

ChemComm

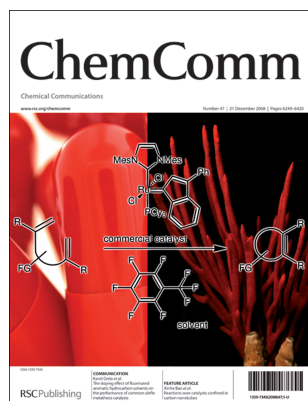
Chemical Communications

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IN THIS ISSUE

ISSN 1359-7345 CODEN CHCOFS (47) 6249-6420 (2008)



Cover

See Karol Grela *et al.*, pp. 6282–6284. Aromatic fluorinated hydrocarbons, used as solvents for olefin metathesis reactions catalysed by standard Ru-precatalysts, allow to obtain substantially higher yields, especially of challenging substrates including biologically active compounds. Doug Anderson and Thijs van Exel kindly provided the photographs used in the background. Image reproduced by permission of Cezary Samojłowicz, Michał Bieniek, Andrzej Zarecki, Renat Kadyrov and Karol Grela from *Chem. Commun.*, 2008, 6282.

CHEMICAL SCIENCE

C89

Drawing together research highlights and news from all RSC publications, *Chemical Science* provides a 'snapshot' of the latest developments across the chemical sciences, showcasing newsworthy articles and significant scientific advances.

Chemical Science

December 2008/Volume 5/Issue 12

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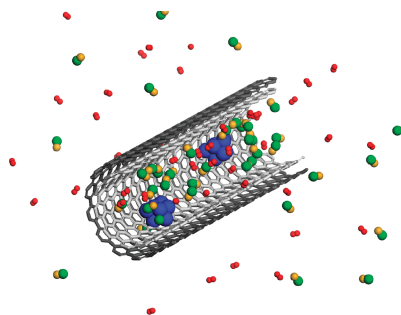
FEATURE ARTICLE

6271

Reactions over catalysts confined in carbon nanotubes

Xiulian Pan and Xinhe Bao*

Carbon nanotubes provide an intriguing confinement environment for catalysis due to their well defined nanochannel morphology and unique electron structure with deformed sp^2 hybridization.



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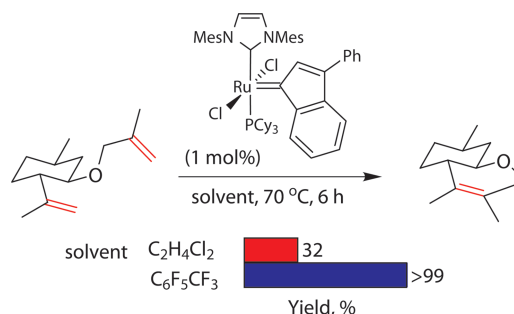
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6282

The doping effect of fluorinated aromatic hydrocarbon solvents on the performance of common olefin metathesis catalysts: application in the preparation of biologically active compounds

Cezary Samojłowicz, Michał Bieniek, Andrzej Zarecki, Renat Kadyrov and Karol Grela*

Aromatic fluorinated solvents allow higher yields to be obtained in the olefin metathesis of challenging substrates, including natural and biologically active compounds.

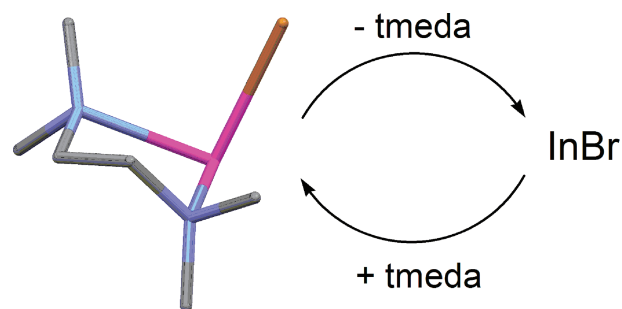


6285

Synthesis and structural characterisation of a soluble, metastable indium(i) halide complex, [InBr(tmeda)]

Shaun P. Green, Cameron Jones* and Andreas Stasch

The first example of a structurally characterised indium(i) halide complex, [InBr(tmeda)], has been prepared by the dissolution of InBr in a tmeda–toluene mixture. The metastable compound decomposes to either InBr or [In₂Br₄(tmeda)₂] in solution.

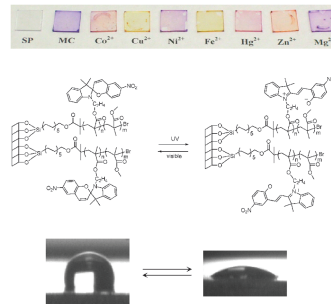


6288

Reversible colorimetric ion sensors based on surface initiated polymerization of photochromic polymers

Kristen Fries, Satyabrata Samanta, Sara Orski and Jason Locklin*

The authors have synthesized spiropyran-containing polymer brushes for use as reversible, photoswitchable optical sensors that show selectivity for different metal ions. Different metal complexation was also used to create surfaces with drastic changes in wettability.

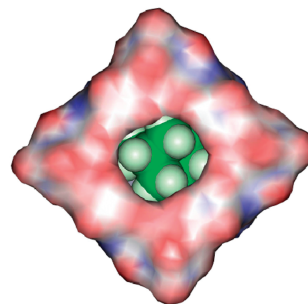


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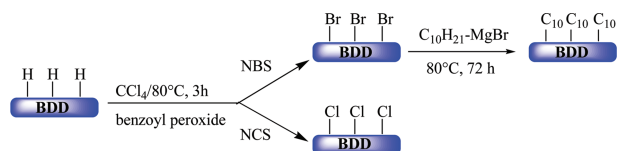
A cavitand with a fluororous rim acts as an amine receptor

Richard J. Hooley, Per Restorp and Julius Rebek, Jr*

A deep cavitand presents two domains for the control of guest binding. The combination provides selectivity for amines and small guests that other self-folding cavitands cannot.



6294

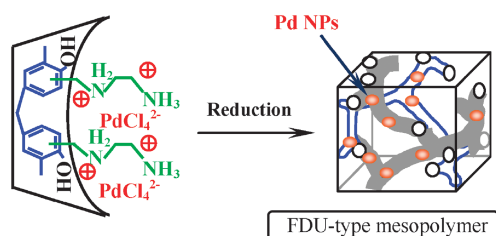


Wet-chemical approach for the halogenation of hydrogenated boron-doped diamond electrodes

Mei Wang, Manash R. Das, Vera G. Praig, Francois LeNormand, Musen Li, Rabah Boukherroub* and Sabine Szunerits*

Brominated and chlorinated boron-doped diamond electrodes were prepared through a radical substitution reaction and reacted further with alkyl-Grignard reagents.

6297

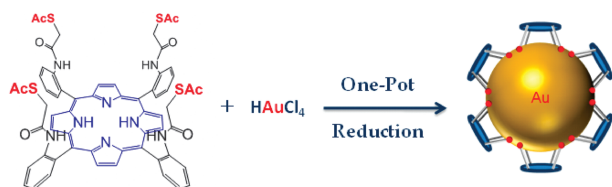


Preparation of active and robust palladium nanoparticle catalysts stabilized by diamine-functionalized mesoporous polymers

Rong Xing, Yueming Liu, Haihong Wu, Xiaohong Li, Mingyuan He and Peng Wu*

Amino group-functionalized mesoporous phenolic resins capture effectively the anionic palladium species which form highly dispersed Pd nanoparticles (NPs) confined inside the mesopores after reduction; the Pd NPs serve as efficient and reusable catalysts for Heck reaction and alkene hydrogenation.

6300

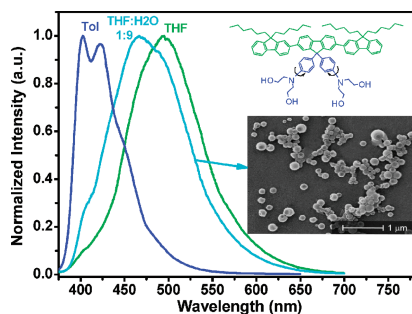


One-phase synthesis of small gold nanoparticles coated by a horizontal porphyrin monolayer

Junya Ohyama, Yutaka Hitomi,* Yasuhiro Higuchi, Masashi Shinagawa, Hidefumi Mukai, Masahito Kodera, Kentaro Teramura, Tetsuya Shishido and Tsunehiro Tanaka

A porphyrin-cored tetradentate passivant gives horizontal porphyrin monolayer-coated gold nanoparticles, whose particle size is smaller than those made using monodentate passivants under identical conditions.

6303



An aggregation-induced blue shift of emission and the self-assembly of nanoparticles from a novel amphiphilic oligofluorene

Linna Zhu, Chuluo Yang* and Jingui Qin

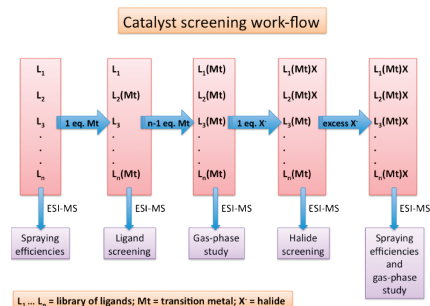
An aggregation-induced blue shift of emission was observed from a novel amphiphilic trifluorene, and tentatively attributed to a similar TICT mechanism. Its optical properties and self-assembly behaviors are presented.

