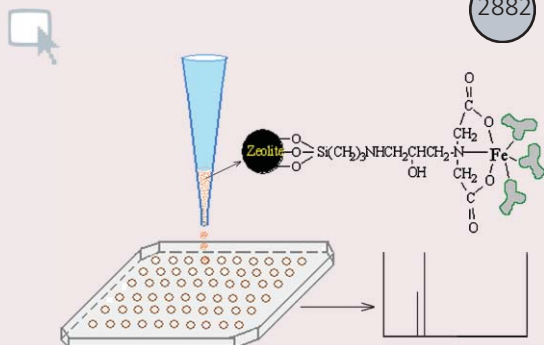


A novel catalyst with high activity for polyhydric alcohol oxidation: nanosilver/zeolite film

Jiang Shen, Wei Shan, Yahong Zhang, Junming Du, Hualong Xu, Kangnian Fan, Wei Shen* and Yi Tang*

A novel nanosilver/zeolite film catalyst was fabricated and it showed high activity and selectivity for the partial oxidation of polyhydric alcohols at a relatively low temperature.

2882

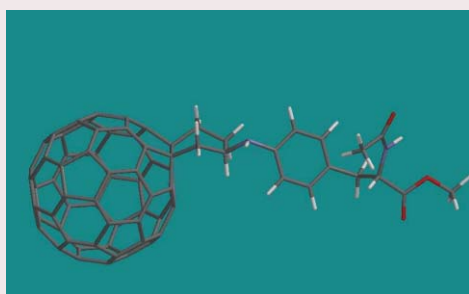


Zeolite nanoparticles with immobilized metal ions: isolation and MALDI-TOF-MS/MS identification of phosphopeptides

Yahong Zhang, Xijuan Yu, Xiaoyan Wang, Wei Shan, Pengyuan Yang* and Yi Tang*

Zeolite nanoparticles containing immobilized Fe^{3+} ion have been applied to isolate and identify phosphopeptides from tryptic β -casein digest *via* a direct MALDI-TOF-MS/MS analysis. The specifically external surface chelation with the phosphopeptides and high dispersibility of Fe^{3+} -nanozeolites facilitate the MALDI identification of phosphopeptides.

2884

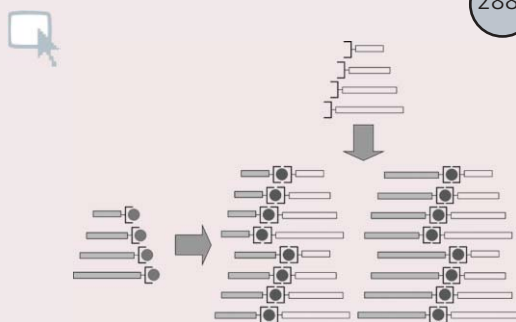


A new route to fullerene substituted phenylalanine derivatives

Jianzhong Yang and Andrew R. Barron*

Fullerene substituted phenylalanines have been prepared by the condensation of 1,2-(4'-oxocyclohexano)fullerene with (4-amino)-phenylalanine derivatives and selective conversion of the imine to the corresponding amine.

2886

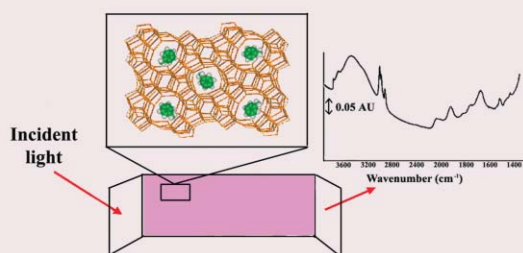


Block copolymer libraries: modular versatility of the macromolecular Lego® system

Bas G. G. Lohmeijer, Daan Wouters, Zhihui Yin and Ulrich S. Schubert*

The synthesis and characterization of a new 4×4 library of metallo-supramolecular block copolymers based on polystyrene and poly(ethylene oxide) having an asymmetrical octahedral bis(terpyridine) ruthenium complex at the block junction are described.

2888

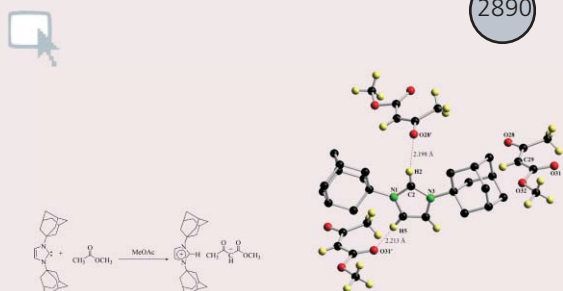


Zeolite coated ATR crystals for new applications in FTIR-ATR spectroscopy

Zheng Wang, Margareta L. Larsson, Mattias Grahn, Allan Holmgren* and Jonas Hedlund*

Thin silicalite-1 films were grown on ATR crystals and used for detection of low amounts of organic molecules in a gas flow by FTIR spectroscopy.

2890

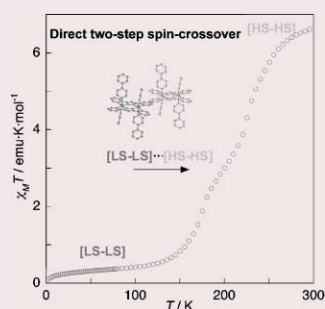


Reactivity of a *N*-heterocyclic carbene, 1,3-di-(1-adamantyl)imidazol-2-ylidene, with a pseudo-acid: structural characterization of Claisen condensation adduct

Gabriela A. Grasa, Rohit Singh, Natalie M. Scott, Edwin D. Stevens and Steven P. Nolan*

Reaction of a pseudo-acid (ester) with NHC allowed the formation of a Claisen condensation type adduct. An X-ray diffraction study revealed an unusual hydrogen bond stabilization in the adduct structure.

2892

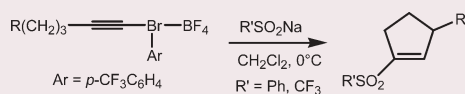


Direct two-step spin-crossover through [HS–HS][LS–LS] at the plateau in dinuclear diiron(II) complex $[\{\text{Fe}(\text{NCBH}_3)(4\text{phpy})\}_2(\mu\text{-bpyppz})_2]$

Keisaku Nakano, Satoshi Kawata, Ko Yoneda, Akira Fuyuhiro, Takashi Yagi, Saburo Nasu, Syotaro Morimoto and Sumio Kaizaki*

A new type of two-step spin-crossover through a like-spin pair state of [HS–HS] and [LS–LS] is demonstrated in contrast to the previously reported mixed spin state [HS–LS].

2894

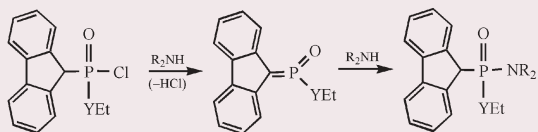


Tandem Michael addition–carbene insertion reaction of 1-alkynyl(aryl)(tetrafluoroborato)- λ^3 -bromanes: 1-(phenylsulfonyl)- and 1-(trifluoromethylsulfonyl)cyclopentene annulation

Masahito Ochiai,* Norihiro Tada, Yoshio Nishi and Kentaro Murai

Exposure of 1-alkynyl [*p*-(trifluoromethyl)phenyl](tetrafluoroborato)- λ^3 -bromanes to sodium benzenesulfinate or sodium trifluoromethanesulfinate in dichloromethane at 0 °C under argon resulted in tandem Michael–carbene insertion reactions to produce 1-sulfonylcyclopentenes selectively.

2896



Phosphonyl transfer by the elimination–addition mechanism: accelerated formation of an alkylideneoxophosphorane (phosphene) intermediate when a P–O single bond is replaced by P–S

Martin J. P. Harger

Rate-limiting formation of the alkylideneoxophosphorane (phosphene) intermediate is *ca.* 10^3 times faster when Y = S than when Y = O, suggesting substantial stabilisation of a three-coordinate P^V centre by singly-bonded sulfur.

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New Draft IUPAC Nomenclature of Organic Chemistry

A draft new edition of Nomenclature of Organic Chemistry (the IUPAC “Blue Book”) has been issued for public review by the International Union of Pure and Applied Chemistry. The deadline for comment is 31st March 2005.

This new edition, which supersedes both the 1979 Blue Book and the 1993 Guide to IUPAC Nomenclature of Organic Compounds, represents a major new development in IUPAC nomenclature recommendations. Previously IUPAC has provided rules enabling the generation of unambiguous names, by codifying, rationalising and extending existing practice, but in many cases has not expressed a preference between legitimate synonyms (e.g. decahydronaphthalene and bicyclo[4.4.0]decane). However, it has become clear that various communities require a single IUPAC name for a given chemical structure, which can be used for legal and regulatory purposes. Such names are needed in patents, in export-import regulations, and in environmental and health and safety information, etc.

Rather than recommend only a single name for each structure, IUPAC has now developed rules for assigning Preferred IUPAC Names (PINs), while continuing to allow considerable freedom in the use of alternatives according to the diverse needs of the chemical community. This freedom of usage extends, as previously, to a variety of trivial and traditional names; indeed several such names (e.g. acetic acid, benzene and pyridine) are

designated as IUPAC-preferred. Thus the present draft should enable users to derive Preferred IUPAC Names if required, while allowing alternatives in a broader context; it will also provide the protocols for developers of naming software to incorporate into their products for PIN generation.

In preparing this new edition, IUPAC has also taken the opportunity to rationalise, clarify and extend nomenclature systems described in previous editions, and has incorporated new nomenclature (e.g. that of phanes and fullerenes) that has appeared in *Pure Appl. Chem.* since publication of the 1993 Guide.

The IUPAC draft can be downloaded from the following web address:

www.iupac.org/reports/provisional/abstract04/favre_310305.html

as a single pdf file (~1300 pages) or as smaller files corresponding to designated sections of the book. In case of difficulty, paper copies of specified sections can be obtained from Dr Alan McNaught (adm@rsc.org) at the RSC's Cambridge office. Comments should be addressed to (both) Prof Henri Favre (halfa@contact.net) and Dr Warren Powell (wpowell2@juno.com). Users should bear in mind the provisional nature of this material; it would be unwise to regard PIN specifications in this draft as definitive.

RSCAD18110421