6306

Rapid screening of atom transfer radical polymerization catalysts by electrospray ionization mass spectrometry

Fabio di Lena and Krzysztof Matyjaszewski*

An ESI-MS-based strategy provides an effective tool for the rapid assay of ATRP catalyst performance without prior polymerization experiments, using only a few milligrams of compounds, and with no reaction workup necessary.

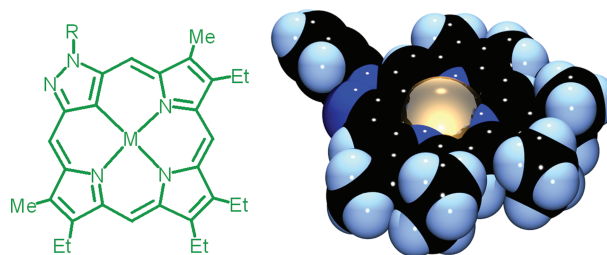


6309

Adding to the confusion! Synthesis and metalation of porphyrin analogues of the porphyrins

Timothy D. Lash,* Alexandra M. Young,
Amber L. Von Ruden and Gregory M. Ferrence

N-substituted pyrazole dialdehydes are shown to react with a tripyrrane under '3 + 1' conditions to give aza-analogues of the N-confused porphyrins; these novel porphyrinoids show borderline aromatic properties and readily afford organometallic derivatives (M = Ni or Pd).

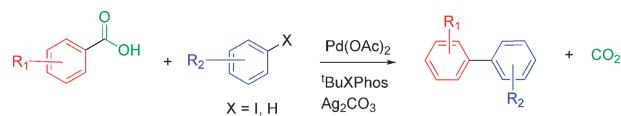


6312

Palladium-catalyzed decarboxylative coupling of aromatic acids with aryl halides or unactivated arenes using microwave heating

Adelina Voutchkova, Abigail Coplin,
Nicholas E. Leadbeater and Robert H. Crabtree*

An efficient microwave-assisted protocol for decarboxylative couplings of aromatic acids to either aryl iodides or simple arenes is described.

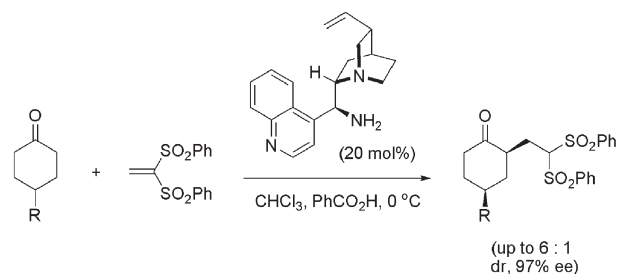


6315

Asymmetric organocatalytic Michael addition of ketones to vinyl sulfone

Qiang Zhu, Lili Cheng and Yixin Lu*

Organocatalytic Michael addition of ketones to vinyl sulfone catalyzed by a cinchona alkaloid-derived primary amine is reported for the first time. Excellent enantioselectivities (88–97% ee) were achieved, and the methodology was applied to the synthesis of sodium cyclamate.



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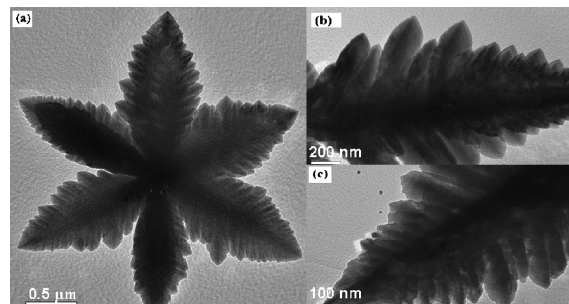
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6318

The synthesis and applications of a micro-pine-structured nanocatalyst

Vivek Polshettiwar, Mallikarjuna N. Nadagouda and Rajender S. Varma*

Dendritic nanoferrites with a micro-pine morphology have been synthesized for the first time under microwave irradiation conditions without using any reducing or capping reagent; the nanoferrites were then functionalized and coated with Pd metal, which catalyzes various organic transformations.

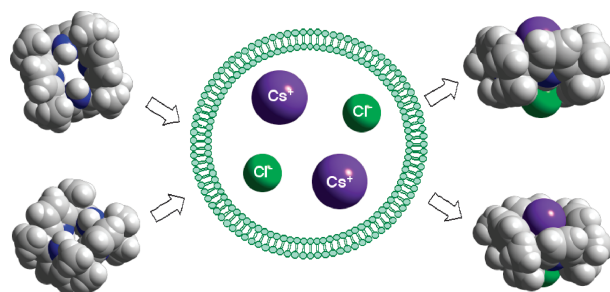


6321

meso-Octamethylcalix[4]pyrrole: an old yet new transmembrane ion-pair transporter

Christine C. Tong, Roberto Quesada,* Jonathan L. Sessler and Philip A. Gale*

The first example of lipid bilayer membrane transport of a salt by a calix[4]pyrrole is reported.

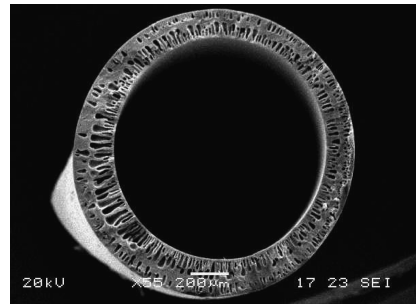


6324

Polyaniline hollow fibres for organic solvent nanofiltration

Xun Xing Loh, Malladi Sairam, Joachim Hans Georg Steinke, Andrew Guy Livingston, Alexander Bismarck and Kang Li*

Intrinsically-skinned asymmetric PANi hollow fibres, fabricated using a process of directly adding large organic acids to PANi solutions, show stability in a wide variety of organic solvents and have shown promising nanofiltration properties, giving high rejections of nanosolutes in acetone.

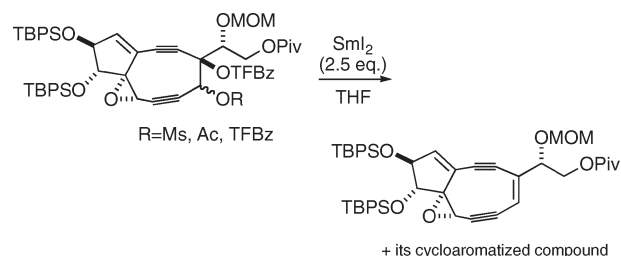


6327

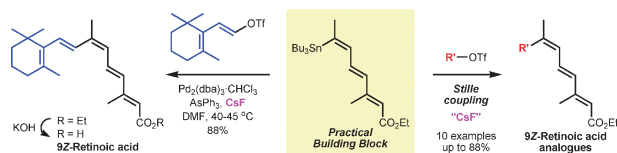
Secure route to the epoxybicyclo[7.3.0]dodecadienediylne core of the kedarcidin chromophore

Kouki Ogawa, Yasuhito Koyama, Isao Ohashi, Itaru Sato and Masahiro Hirama*

The construction of the epoxybicyclo[7.3.0]dodecadienediylne core of the kedarcidin chromophore was realized *via* highly chemoselective reductive olefination in the presence of the epoxide.



6330

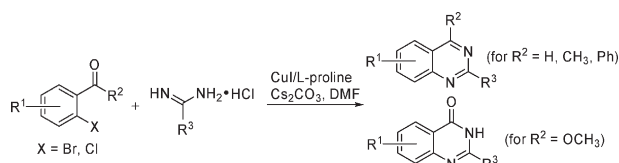


Caesium fluoride-promoted Stille coupling reaction: an efficient synthesis of 9Z-retinoic acid and its analogues using a practical building block

Takashi Okitsu, Kinya Iwatsuka and Akimori Wada*

A highly efficient and rapid total synthesis of 9Z-retinoic acid was accomplished by CsF-promoted Stille coupling reaction. Using a common building block, their analogues were also prepared without isomerisation of the Z-double bond.

6333

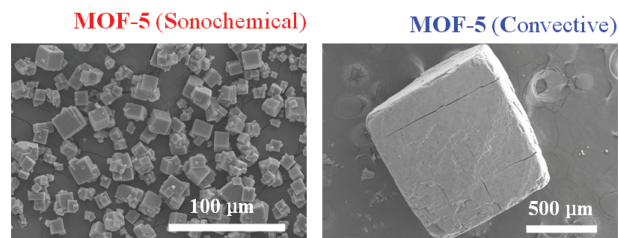


Highly efficient copper-catalyzed cascade synthesis of quinazoline and quinazolinone derivatives

Cheng Huang, Yuan Fu, Hua Fu,* Yuyang Jiang* and Yufen Zhao

We have developed a general and highly efficient copper-catalyzed method for synthesis of quinazoline and quinazolinone derivatives *via* cascade reactions of amidines with substituted 2-halobenzaldehydes, 2-halophenylketones, or methyl 2-halobenzoates.

6336

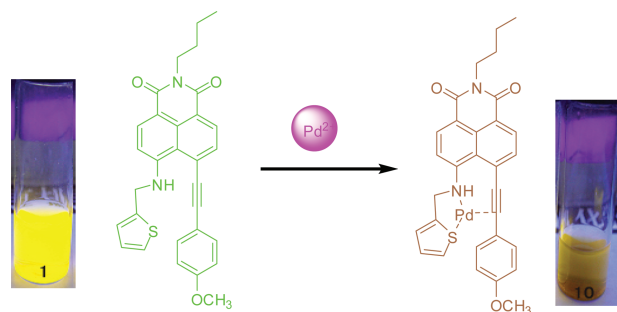


Sonochemical synthesis of MOF-5

Won-Jin Son, Jun Kim, Jaheon Kim* and Wha-Seung Ahn*

High quality MOF-5 crystals of 5–25 μm in size were prepared for the first time using a sonochemical method in substantially reduced synthesis time (*ca.* 30 min) compared with conventional solvothermal synthesis (24 h).

6339



Highly sensitive and selective Pd²⁺ sensor of naphthalimide derivative based on complexation with alkynes and thio-heterocycle

Liping Duan, Yufang Xu and Xuhong Qian*

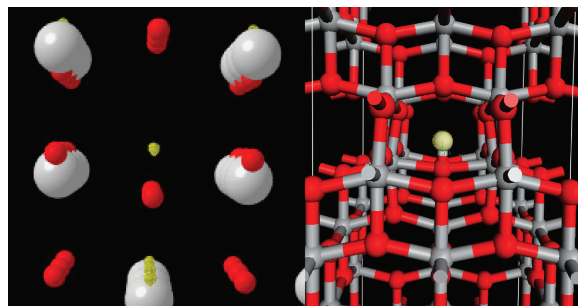
N-butyl-4-(*p*-methoxy)-phenylethynyl-5-thiophenemethylamino-1,8-naphthalimide (**1**) showed highly selective on-off fluorescence and chromogenic changes for Pd²⁺ in buffer solution.

6342

Direct observation of space charge induced hydrogen ion insertion in nanoscale anatase TiO₂

Wing K. Chan, Wouter J. H. Borghols and Fokko M. Mulder*

Nanoscale TiO₂ in an acidic environment shows significant hydrogen densities induced by space charge effects, as is observed by neutron diffraction. Modelling reproduces the hydrogen position and reveals that, consistent with experimental results in fuel cells, these ions show rapid self diffusion.

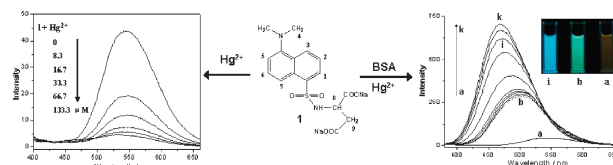


6345

A protein-supported fluorescent reagent for the highly-sensitive and selective detection of mercury ions in aqueous solution and live cells

Li-Jun Ma, Yue Li, Lei Li, Jian Sun, Chunjuan Tian and Yuqing Wu*

Hg²⁺ strongly quenched sodium dansyl-L-aspartic acid (**1**) in aqueous solution, while in the presence of BSA it induced both blue shift and enhancement of the fluorescence emission of **1**, supplying a highly-sensitive and selective detection of Hg²⁺ in aqueous solution and in live cells.

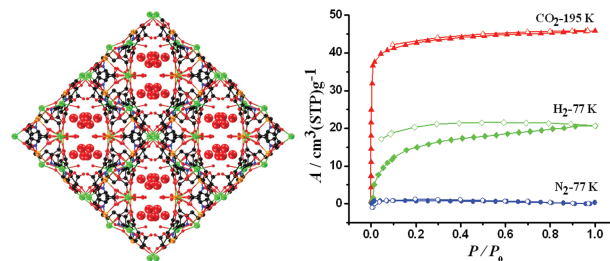


6348

Novel three-dimensional 3d–4f microporous magnets exhibiting selective gas adsorption behavior

Cui-Jin Li, Zhuo-jia Lin, Meng-Xia Peng, Ji-Dong Leng, Ming-Mei Yang and Ming-Liang Tong*

Three stable 3D Ln-Co microporous magnets having hydrophilic channels that exhibit a size-selective adsorption ability for H₂ over N₂ and CO₂ over N₂ were obtained from hydrothermal reactions of Ln(NO₃)₃·6H₂O (Ln = Sm, Eu and Gd), Co(NO₃)₂·6H₂O and H₃pyta.

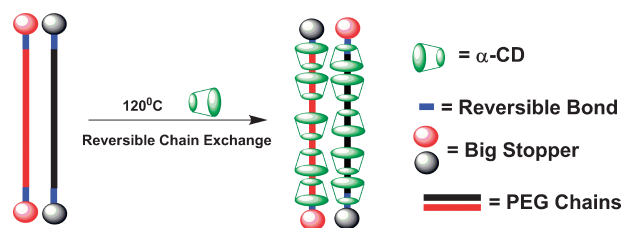


6351

Construction of polyrotaxanes *via* reversible chain exchange between acylhydrazone bonds

Yi Jiang, Jieli Wu, Lin He, Chunlai Tu, Xinyuan Zhu,* Qun Chen, Yefeng Yao* and Deyue Yan*

Polyrotaxanes form spontaneously *via* chain exchange between reversible covalent bonds, by simply heating mixtures of α -cyclodextrins and dumbbell-like poly(ethylene glycol) derivatives at 120 °C.



Dynamic Stereochemistry of Chiral Compounds

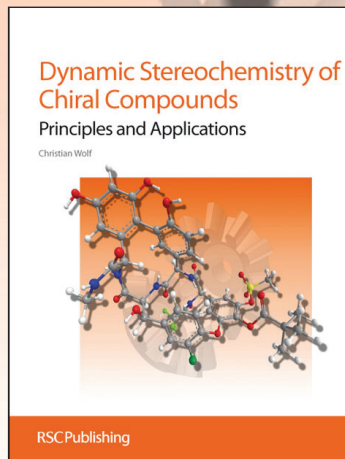
This book provides an overview of fundamental concepts of asymmetric synthesis highlighting the significance of stereochemical and stereodynamic reaction control. Topics include kinetic resolution (KR), dynamic kinetic resolution (DKR), dynamic kinetic asymmetric transformation (DYKAT), and dynamic thermodynamic resolution (DTR). In-depth discussions of asymmetric synthesis with chiral organolithium compounds, atropisomeric biaryl synthesis, self-regeneration of stereogenicity (SRS), chiral amplification with chiral relays and other commonly used strategies are also provided. Particular emphasis is given to selective introduction, interconversion and translocation of central, axial, planar, and helical chirality.

A systematic coverage of stereochemical principles and stereodynamic properties of chiral compounds guides the reader through the book and establishes a conceptual linkage to asymmetric synthesis, interconversion of stereoisomers, molecular devices that resemble the structure and stereomutations of propellers, bevel gears, switches and motors, and topologically chiral assemblies such as catenanes and rotaxanes. Racemization and diastereomerization reactions of numerous chiral compounds are discussed as well as the principles, scope and compatibility of commonly used analytical techniques.

- More than 550 figures, schemes and tables illustrating mechanisms of numerous asymmetric reactions and stereomutations of chiral compounds
- Technical drawings illustrating the conceptual linkage between macroscopic devices such as turnstiles, ratchets, brakes, bevel gears, propellers or knots and molecular analogs
- More than 3000 references to encourage further reading and facilitate additional literature research
- A comprehensive glossary with stereochemical definitions and terms which facilitate understanding and reinforce learning

This book will be of particular interest to advanced undergraduates, graduates and professionals working and researching in the fields of synthetic organic chemistry and stereochemistry.

030804



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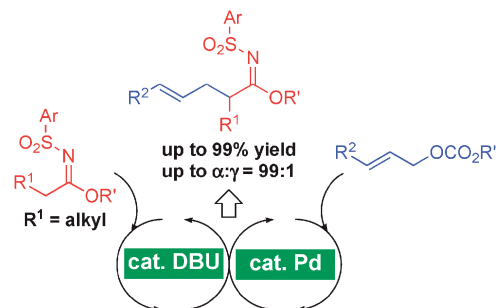
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6354

Catalytic direct-type substitution reaction of α -alkyl enolates: a Pd/Brønsted base-catalysed approach to the decarboxylative allylation of sulfonylimidates

S. B. Jennifer Kan, Ryosuke Matsubara, Florian Berthiol and Shū Kobayashi*

A mild and efficient process for the direct-type catalytic allylation of sulfonylimidates has been developed. This reaction represents the first example of Brønsted base-catalysed, *in situ* generation and use of α -alkyl enolates in substitution reactions.

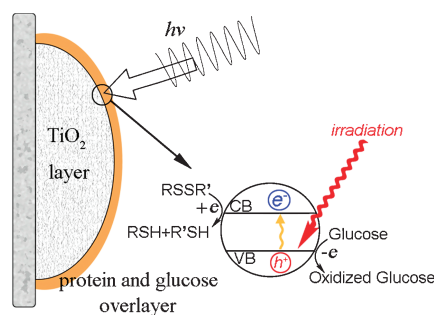


6357

In-source photocatalytic reduction of disulfide bonds during laser desorption/ionization

Liang Qiao, Hongyan Bi, Jean-Marc Busnel, Baohong Liu* and Hubert H. Girault*

A photosensitive plate based on TiO₂ nanoparticles has been developed to carry out photo-induced reductions using glucose as a hole scavenger during laser desorption/ionization process, where in-source cleavage of disulfide bridges is employed to demonstrate the concept.

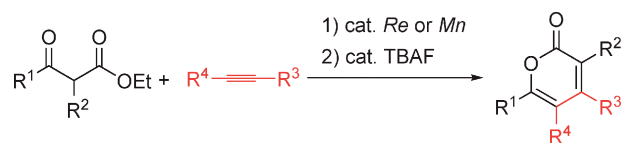


6360

Rhenium- and manganese-catalyzed insertion of acetylenes into β -keto esters: synthesis of 2-pyranones

Yoichiro Kuninobu,* Atsushi Kawata, Mitsumi Nishi, Hisatsugu Takata and Kazuhiko Takai*

Rhenium- and manganese-catalyzed reactions between β -keto esters and acetylenes, followed by treatment with tetrabutylammonium fluoride, gave 2-pyranone derivatives regioselectively.

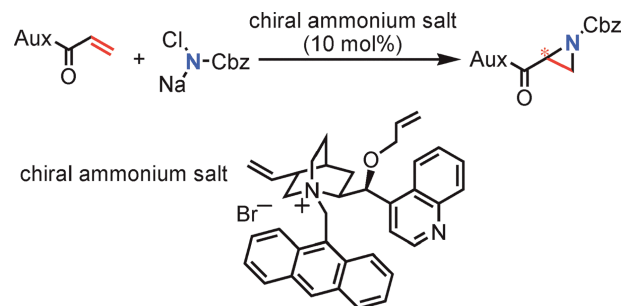


6363

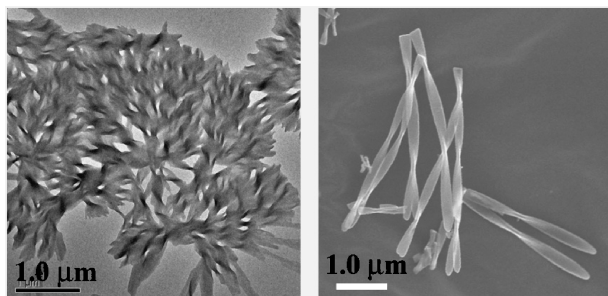
Catalytic aziridination of electron-deficient olefins with an *N*-chloro-*N*-sodio carbamate and application of this novel method to asymmetric synthesis

Satoshi Minakata,* Yuta Murakami, Ryoji Tsuruoka, Shinsuke Kitanaka and Mitsuo Komatsu

A new method for the aziridination of electron-deficient olefins using an *N*-chloro-*N*-sodio carbamate is described. The reaction was promoted by phase-transfer catalysis and afforded aziridines from α,β -unsaturated ketones, esters, sulfones and amides. This process was applied to asymmetric synthesis using *Cinchona* alkaloid derivatives as catalysts.



6366

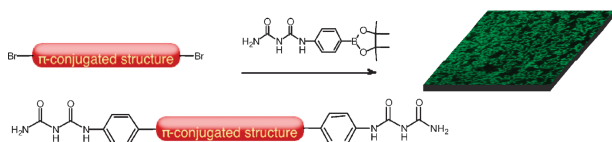


From branched self-assemblies to branched mesoporous silica nanoribbons

Baozong Li, Yuanli Chen, Huanyu Zhao, Xianfeng Pei, Lifeng Bi, Kenji Hanabusa and Yonggang Yang*

Branched left-handed twisted mesoporous silica nanoribbons were prepared *via* a template method.

6369

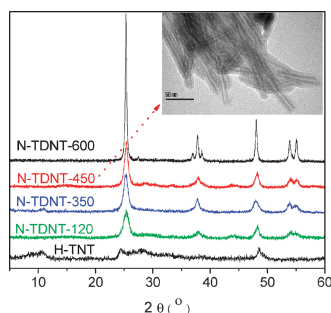


Versatile one-step introduction of multiple hydrogen-bonding sites onto extended π -conjugated systems

Fu-Chuan Fang, Cheng-Che Chu, Chih-Hao Huang, Guillaume Raffy, André Del Guerzo, Ken-Tsung Wong* and Dario M. Bassani*

A new synthon allows the one-step introduction of biuret hydrogen-bonding units onto π -conjugated structures, affording materials that display interpenetrated networks in which energy transfer is highly efficient.

6372

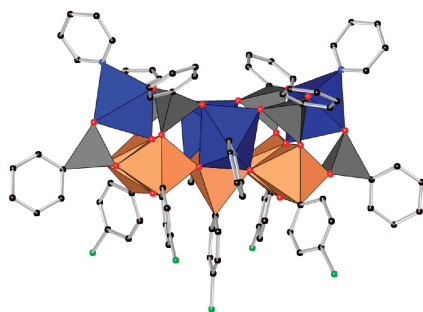


Solvothermal synthesis of N-doped TiO_2 nanotubes for visible-light-responsive photocatalysis

Zheng Jiang,* Fan Yang, Nianjun Luo, Bryan T. T. Chu, Deyin Sun, Huahong Shi, Tiancun Xiao and Peter P. Edwards*

Thermally stable and visible-light-responsive N-doped TiO_2 nanotubes were synthesized *via* a low-temperature solvothermal treatment of protonated titanate nanotubes in NH_4Cl /ethanol/water solution, and subsequent calcination.

6375



Mixed antimonate-phosphonate ligands as polydentate bridging oxygen donors

Shoaib Ali, Viswanathan Baskar, Christopher A. Muryn and Richard E. P. Winpenny*

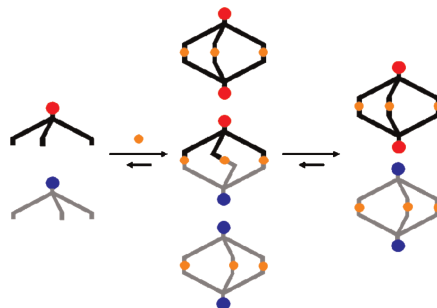
The synthesis of two new $\text{Sb}_x\text{-O-P}_y$ pro-ligands are described; both pro-ligands react with cobalt acetate to give new polymetallic cage complexes, for example the $\{\text{Co}_4\}$ butterfly shown.

6378

Post-assembly error-checking in subphthalocyanine based M_3L_2 metallosupramolecular capsules

Christian G. Claessens,* M. Jesús Vicente-Arana and Tomás Torres*

A kinetic mixture of self-assembled subphthalocyanine-based capsules was shown to gradually reorganize into its more stable symmetrical components by electrospray mass spectrometry.

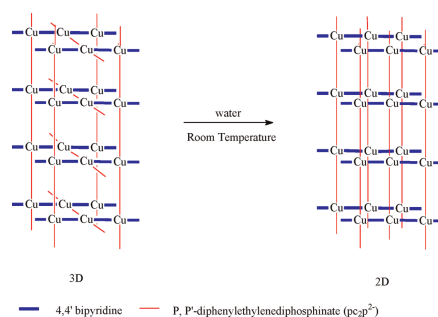


6381

A snapshot of a coordination polymer self-assembly process: the crystallization of a metastable 3D network followed by the spontaneous transformation in water to a 2D pseudopolymorphic phase

Thierry Bataille, Ferdinando Costantino,* Andrea Ienco,* Annalisa Guerri, Fabio Marmottini and Stefano Midollini

A metastable Cu(II) 3D hybrid with 4,4'-bipy and pc_2p^{2-} undergoes a spontaneous, quantitative transformation to a stable 2D polymorphic species either in water or after thermal dehydration followed by hydration.

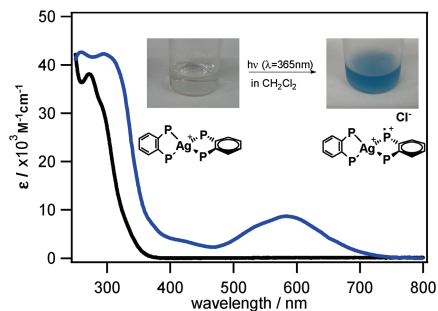


6384

Photochemistry and photophysics of the tetrahedral silver(I) complex with diphosphine ligands: $[Ag(dppb)_2]PF_6$ (dppb = 1, 2-bis[diphenylphosphino]benzene)

Masahisa Osawa* and Mikio Hoshino

The photophysical and photochemical properties of $[Ag(dppb)_2]PF_6$ having a tetrahedral coordination geometry have been described.

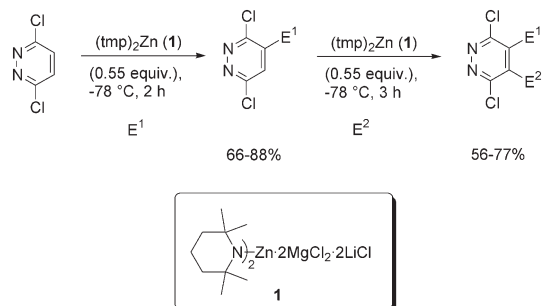


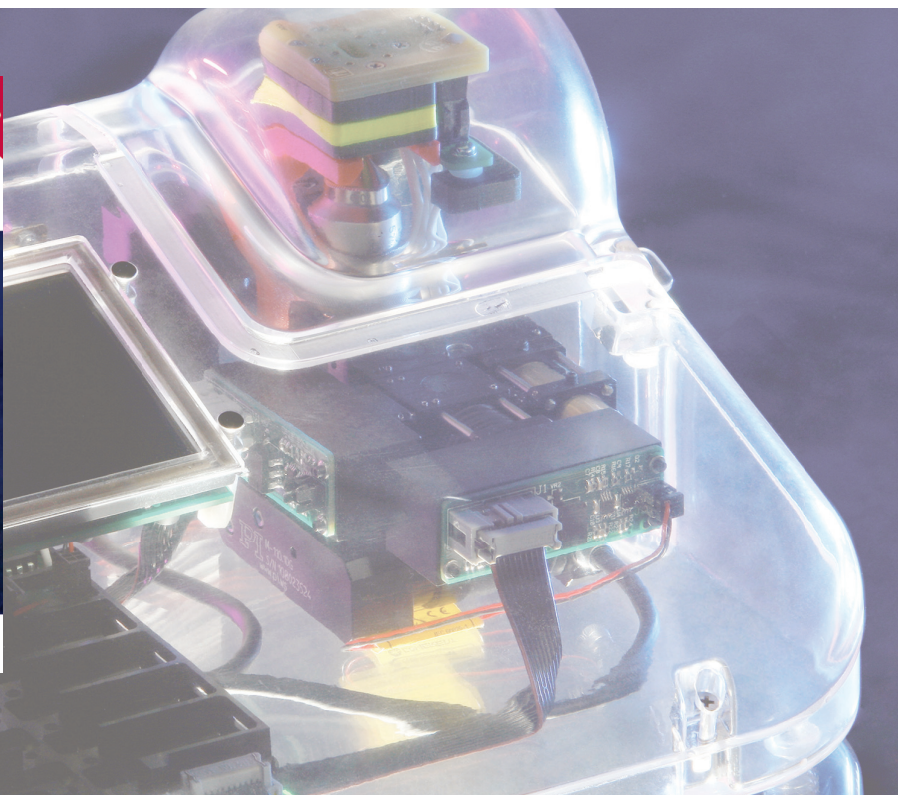
6387

Efficient *mono-* and *bis-*functionalization of 3,6-dichloropyridazine using $(tmp)_2Zn \cdot 2MgCl_2 \cdot 2LiCl$

Stefan Wunderlich and Paul Knochel*

3,6-Dichloropyridazine undergoes a smooth metallation using $(tmp)_2Zn \cdot 2MgCl_2 \cdot 2LiCl$. The resulting *bis*-organozinc species react with various electrophiles providing the desired products in good to excellent yields. Subsequent functionalization *via* a second metallation proceeds readily.





Point-of-Care Diagnostics themed issue

Lab on a Chip issue 12, 2008, is a themed issue devoted to point-of-care microfluidic-based diagnostics capturing some of the leading directions and themes of today's research. As this new emerging area has seen a marked increase in recent years, this issue of *Lab on a Chip* collects nineteen papers containing the latest research on microfluidics for point-of-care.

Papers include:

Egg Beater as Centrifuge:

Isolating Human Blood Plasma from Whole Blood in Resource-poor Settings

George Whitesides

Enabling a microfluidic immunoassay for the developing world by integration of on-card dry-reagent storage

Dean Stevens

Towards non- and minimally instrumented, microfluidics-based diagnostic devices

Bernhard Weigl

Neutrophil Migration Assay from a Drop of Blood

Daniel Irimia

An Integrated Microfluidic Platform for Ultrasensitive and Rapid Detection of Biological Toxins

Anup Singh

Optimizing Capture of Analytes in Microfluidic Heterogeneous Immunoassays Under Real-World Conditions

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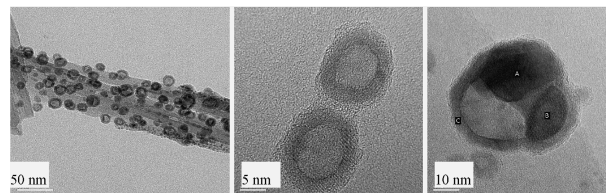
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6390

A template-free nano-wrapping technique for the fabrication of copper hollow nanospheres smaller than 20 nm

Frank Leung-Yuk Lam, Tommy Chi-Yan Martin and Xijun Hu*

A new template-free “nano-wrapping” method has been developed for the fabrication of copper hollow nanospheres with the smallest size of around 15 nm and its significance is highlighted to its composition tunability of the metal encapsulated inside the copper nanoshell.

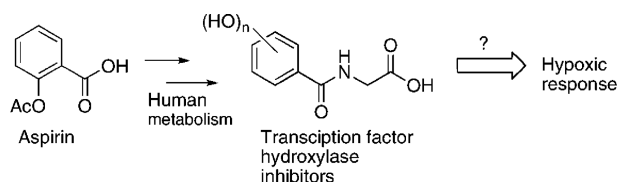


6393

Evaluation of aspirin metabolites as inhibitors of hypoxia-inducible factor hydroxylases

Benoit M. Lienard, Ana Conejo-García, Ineke Stolze, Christoph Loenarz, Neil J. Oldham, Peter J. Ratcliffe and Christopher J. Schofield*

Known and potential aspirin metabolites were evaluated as inhibitors of oxygen-sensing hypoxia-inducible transcription factor (HIF) hydroxylases; some of the metabolites were found to stabilise HIF- α in cells.

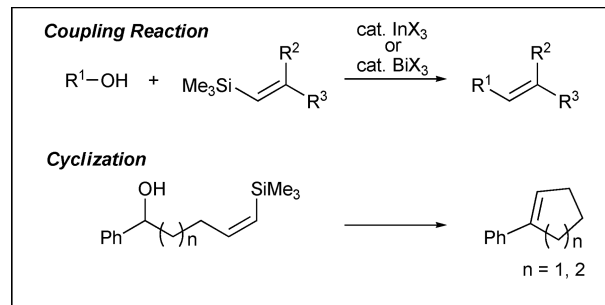


6396

Direct coupling of alcohols with alkenylsilanes catalyzed by indium trichloride or bismuth tribromide

Yoshihiro Nishimoto, Masayuki Kajioka, Takahiro Saito, Makoto Yasuda and Akio Baba*

Indium halides or bismuth halides catalyzed the coupling of various alcohols with alkenylsilanes to give the corresponding alkenes stereospecifically without any other activators.

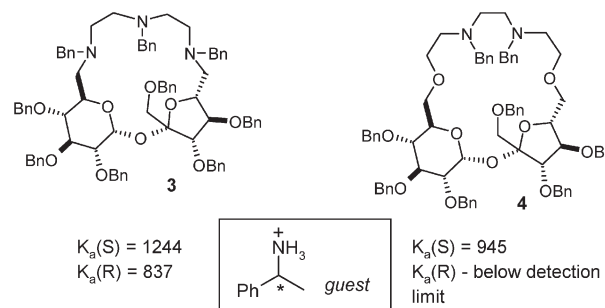


6399

Chiral recognition of α -phenylethylamine by sucrose-based macrocyclic receptors

Bartosz Lewandowski and Slawomir Jarosz*

Sucrose-based aza-crown ethers display *unprecedented* enantioselectivity as supramolecular receptors for phenylethylamine derivatives.



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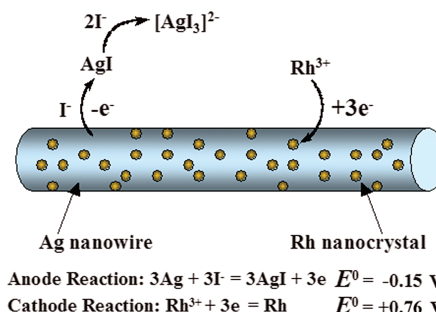
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6402

Iodide ions control galvanic replacement growth of uniform rhodium nanotubes at room temperature

Yingpu Bi and Gongxuan Lu*

Hollow rhodium nanotubes with uniform and perfect structures have been successfully synthesized through the replacement reaction between Ag nanowires and RhCl₃ in saturated NaI solutions at room temperature, and the main effect of iodide ions is found to reduce the redox potential of Ag species and resolve the formed AgI precipitation.

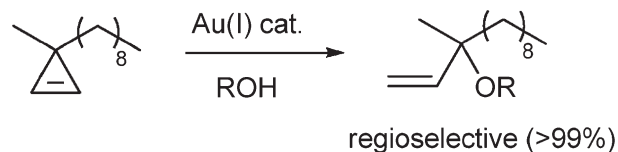


6405

Gold catalysed reactions with cyclopropenes

Jürgen T. Bauer, Maximillian S. Hadfield and Ai-Lan Lee*

A gold(I) catalysed addition of alcohols to cyclopropenes to yield *tert*-allylic ethers is described. The reaction is highly regioselective, mild and facile. Gold(I) catalysts were found to be unique and superior in terms of reactivity and regioselectivity.

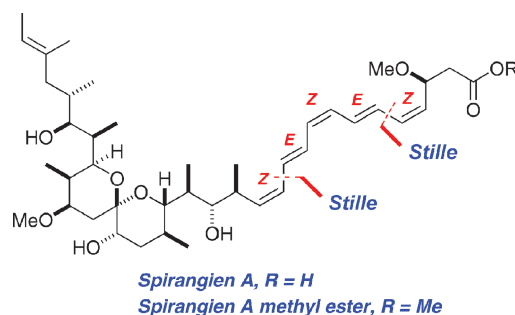


6408

Total synthesis of (–)-spirangien A and its methyl ester

Ian Paterson,* Alison D. Findlay and Christian Noti

The first total synthesis of (–)-spirangien A, a cytotoxic and antifungal polyketide of myxobacterial origin, is reported; this exploits a Stork–Wittig olefination and double Stille cross-coupling sequence to install the sensitive pentaene side chain onto a fully elaborated spiroacetal core, leading initially to the methyl ester of spirangien A.

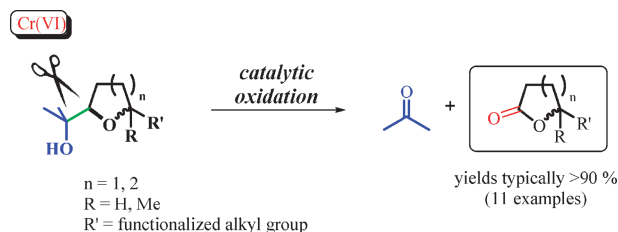


6411

A new catalytic oxidative cleavage reaction to furnish lactones

Stefanie Roth and Christian B. W. Stark*

A highly efficient catalytic oxidative cleavage reaction of THF and THP alcohols to γ - and δ -lactones using PCC (1 mol%) and periodic acid as terminal oxidant is presented.



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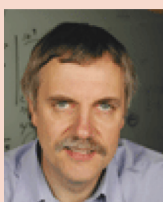
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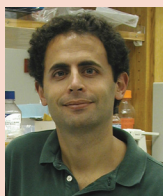
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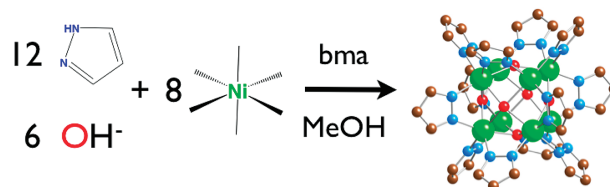
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6414

The self-assembly and magnetic properties of a Ni(II)₈(μ₄-hydroxo)₆ cube with μ₂-pyrazolate as an exogenous ancillary ligand

Jing-Yuan Xu, Xin Qiao, Hai-Bin Song, Shi-Ping Yan,*
Dai-Zheng Liao, Song Gao, Yves Journaux* and
Joan Cano

A novel octanuclear hydroxonickel(II) complex possessing a unprecedented cube molecular structure has been synthesized and its magnetic properties investigated.




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Chemical Science

Egg white proteins aid formation of magnetite nanotubes

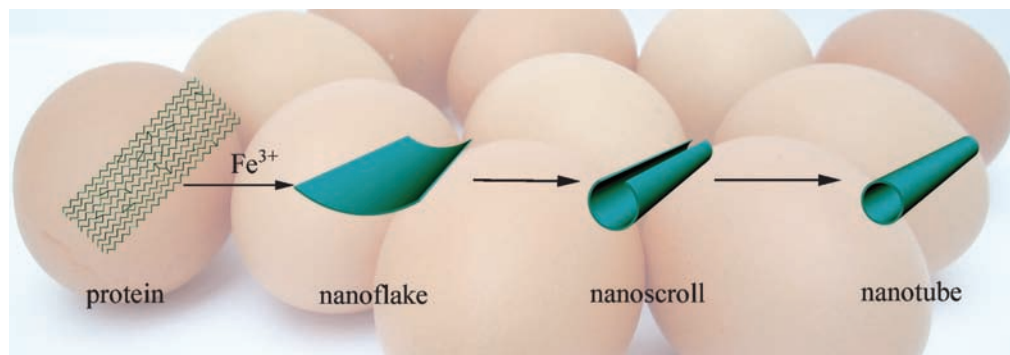
Which came first, the nanotube or the egg?

Egg whites have found a novel use as a template for making inorganic nanotubes, thanks to Chinese scientists.

Baoyou Geng and colleagues at the Anhui Normal University, Wuhu, made magnetite (Fe_3O_4) nanotubes in an egg white solution. The egg white protein – which has a high affinity for metal ions – forms organic–inorganic complexes with Fe(III) . The complexes then aggregate to form nanosheets, a process that generates heat. The increase in temperature ruptures hydrogen and peptide–iron bonds so that the iron oxide dissociates from the egg white template. The iron oxide sheets then roll up to form hollow nanotubes.

The use of proteins from bones and shells as templates is well known, but most need time consuming and complex methodologies to generate the biological template. Geng explains that their new strategy uses a cheap and easily obtainable protein template.

Inorganic nanotubes have a wide



range of applications from drug delivery to solar energy conversion devices. And magnetite – one of the most magnetic minerals – is particularly interesting for magnetism related applications.

Xitian Zhang – a specialist in the preparation and applications of nanotubes from the Chinese University of Hong Kong, Shatin – says that this research ‘provides a simple, novel and feasible method for the preparation of single-crystalline iron oxide nanotubes.’ ‘This approach not only enriches magnetite chemistry, but also

Iron oxide nanotubes have magnetism related applications

provides a new strategy to synthesise similar materials,’ he adds.

The next challenge is to investigate ‘the reaction conditions on the egg white structure, which may result in morphology changes to the product,’ says Geng. Geng and his team will also try synthesising other nanotubes to investigate the effects of different metal ions on egg white.

Michael Brown

Reference

B Geng *et al*, *Chem. Commun.*, 5773, 2008 (DOI:10.1039/b813071j)

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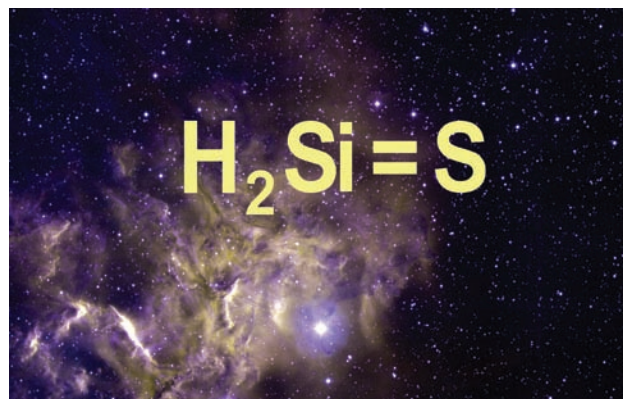
A 'plausible astronomical molecule' has been characterised for the first time

Silanethiones reach for the stars

German researchers have identified experimentally $\text{H}_2\text{Si}=\text{S}$, a molecule thought to exist in outer space, for the first time.

A team led by Sven Thorwirth at the Max Planck Institute for Radioastronomy, Bonn, were able to characterise this elusive molecule using microwave spectroscopy. 'Cosmically, silicon and sulfur are very abundant elements,' says Thorwirth. This unsubstituted silanethione is 'a plausible astronomical molecule' that may exist in the shells of dust surrounding dying stars, he explains.

Several substituted silanethiones, $\text{RR}'\text{Si}=\text{S}$, stabilised by bulky alkyl (R) groups have already been synthesised and their structures determined using X-ray crystallography. But the unsubstituted silanethione – the second-row analogue of



formaldehyde – had never been seen before.

Thorwirth used microwave spectroscopy – which measures the difference between the electromagnetic radiation absorbed by a molecule and that emitted – to look for the molecule. The radiation

Silanethione may exist in the shells of dust surrounding dying stars

Reference
S Thorwirth *et al*, *Chem. Commun.*, 2008, 5292 (DOI: 10.1039/b814558j)

difference is associated with the molecule's rotation, and is used to identify molecular species and isotopes. The team then backed up their experimental results with high-level quantum chemical calculations. Explaining the significance of this work, Thorwirth says that the 'data provide the laboratory basis needed for future radio astronomical searches for this molecule in space.'

The research is welcomed by Paul Davies, a member of the infrared laser spectroscopy group at the University of Cambridge, UK, who says that this combination of spectroscopy and high-level calculations 'should be generally applicable for unravelling the spectra from increasingly complicated molecules, hence enabling the full potential of microwave spectroscopy to be realised.'

Vikki Chapman

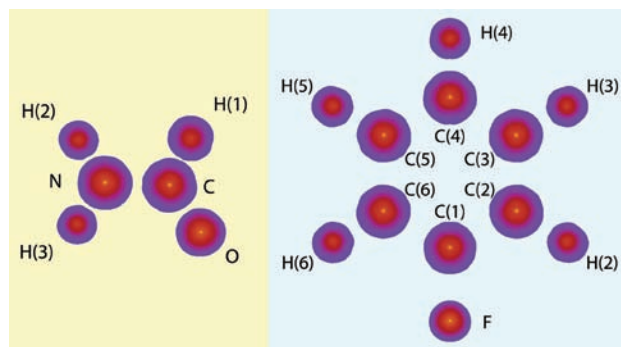
Scientists solve the 'how many electrons are on each atom in a molecule' puzzle

Cracking charge density

A new computational approach to accurately and reliably divide a molecule's electronic properties into its component atom parts has been developed by scientists in the UK.

While chemists typically think of the properties of molecules as a sum of their atomic parts, molecular characteristics such as electron density are impossible to experimentally divide into their atomic components, and have proven difficult to derive computationally. Now, Timothy Lillestolen and Richard Wheatley at the University of Nottingham have developed a simple algorithm that they say gives atoms with the smooth, spherical shapes and charges that would intuitively be expected.

'If you ask a chemist whether the properties of a molecule can be understood in terms of the properties of its constituent atoms, you are likely to get an affirmative answer,' says Wheatley. 'However, the tools available for accurate chemical



calculations treat the molecule holistically, and do not allow information on separate atoms to be easily extracted.'

To tackle the problem, the team developed an iterative stockholder approach to calculate the electron density of each atom. Electronegative atoms were correctly predicted to have negative charges, while hydrogen atoms bonded to electronegative atoms had a positive charge.

'The beautiful results produced

A simple algorithm has allowed electron density to be divided up into atomic components

Reference
R Wheatley and T Lillestolen, *Chem Commun.*, 2008, DOI: 1039/b812691g

by the iterated stockholder method have taken us by surprise: if it has an Achilles' heel, then we have yet to discover it!' says Wheatley. 'However, our results so far are preliminary, and we are still working on applications of the method to a wider range of chemicals,' he adds. The team are in talks with several software companies over the possibility of incorporating the work in quantum chemistry programmes.

'This is a slick and simple idea that provides a way to answer a question that is in most chemists' minds: how many electrons are there on each atom of a molecule?' says Peter Knowles, who develops computational methods at Cardiff University, UK. 'Further work should answer the question as to whether there is a practical use for this simple theory – can we use it to predict relative chemical reactivity, or to construct a simple force field for intermolecular interactions, using these atomic charges?'

James Mitchell Crow

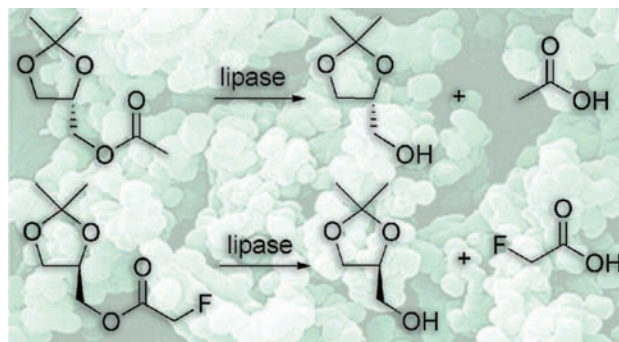
Suicidal yeasts assist in the search for enantioselective enzymes

Underperforming yeasts opt out of life

German scientists looking to evolve yeast enzymes to catalyse asymmetric organic reactions have used a chemical trick to force underperforming yeasts to commit suicide even before they have to be screened.

Manfred Reetz and co-workers, at the Max Planck Institute for Coal Research, Mülheim, were searching for a better enantioselective enzyme to catalyse cleavage reactions of a chiral ester to make a chiral alcohol. The standard way of doing this, directed evolution, involves generating libraries of mutant enzymes from host yeasts containing the enzyme of interest, sorting through the new enzymes to pick out the best progeny, and continuing until the desired degree of catalyst improvement has been reached. But, as Reetz explains, 'screening large libraries of mutant enzymes in order to fish out the best ones is very time-consuming and costly.'

Instead, Reetz's team designed



a selection system so that yeasts producing a lipase which cleaved the wrong chiral ester killed themselves, while yeasts whose enzymes were on the right track grew faster. They fed the yeasts with two almost identical esters of chiral isopropylidene glycol, a test compound. When the *S*-enantiomer was cleaved (the desired reaction) it generated acetate as a byproduct, which acts as an energy source for the yeast. The mirror-image ester, the undesired

The yeasts die if the enzyme their gene encodes for generates the toxic byproduct

Reference
M T Reetz *et al*, *Chem. Commun.*, 2008, 5502 (DOI: 10.1039/b814538e)

R-enantiomer, was in fact a pseudo-enantiomer with a fluorine atom attached. Cleavage of this compound produced poisonous fluoroacetate, which kills the yeast. So the yeasts effectively commit suicide if the enzyme their gene encodes for cleaves the wrong enantiomer.

'Here the undesired enzyme mutants are not formed, which is of great advantage relative to screening systems in which mostly junk mutants are generated,' explains Reetz.

Stefan Lutz, who is a US expert on protein engineering and biomolecular chemistry at Emory University, Atlanta, says the findings represent a significant advance in the field. 'It is a classic example of a carrot-and-stick idea, Reetz and colleagues have devised a system that uses easily synthesised substrates (acetate versus fluoroacetate esters of their alcohol of interest). It is hard to imagine that one could find something simpler.' *Kathleen Too*

Organic ligands bound to quantum dots improve metal ion detection in water

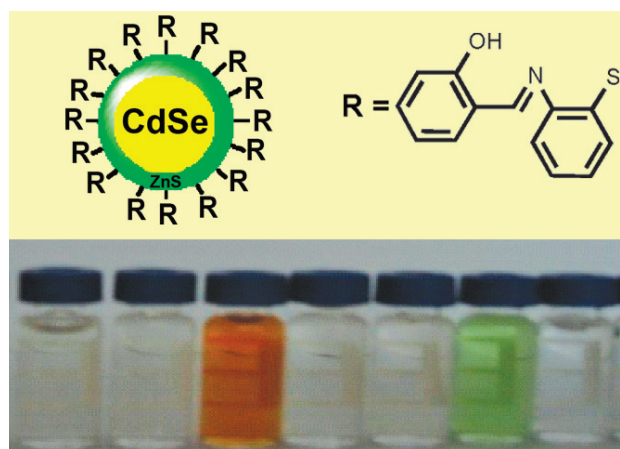
Quantum leap in chemical sensing

Small molecules that bind to many types of metal ions in water can be transformed into highly selective multi-functional sensors by harnessing them to quantum dots, UK scientists have demonstrated.

John Callan and colleagues at the Robert Gordon University, Aberdeen, created nanocrystals that can simultaneously detect copper and iron in water. The sample solution visibly changes colour when metals come into contact with the sensor: from colourless to green for copper, or to orange for iron.

'The remarkable aspect of the work is that the receptor itself shows no selectivity for any particular metal ion, but displays dual selectivity when anchored to the quantum dot surface,' says Callan.

Once the organic ligands attach to the dots – which are cadmium selenide/zinc sulfide



Iron and copper can be detected simultaneously in water samples

semiconductor nanoparticles – they are confined by the surrounding three-dimensional structure, and form binding sites that complement the size, shape and electronic properties of copper and iron ions. Because the ultraviolet-visible

spectra of detected copper and iron metals in solution don't overlap, each metal can be tracked simultaneously using ultraviolet-visible spectroscopy.

'This fine work brings multi-functionality to quantum dot sensors for the first time,' comments A P De Silva, an expert in sensors from Queens University, Belfast, UK.

Callan's sensor is straightforward to prepare and gives results in real time. It compares well with other multi-analyte sensors which often involve long-winded methods for receptor synthesis and data processing. And, Callan claims, it also has superior optical properties compared with the organic dyes currently used in optical sensors. *Ziva Whitelock*

Reference
N Singh *et al*, *Chem. Commun.*, 2008, 4900 (DOI:10.1039/b813423e)



Journal of Environmental Monitoring

Focus on Medical Geology & Air- and Biomonitoring

Journal of Environmental Monitoring (JEM) issue 12, 2008, is focusing on the areas of Medical Geology & Air- and Biomonitoring.

Medical Geology has seen immense growth and maturation allowing biomedical/health professionals and geoscientists to take strong root in the international arena. The journal anticipates publishing many articles in this field. The first two reviews, included in this issue, are:

The utility of mosquito-borne disease as an environmental monitoring tool in tropical ecosystems

Andrew Jardine, Angus Cook and Philip Weinstein

10th Anniversary Critical Review: Naturally occurring asbestos

Martin Harper

Air- and Biomonitoring features six selected papers on exposure monitoring within the preventive framework of identifying and controlling health hazards within the workplace and in the environment presented at AIRMON 2008, held at Geilo, Norway, January 28-31, 2008.

Highlighted papers:

Three dimensional modeling of air flow, aerosol distribution and aerosol samplers for unsteady conditions

Albert Gilmutdinov and Ilya Zivliskii

Experimental methods to determine inhalability and personal sampler performance for aerosols in ultra-low windspeed environments

Darrah K. Schmees, Yi-Hsuan Wu and James H. Vincent

A study of the bio-accessibility of welding fumes

Balázs Berlinger, Dag G. Ellingsen, Miklós Náray, Gyula Zárny and Yngvar Thomassen

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Asbestos comes naturally

Martin Harper, National Institute for Occupational Safety and Health, Morgantown, WV, US, points out a hazard in the natural environment

The standard reaction to pollution is to blame the polluter – in most cases man and his activities. But what happens when the polluter is the environment? Recently, we have started to view the environment as a source of substances likely to be harmful to human health. A high-profile example of this ‘natural pollution’ is the contamination of groundwater by arsenic from natural sources in Bangladesh and India.

Another, less well-known problem is asbestos that occurs naturally in rock. Naturally occurring asbestos (NOA) is the name given to the silicate minerals serpentine and amphibole that, in certain environmental conditions, form exceedingly thin crystals in parallel alignment – with the appearance of cotton or silk. The term NOA can also be used to describe different minerals that crystallise in a finely fibrous manner resembling asbestos, and minerals that can produce elongated particles when broken or crushed.

The most significant risk from NOA is serious illness that may occur through exposure through inhalation. The illnesses include asbestosis – the chronic inflammation of the inside of the lungs (which is a result of exposure to high concentrations of asbestos), lung cancer and mesothelioma – a cancer that occurs in the protective lining that covers most of the body’s internal organs. These latter two diseases result from exposure to lower concentrations and are the largest concern for NOA. Not all particles that might find themselves classified as NOA are likely to have the same disease risk, and trying to determine the exact risk from low-level environmental exposures is not easy. So far, adverse health effects as serious and widespread as those related to arsenic in groundwater have not been observed. For the asbestos particles to become airborne – and therefore pose a health risk



– the rock or soil normally needs to be disturbed. The nature of the soil and local climate are also important, as well as the type of activity causing disturbance. Simple erosion isn’t as much of a risk as man’s activities – such as mining and quarrying, excavation for construction, farming, landscaping and gardening. People carrying out these activities have the highest risk occupations, but second-hand exposure is also possible for local residents. Exposure can also occur through recreational activities that seriously disturb the soil such as riding motorised vehicles, bicycles, jogging and other sports. The trailing members of a group of riders, cyclists or runners are known to be exposed to much greater quantities than the leaders, and children may suffer higher exposure than adults.

A community may have lived for many generations in an area with NOA without realising it. Such communities may be more comfortable in dealing with the presence of NOA when discovered than people moving into new developments would be – especially those where there is ongoing major construction activity.

Once NOA is identified, risk assessment is required in order to assess the problem, and this

Shovelling and raking of gravel containing asbestos minerals can cause asbestos particles to become airborne

can be challenging and hard to communicate effectively when there is not a consensus on the risk.

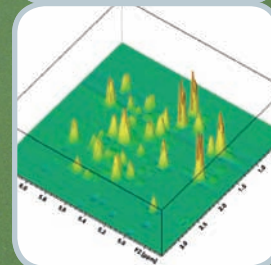
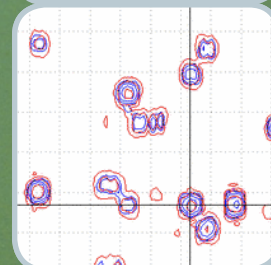
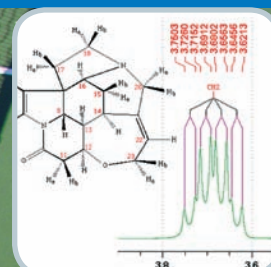
Once it is known that a region has NOA, the local population must determine whether the risk is tolerable, and this becomes more difficult with increasing uncertainty in the assessment. Risk tolerance is a function of many socio-economic factors, which may involve politics and the law, and the role of government. In each situation where communities deal with NOA there is a unique combination of risk assessment and social issues – which include employment, income and property values. A different combination of the following groups of people get involved in each case – local activists, people with commercial interests, politicians, media, scientific experts, local and national government agencies, and courts of law. Failure to come up with an acceptable solution to the issue of NOA is not pretty; leading to litigation and political and social recriminations, in addition to loss of amenity, reduction of property value, and ultimately the possibility of impaired future health. With all these factors to consider it is clear that this isn’t a situation where the one-size-fits-all approach could work, and how each ‘newly’ contaminated area is dealt with will have to be custom-fitted.

NOA is an issue of study, debate and concern within the affected areas of the US today, and also for some countries around the Mediterranean, such as Italy and Turkey, where NOA is relatively common. However, the widespread occurrence of these minerals suggests that this matter will become an issue for many other countries in the future.

Read Martin Harper’s critical review ‘Naturally occurring asbestos’ in issue 12, 2008 of Journal of Environmental Monitoring

Reference
M Harper, *J. Environ. Monit.*, 2008, DOI: 10.1039/b810541n

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A total mismatch

Penny Brothers tells Michael Brown about porphyrins, the porphyrin–boron mismatch and their potential role in neutron capture therapy



Penny Brothers

Penny Brothers is an associate professor at the University of Auckland, New Zealand. Her research brings together her interests in porphyrin chemistry, the main group elements and organometallic chemistry. She investigates how the porphyrin ligand can be used to modify the chemistry of elements such as boron and bismuth. She has recently begun to explore the chemistry of main group elements with the related macrocycle corrole.

What motivated you to specialise in organometallics and porphyrins?

At the University of Auckland, where my father was a geology professor, there were display cases full of minerals that I loved looking at. All the beautiful crystals, with all their different morphologies and colours, helped attract me to inorganic chemistry. When I was choosing my masters research subject area, Professor Warren Roper, an organometallic chemist, was my mentor. Warren Roper had a long association with Jim Collman and I went to Stanford to do a PhD in his group, which was focused on porphyrin chemistry. I worked on a porphyrin project, which I enjoyed, and that was how I got into porphyrin chemistry. I have been there ever since.

Can you explain the significance of your work?

Boron–porphyrin chemistry is where my attention is at present. In terms of significance there are potential applications of boron porphyrins in sugar sensing and in neutron capture therapy. Porphyrins are known to localise on the surface of a tumour and the boron serves as the neutron capture element. Others have investigated boron attached to the periphery of the porphyrin, but my research involves boron coordinated to the centre of the porphyrin. In coordination chemistry, a ligand is often designed for a specific coordination geometry and metal centre, producing a thermodynamically stable complex. In our research, we do the reverse. Porphyrins are a total mismatch for boron, with the wrong coordination geometry and the wrong size, and this mismatch can stimulate some unusual and interesting chemistry. This fundamental interest is my main motivation.

What are the advantages of collaborations and have they been beneficial?

Absolutely. Students view chemistry as something rather dry that you read about in text books and journal articles. If you can show students the link between the research and the people that are committed to chemistry, then it becomes more interesting and easier to understand. I think chemistry becomes more alive and a richer subject when you know the people that are involved in it. When you read the work of someone you know

personally, you can find it easier to understand because chemists, like anybody else involved in creative endeavours, express their personalities through their work. We have no hesitation in understanding this for artists and musicians, but it is also true in science. With collaborations, you not only get the experience of someone else's expertise, you get their intellectual input, and a personal interaction that means it becomes the creative endeavour of a bigger team.

Did you face any challenges as a woman in science?

Because I grew up in a household of scientists, I never felt I had a barrier, either as an individual or as a woman, to overcome. I had a lot of support from my family, teachers, mentors and advisors, so I had a very straightforward pathway through the system. Women often have a more difficult journey into an academic career, as they may have family responsibilities or may have to fit with the career plans of a partner. For my generation in particular, the career aspirations of women began to be valued for the first time, so I was very lucky to start my career at the time I did. I have never encountered any overt discrimination, but I do recognise that there are barriers in the system. I think that we often generate some of the barriers ourselves and women can lack the confidence to strive for their goals.

What do you enjoy most about your role on the Chemical Communications editorial board?

The more diverse the network of people I know in the world of chemistry, the more I enjoy it. When I was appointed to the editorial board, my first reaction was to think that I need to get over my lack of confidence. I can make as much of a contribution to the editorial board as anyone else. Particularly, I can add a perspective from a smaller country that is outside the big hubs of activity like the US, the UK, Europe and Asia. I have always been interested in publishing, but felt that it was inevitable to end up in an academic position as I grew up in that environment. If I hadn't ended up doing academic chemistry, I would have liked to be involved in science publishing, so this is a really good opportunity for me to learn a bit more about that and make a contribution to a different area.

Board member wins Nobel Prize

The Nobel Prize in Chemistry 2008 has been awarded to Roger Tsien (below right), University of California, San Diego, US, a member of the editorial board for the upcoming RSC journal *Integrative Biology* (to be launched in January 2009), and colleagues for their work in the development of the gene marker green fluorescent protein (GFP).

Harp Minhas, editor of *Integrative Biology*, says: 'Congratulations to Professor Tsien, from all of us at the RSC. We are all immensely pleased that 2008 Nobel Prize winner Roger Tsien is an editorial board member for *Integrative Biology*; his work typifies the quality of material we are seeking in the development of biology through new tools and technologies.'

Derivatives of GFP are used in experiments to observe



cell dynamics and behaviour – their fluorescent glow allows scientists to visualise processes inside cells.

Furthermore, as it is non-toxic to cells it can be used in live



cell (in vitro) studies meaning that real time analysis of cells is possible.

GFP is a protein first extracted from the jellyfish *Aequorea victoria* in the 1960s by Osamu Shimomura, who was jointly awarded this year's prize with Tsien and Martin Chalfie.

Variants of GFP can fluoresce in different colours, allowing several different proteins in a cell to be studied simultaneously.

Find out more about our new journal *Integrative Biology* at www.rsc.org/ibiology

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This textbook has been fully revised and updated and includes a foreword written by Heston Blumenthal. Look out for other exciting new food science books in 2009 such as *Kitchen Chemistry* (new volume), *Handbook of Culture Media for Food and Water Microbiology* and *Nanotechnologies in Food*.

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Announcing *Lab on a Chip* prize winners

Lab on a Chip, the miniaturisation journal for chemistry, biology and bioengineering, has yet again shown extensive community support by sponsoring some of the most prestigious prizes in the miniaturisation field. At this year's μ -TAS meeting in San Diego the journal, together with Corning Inc., awarded the 'Pioneers in Miniaturisation Prize' to Patrick Doyle, professor at the department of chemical engineering at MIT, US. Jean-Louis Viovy from the Institute Curie comments on Doyle's

work: '[Patrick] developed the "stop-flow lithography" technological platform, which I consider a major breakthrough in microfluidics.'

Lab on a Chip also awarded the 'Widmer Young Researcher Poster Award' to Maged Fouad for best poster and presentation. Among 589 candidates, this poster titled 'Nanotechnology meets plant biotechnology: carbon nanotubes deliver DNA and incorporate into the plant cell structure' caught the judges' eyes.

A new award named 'Art in

Science' recognised the aesthetic value in scientific illustrations. 'The winner, Yu Wen Huang (Texas A & M University) clearly understood the principles of this award and produced an image that was reminiscent of a tall city building seen in an early morning fog. The picture is an optical effect generated by concentrated double-stranded DNA in the vicinity of a 50 micrometre wide electrode inside a microchannel,' comments Harp Minhas, editor of *Lab on a Chip*, who proudly presented all awards to the winners.

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